# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:58 PM BST

| | | |
|---|---|---|
| PDB ID | : | 5NDV |
| Title | : | Crystal structure of Paromomycin bound to the yeast 80S ribosome |
| Authors | : | Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G. |
| Deposited on | : | 2017-03-09 |
| Resolution | : | 3.30 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

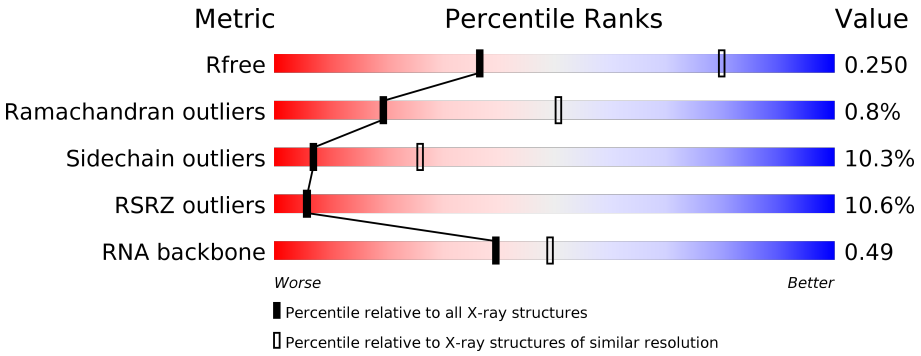
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.13 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.13 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



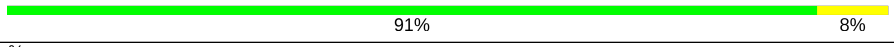

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1149 (3.34-3.26) |
| Ramachandran outliers | 138981 | 1183 (3.34-3.26) |
| Sidechain outliers | 138945 | 1182 (3.34-3.26) |
| RSRZ outliers | 127900 | 1115 (3.34-3.26) |
| RNA backbone | 3102 | 1117 (3.70-2.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 3396 | 70% 19% • 9% |
| 1 | 5 | 3396 | % 70% 20% • 9% |
| 2 | 3 | 121 | 79% 21% |
| 2 | 7 | 121 | 83% 17% |
| 3 | 4 | 158 | % 77% 20% • • |
| 3 | 8 | 158 | % 77% 19% • |

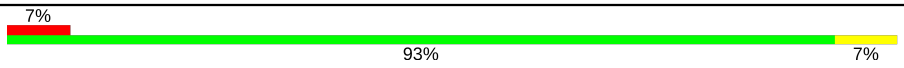
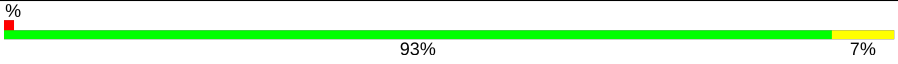
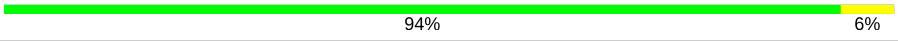
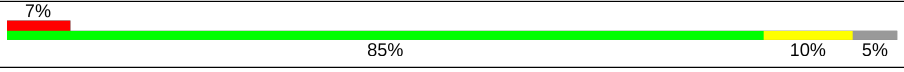
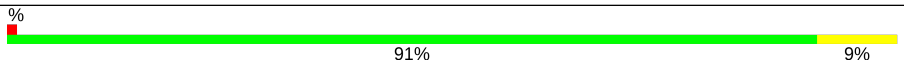
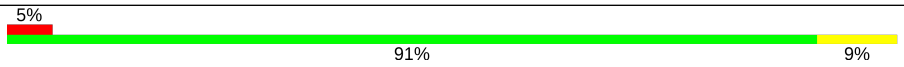
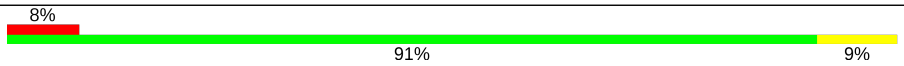
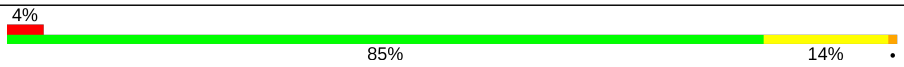
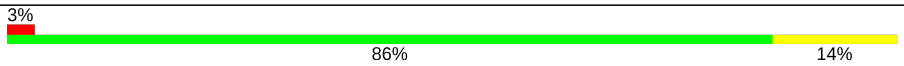
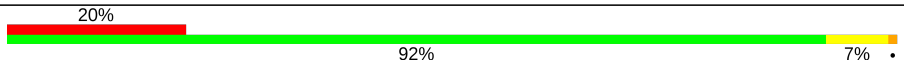
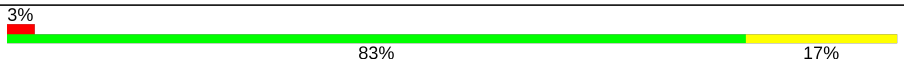
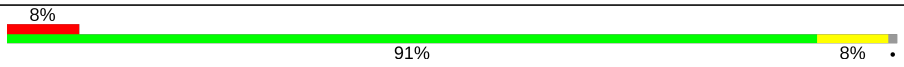
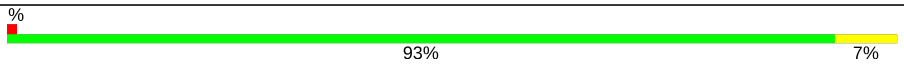
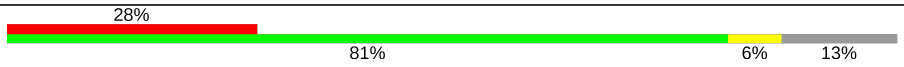
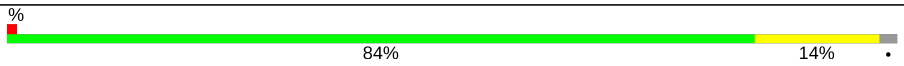
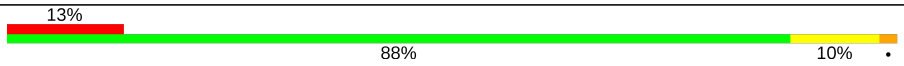
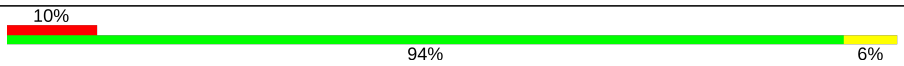
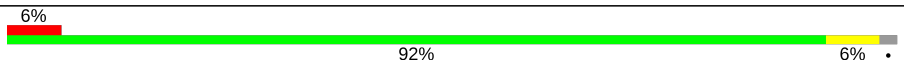
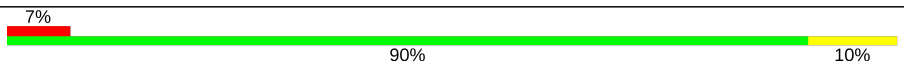
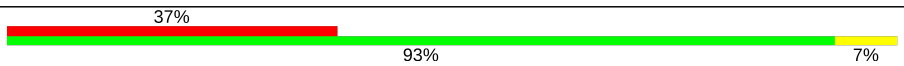
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | L2 | 248 | |
| 4 | l2 | 248 | |
| 5 | L3 | 386 | |
| 5 | l3 | 386 | |
| 6 | L4 | 361 |   |
| 6 | l4 | 361 | |
| 7 | L5 | 296 | |
| 7 | l5 | 296 | |
| 8 | L6 | 176 | |
| 8 | l6 | 176 | |
| 9 | L7 | 226 | |
| 9 | l7 | 226 | |
| 10 | L8 | 231 | |
| 10 | l8 | 231 | |
| 11 | L9 | 191 | |
| 11 | l9 | 191 | |
| 12 | M0 | 221 | |
| 12 | m0 | 221 | |
| 13 | M1 | 169 | |
| 13 | m1 | 169 | |
| 14 | M3 | 194 | |
| 14 | m3 | 194 | |
| 15 | M4 | 137 | |
| 15 | m4 | 137 | |
| 16 | M5 | 203 | |

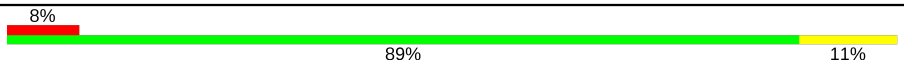
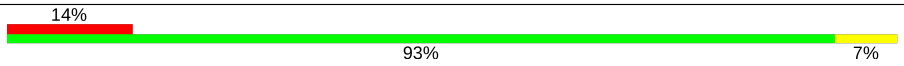
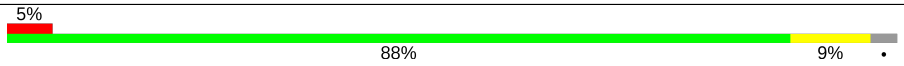
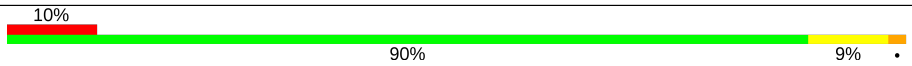
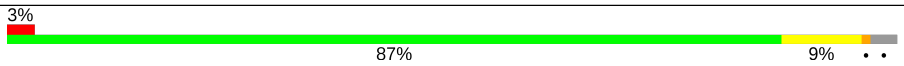
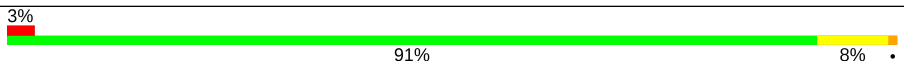
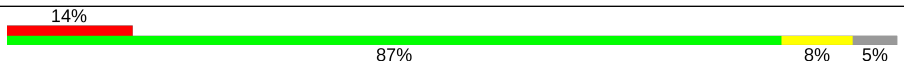
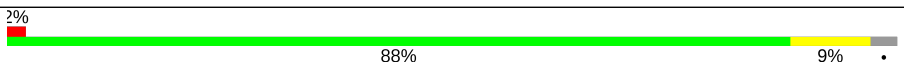
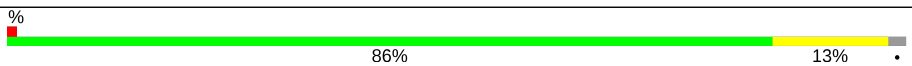
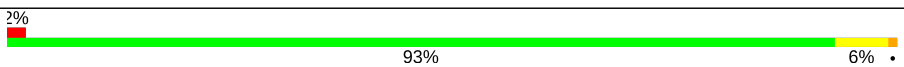
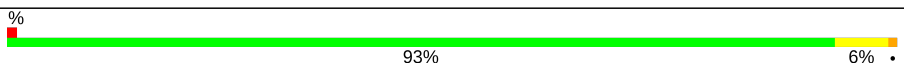
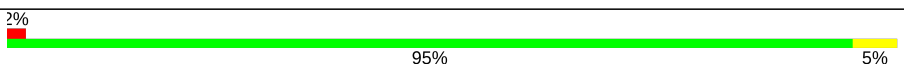
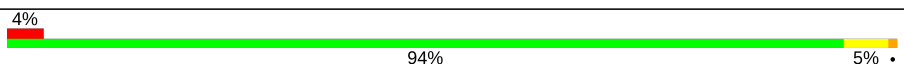
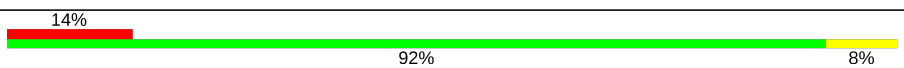
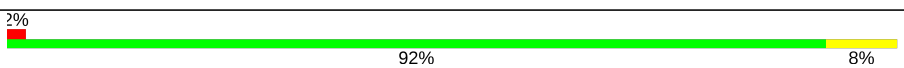
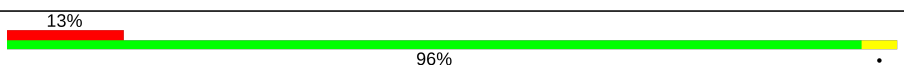
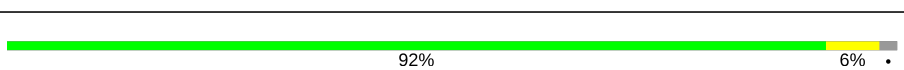
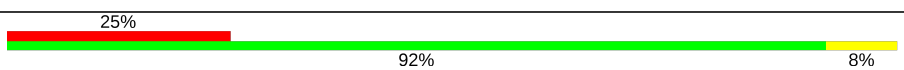
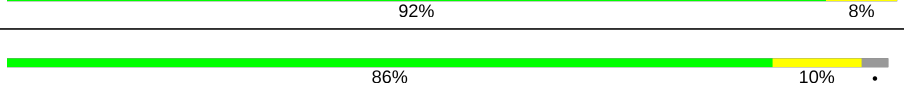
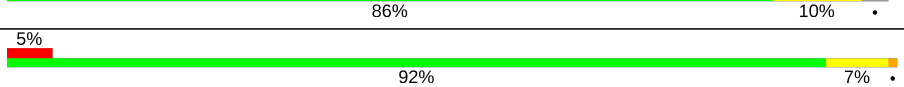
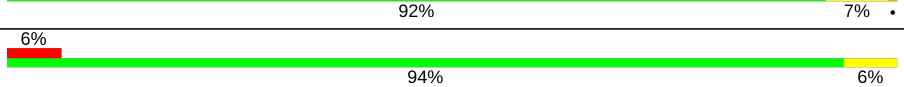
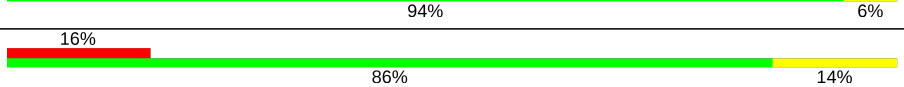
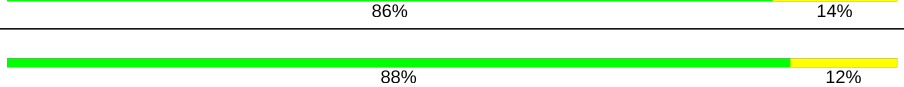
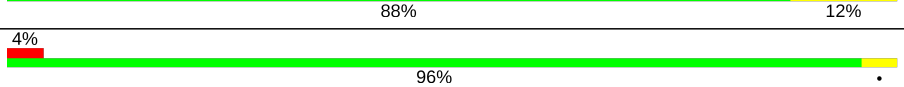
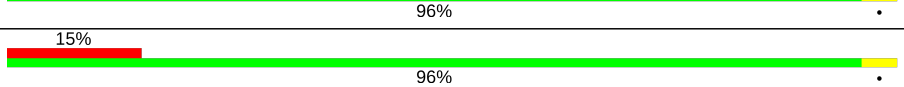
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 16 | m5 | 203 |   |
| 17 | M6 | 197 |   |
| 17 | m6 | 197 |   |
| 18 | M7 | 184 |   |
| 18 | m7 | 184 | |
| 19 | M8 | 185 |   |
| 19 | m8 | 185 |   |
| 20 | M9 | 188 | |
| 20 | m9 | 188 |   |
| 21 | N0 | 172 |   |
| 21 | n0 | 172 | |
| 22 | N1 | 159 |   |
| 22 | n1 | 159 |   |
| 23 | N2 | 99 |   |
| 23 | n2 | 99 |   |
| 24 | N3 | 136 | |
| 24 | n3 | 136 |   |
| 25 | N4 | 155 | |
| 25 | n4 | 155 |   |
| 26 | N5 | 120 |   |
| 26 | n5 | 120 |   |
| 27 | N6 | 125 |   |
| 27 | n6 | 125 |   |
| 28 | N7 | 135 |   |
| 28 | n7 | 135 |   |

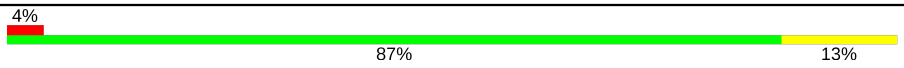
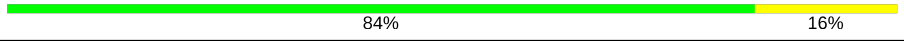
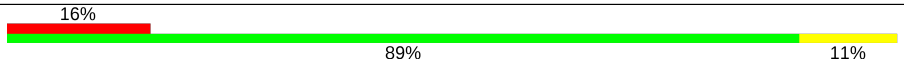
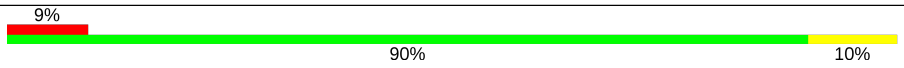
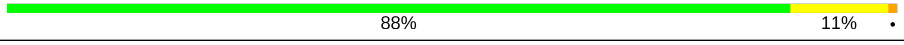
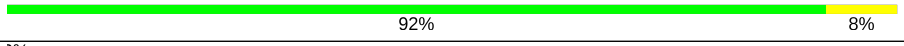
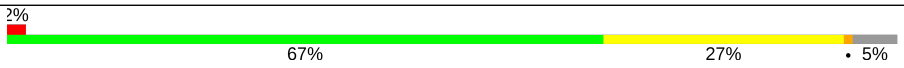
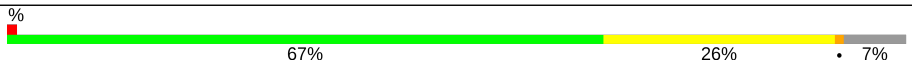
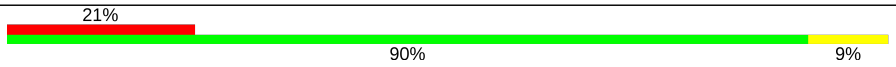
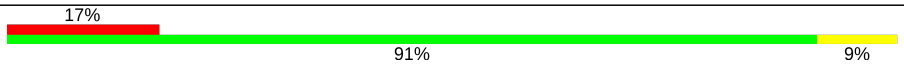
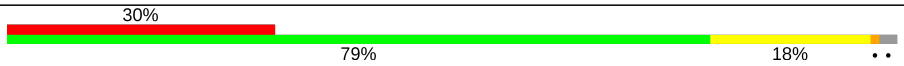
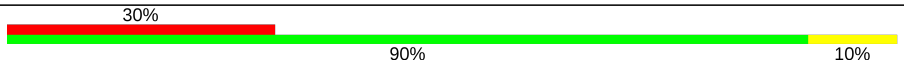
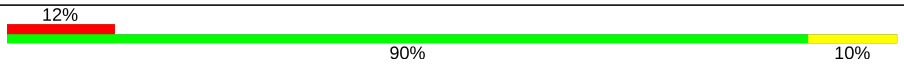
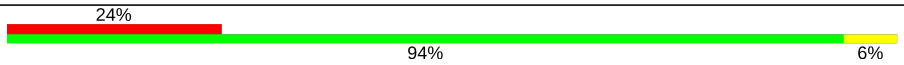
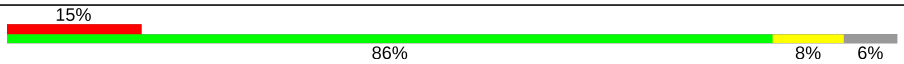
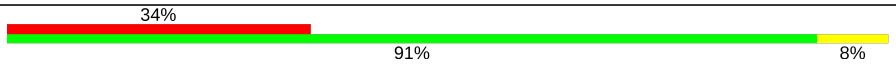
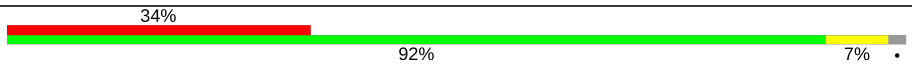
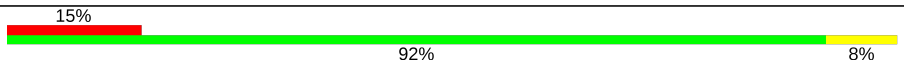
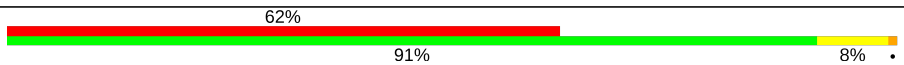
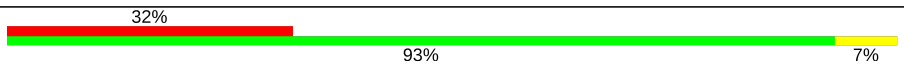
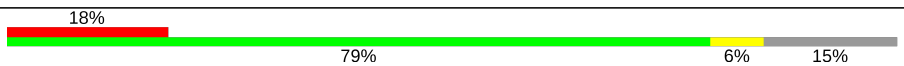
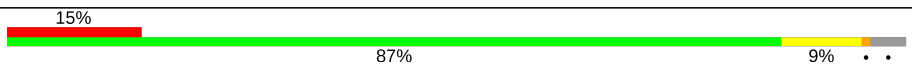
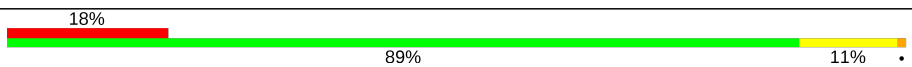
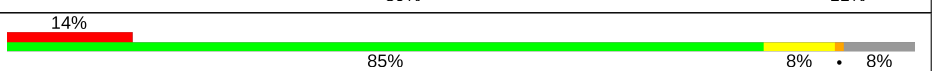
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | N8 | 148 |   |
| 29 | n8 | 148 |   |
| 30 | N9 | 58 |   |
| 30 | n9 | 58 |   |
| 31 | O0 | 100 |   |
| 31 | o0 | 100 |   |
| 32 | O1 | 112 |   |
| 32 | o1 | 112 |   |
| 33 | O2 | 127 |   |
| 33 | o2 | 127 |   |
| 34 | O3 | 106 |   |
| 34 | o3 | 106 |   |
| 35 | O4 | 112 |   |
| 35 | o4 | 112 |   |
| 36 | O5 | 119 |   |
| 36 | o5 | 119 |   |
| 37 | O6 | 99 |   |
| 37 | o6 | 99 |   |
| 38 | O7 | 87 |   |
| 38 | o7 | 87 |   |
| 39 | O8 | 77 |   |
| 39 | o8 | 77 |   |
| 40 | O9 | 50 |   |
| 40 | o9 | 50 |   |
| 41 | Q0 | 52 |   |

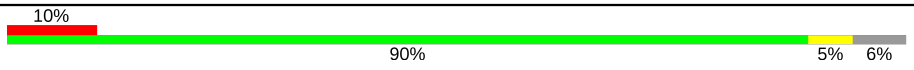
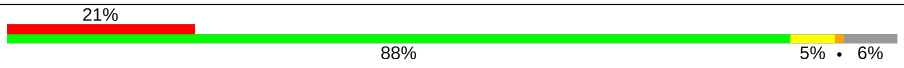
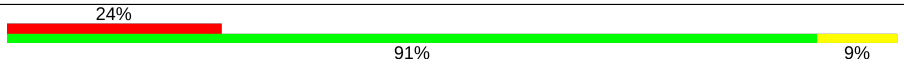
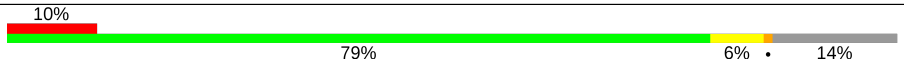
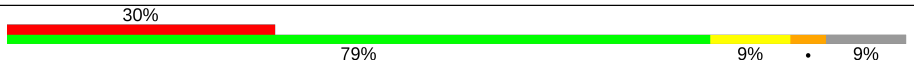
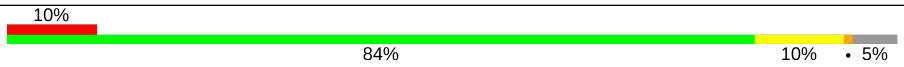
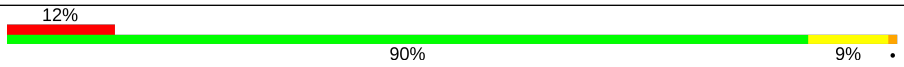
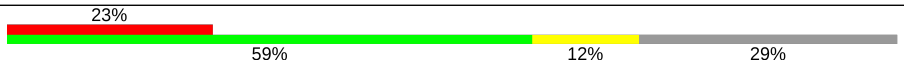
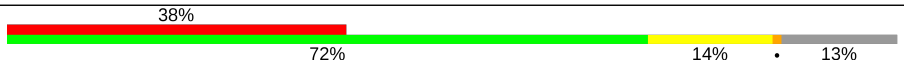
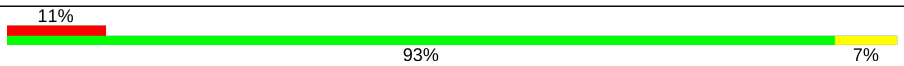
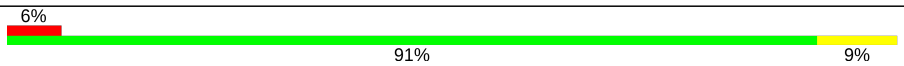
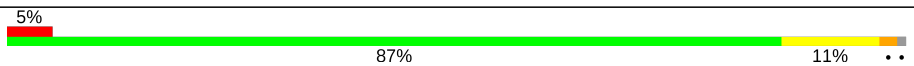
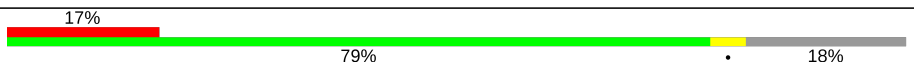
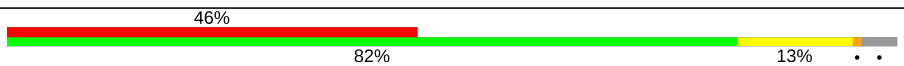
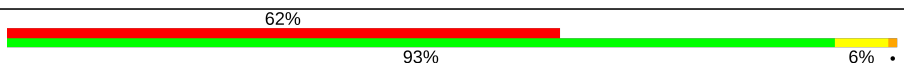
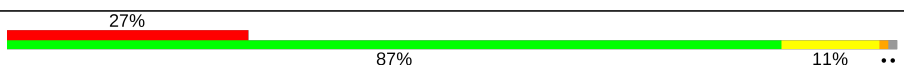
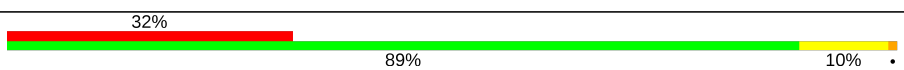
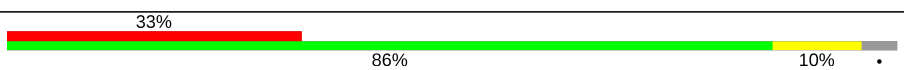
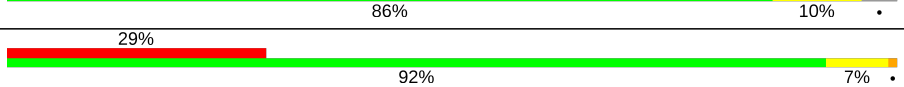
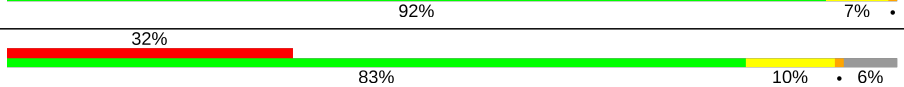
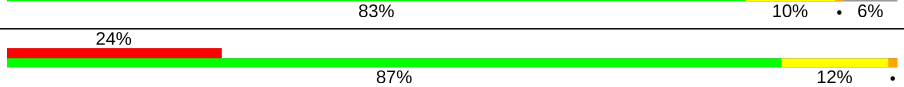
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | q0 | 52 |   |
| 42 | Q1 | 25 |   |
| 42 | q1 | 25 | |
| 43 | Q2 | 105 |   |
| 43 | q2 | 105 |   |
| 44 | Q3 | 91 |   |
| 44 | q3 | 91 |   |
| 45 | 2 | 1800 |   |
| 45 | 6 | 1800 |   |
| 46 | S0 | 206 |   |
| 46 | s0 | 206 |   |
| 47 | S1 | 216 |   |
| 47 | s1 | 216 |   |
| 48 | S2 | 217 |   |
| 48 | s2 | 217 |   |
| 49 | S3 | 223 |   |
| 49 | s3 | 223 |   |
| 50 | S4 | 260 |   |
| 50 | s4 | 260 |   |
| 51 | S5 | 206 |   |
| 51 | s5 | 206 |   |
| 52 | S6 | 236 |   |
| 53 | S7 | 186 |   |
| 53 | s7 | 186 |   |
| 54 | S8 | 200 |   |

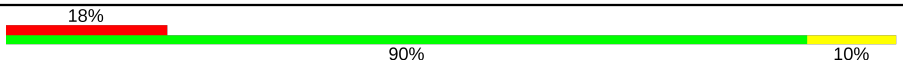
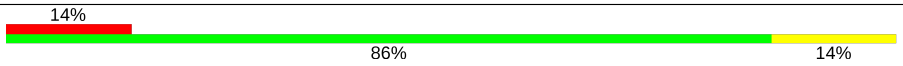
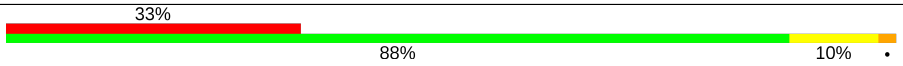
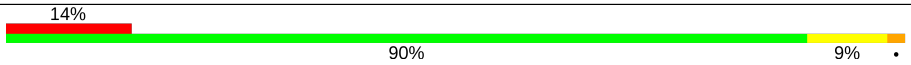
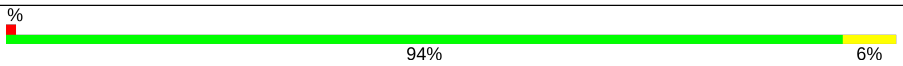
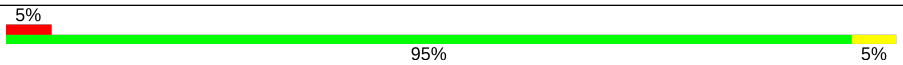
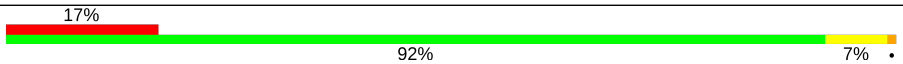
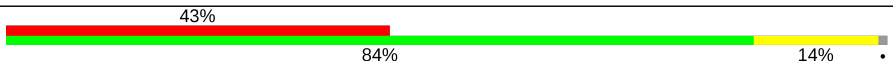
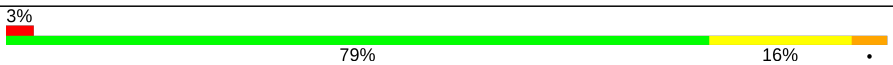
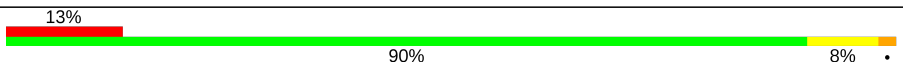
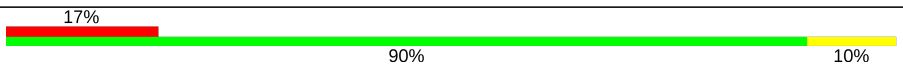
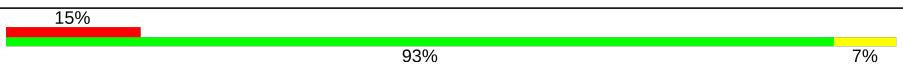
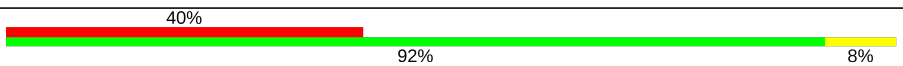
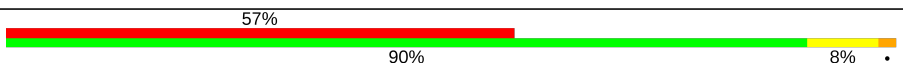
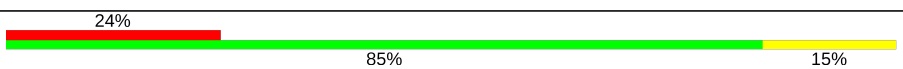
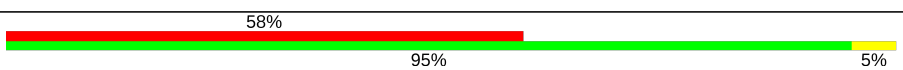
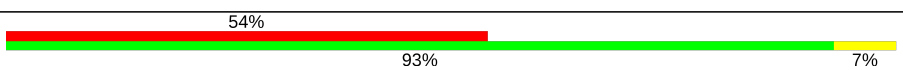
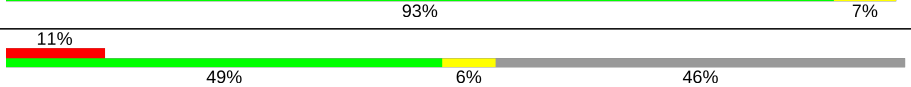
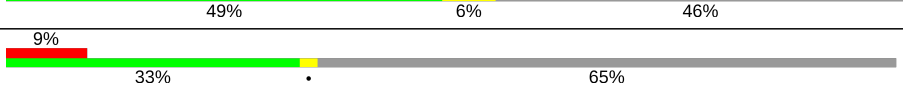
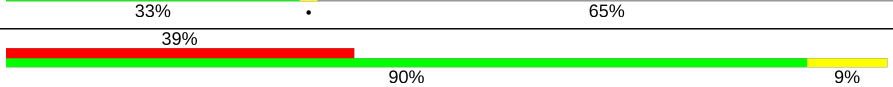
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | s8 | 200 |   |
| 55 | S9 | 185 |   |
| 55 | s9 | 185 |   |
| 56 | C0 | 105 |   |
| 56 | c0 | 105 |   |
| 57 | C1 | 146 |   |
| 57 | c1 | 146 |   |
| 58 | C2 | 143 |   |
| 58 | c2 | 143 |   |
| 59 | C3 | 150 |   |
| 59 | c3 | 150 |   |
| 60 | C4 | 128 |   |
| 60 | c4 | 128 | |
| 61 | C5 | 141 |   |
| 61 | c5 | 141 |   |
| 62 | C6 | 142 | |
| 62 | c6 | 142 |   |
| 63 | C7 | 136 | |
| 63 | c7 | 136 | |
| 64 | C8 | 145 |   |
| 64 | c8 | 145 |   |
| 65 | C9 | 143 |   |
| 65 | c9 | 143 |   |
| 66 | D0 | 109 |   |
| 66 | d0 | 109 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 67 | D1 | 87 |   |
| 67 | d1 | 87 |   |
| 68 | D2 | 129 |   |
| 68 | d2 | 129 |   |
| 69 | D3 | 144 |   |
| 69 | d3 | 144 |   |
| 70 | D4 | 134 | |
| 70 | d4 | 134 |   |
| 71 | D5 | 70 | |
| 71 | d5 | 70 |   |
| 72 | D6 | 97 |   |
| 72 | d6 | 97 |   |
| 73 | D7 | 81 |   |
| 73 | d7 | 81 |   |
| 74 | D8 | 63 |   |
| 74 | d8 | 63 |   |
| 75 | D9 | 53 | |
| 75 | d9 | 53 | |
| 76 | E0 | 62 | |
| 76 | e0 | 62 |   |
| 77 | SR | 318 |   |
| 77 | sR | 318 |   |
| 78 | SM | 272 |   |
| 78 | sM | 272 |   |
| 79 | s6 | 218 |   |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 80 | PAR | 5 | 3423 | - | - | - | X |
| 81 | MG | 1 | 3491 | - | - | - | X |
| 81 | MG | 1 | 3521 | - | - | - | X |
| 81 | MG | 1 | 3548 | - | - | - | X |
| 81 | MG | 1 | 3577 | - | - | - | X |
| 81 | MG | 1 | 3591 | - | - | - | X |
| 81 | MG | 1 | 3593 | - | - | - | X |
| 81 | MG | 1 | 3632 | - | - | - | X |
| 81 | MG | 1 | 3634 | - | - | - | X |
| 81 | MG | 1 | 3682 | - | - | - | X |
| 81 | MG | 1 | 3711 | - | - | - | X |
| 81 | MG | 1 | 3795 | - | - | - | X |
| 81 | MG | 1 | 3830 | - | - | - | X |
| 81 | MG | 1 | 3847 | - | - | - | X |
| 81 | MG | 1 | 3860 | - | - | - | X |
| 81 | MG | 1 | 3871 | - | - | - | X |
| 81 | MG | 1 | 3884 | - | - | - | X |
| 81 | MG | 1 | 3903 | - | - | - | X |
| 81 | MG | 1 | 3904 | - | - | - | X |
| 81 | MG | 1 | 3905 | - | - | - | X |
| 81 | MG | 1 | 3924 | - | - | - | X |
| 81 | MG | 1 | 3946 | - | - | - | X |
| 81 | MG | 1 | 3957 | - | - | - | X |
| 81 | MG | 1 | 3963 | - | - | - | X |
| 81 | MG | 1 | 3975 | - | - | - | X |
| 81 | MG | 1 | 3979 | - | - | - | X |
| 81 | MG | 1 | 3982 | - | - | - | X |
| 81 | MG | 1 | 3993 | - | - | - | X |
| 81 | MG | 1 | 3998 | - | - | - | X |
| 81 | MG | 1 | 4015 | - | - | - | X |
| 81 | MG | 1 | 4018 | - | - | - | X |
| 81 | MG | 1 | 4020 | - | - | - | X |
| 81 | MG | 1 | 4026 | - | - | - | X |
| 81 | MG | 1 | 4033 | - | - | - | X |
| 81 | MG | 1 | 4062 | - | - | - | X |
| 81 | MG | 1 | 4084 | - | - | - | X |
| 81 | MG | 1 | 4089 | - | - | - | X |
| 81 | MG | 1 | 4095 | - | - | - | X |
| 81 | MG | 1 | 4098 | - | - | - | X |
| 81 | MG | 1 | 4099 | - | - | - | X |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 4100 | - | - | - | X |
| 81 | MG | 1 | 4102 | - | - | - | X |
| 81 | MG | 1 | 4107 | - | - | - | X |
| 81 | MG | 1 | 4108 | - | - | - | X |
| 81 | MG | 1 | 4109 | - | - | - | X |
| 81 | MG | 1 | 4118 | - | - | - | X |
| 81 | MG | 1 | 4121 | - | - | - | X |
| 81 | MG | 1 | 4136 | - | - | - | X |
| 81 | MG | 1 | 4139 | - | - | - | X |
| 81 | MG | 1 | 4155 | - | - | - | X |
| 81 | MG | 1 | 4173 | - | - | - | X |
| 81 | MG | 1 | 4175 | - | - | - | X |
| 81 | MG | 1 | 4180 | - | - | - | X |
| 81 | MG | 1 | 4184 | - | - | - | X |
| 81 | MG | 1 | 4186 | - | - | - | X |
| 81 | MG | 1 | 4198 | - | - | - | X |
| 81 | MG | 2 | 1923 | - | - | - | X |
| 81 | MG | 2 | 1932 | - | - | - | X |
| 81 | MG | 2 | 1937 | - | - | - | X |
| 81 | MG | 2 | 1940 | - | - | - | X |
| 81 | MG | 2 | 1982 | - | - | - | X |
| 81 | MG | 2 | 2003 | - | - | - | X |
| 81 | MG | 2 | 2010 | - | - | - | X |
| 81 | MG | 2 | 2011 | - | - | - | X |
| 81 | MG | 2 | 2019 | - | - | - | X |
| 81 | MG | 2 | 2025 | - | - | - | X |
| 81 | MG | 2 | 2026 | - | - | - | X |
| 81 | MG | 2 | 2044 | - | - | - | X |
| 81 | MG | 2 | 2048 | - | - | - | X |
| 81 | MG | 2 | 2059 | - | - | - | X |
| 81 | MG | 2 | 2061 | - | - | - | X |
| 81 | MG | 2 | 2094 | - | - | - | X |
| 81 | MG | 2 | 2103 | - | - | - | X |
| 81 | MG | 2 | 2111 | - | - | - | X |
| 81 | MG | 2 | 2113 | - | - | - | X |
| 81 | MG | 5 | 3529 | - | - | - | X |
| 81 | MG | 5 | 3535 | - | - | - | X |
| 81 | MG | 5 | 3536 | - | - | - | X |
| 81 | MG | 5 | 3537 | - | - | - | X |
| 81 | MG | 5 | 3561 | - | - | - | X |
| 81 | MG | 5 | 3658 | - | - | - | X |
| 81 | MG | 5 | 3677 | - | - | - | X |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3679 | - | - | - | X |
| 81 | MG | 5 | 3681 | - | - | - | X |
| 81 | MG | 5 | 3685 | - | - | - | X |
| 81 | MG | 5 | 3690 | - | - | - | X |
| 81 | MG | 5 | 3700 | - | - | - | X |
| 81 | MG | 5 | 3701 | - | - | - | X |
| 81 | MG | 5 | 3708 | - | - | - | X |
| 81 | MG | 5 | 3729 | - | - | - | X |
| 81 | MG | 5 | 3769 | - | - | - | X |
| 81 | MG | 5 | 3793 | - | - | - | X |
| 81 | MG | 5 | 3794 | - | - | - | X |
| 81 | MG | 5 | 3826 | - | - | - | X |
| 81 | MG | 5 | 3827 | - | - | - | X |
| 81 | MG | 5 | 3828 | - | - | - | X |
| 81 | MG | 5 | 3839 | - | - | - | X |
| 81 | MG | 5 | 3840 | - | - | - | X |
| 81 | MG | 5 | 3841 | - | - | - | X |
| 81 | MG | 5 | 3842 | - | - | - | X |
| 81 | MG | 5 | 3844 | - | - | - | X |
| 81 | MG | 5 | 3845 | - | - | - | X |
| 81 | MG | 5 | 3846 | - | - | - | X |
| 81 | MG | 5 | 3853 | - | - | - | X |
| 81 | MG | 5 | 3878 | - | - | - | X |
| 81 | MG | 5 | 3910 | - | - | - | X |
| 81 | MG | 5 | 3915 | - | - | - | X |
| 81 | MG | 5 | 3927 | - | - | - | X |
| 81 | MG | 5 | 3928 | - | - | - | X |
| 81 | MG | 5 | 3951 | - | - | - | X |
| 81 | MG | 5 | 3952 | - | - | - | X |
| 81 | MG | 5 | 3953 | - | - | - | X |
| 81 | MG | 5 | 3959 | - | - | - | X |
| 81 | MG | 5 | 3966 | - | - | - | X |
| 81 | MG | 5 | 3983 | - | - | - | X |
| 81 | MG | 5 | 3985 | - | - | - | X |
| 81 | MG | 5 | 3987 | - | - | - | X |
| 81 | MG | 5 | 3989 | - | - | - | X |
| 81 | MG | 5 | 3994 | - | - | - | X |
| 81 | MG | 5 | 3998 | - | - | - | X |
| 81 | MG | 5 | 3999 | - | - | - | X |
| 81 | MG | 5 | 4000 | - | - | - | X |
| 81 | MG | 5 | 4003 | - | - | - | X |
| 81 | MG | 5 | 4012 | - | - | - | X |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 4013 | - | - | - | X |
| 81 | MG | 5 | 4019 | - | - | - | X |
| 81 | MG | 5 | 4025 | - | - | - | X |
| 81 | MG | 5 | 4038 | - | - | - | X |
| 81 | MG | 5 | 4057 | - | - | - | X |
| 81 | MG | 5 | 4058 | - | - | - | X |
| 81 | MG | 5 | 4059 | - | - | - | X |
| 81 | MG | 5 | 4062 | - | - | - | X |
| 81 | MG | 5 | 4066 | - | - | - | X |
| 81 | MG | 5 | 4067 | - | - | - | X |
| 81 | MG | 5 | 4068 | - | - | - | X |
| 81 | MG | 5 | 4079 | - | - | - | X |
| 81 | MG | 5 | 4082 | - | - | - | X |
| 81 | MG | 5 | 4085 | - | - | - | X |
| 81 | MG | 5 | 4090 | - | - | - | X |
| 81 | MG | 5 | 4091 | - | - | - | X |
| 81 | MG | 5 | 4098 | - | - | - | X |
| 81 | MG | 5 | 4099 | - | - | - | X |
| 81 | MG | 5 | 4100 | - | - | - | X |
| 81 | MG | 5 | 4105 | - | - | - | X |
| 81 | MG | 5 | 4111 | - | - | - | X |
| 81 | MG | 5 | 4115 | - | - | - | X |
| 81 | MG | 5 | 4116 | - | - | - | X |
| 81 | MG | 6 | 1921 | - | - | - | X |
| 81 | MG | 6 | 1922 | - | - | - | X |
| 81 | MG | 6 | 1937 | - | - | - | X |
| 81 | MG | 6 | 1966 | - | - | - | X |
| 81 | MG | 6 | 1986 | - | - | - | X |
| 81 | MG | 6 | 2011 | - | - | - | X |
| 81 | MG | 6 | 2013 | - | - | - | X |
| 81 | MG | 6 | 2020 | - | - | - | X |
| 81 | MG | 6 | 2058 | - | - | - | X |
| 81 | MG | 6 | 2060 | - | - | - | X |
| 81 | MG | 6 | 2064 | - | - | - | X |
| 81 | MG | 6 | 2065 | - | - | - | X |
| 81 | MG | 6 | 2067 | - | - | - | X |
| 81 | MG | 6 | 2070 | - | - | - | X |
| 81 | MG | 6 | 2071 | - | - | - | X |
| 81 | MG | 7 | 204 | - | - | - | X |
| 81 | MG | 7 | 211 | - | - | - | X |
| 81 | MG | 8 | 209 | - | - | - | X |
| 81 | MG | 8 | 212 | - | - | - | X |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 81 | MG | 8 | 219 | - | - | - | X |
| 81 | MG | 8 | 220 | - | - | - | X |
| 81 | MG | 8 | 222 | - | - | - | X |
| 81 | MG | 8 | 223 | - | - | - | X |
| 81 | MG | D3 | 202 | - | - | - | X |
| 81 | MG | L3 | 402 | - | - | - | X |
| 81 | MG | L7 | 302 | - | - | - | X |
| 81 | MG | N8 | 203 | - | - | - | X |
| 81 | MG | O2 | 202 | - | - | - | X |
| 81 | MG | d3 | 204 | - | - | - | X |
| 81 | MG | m9 | 204 | - | - | - | X |
| 81 | MG | o2 | 204 | - | - | - | X |
| 81 | MG | q3 | 502 | - | - | - | X |

# 2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 397978 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 3078 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 65834 | 29406 | 11864 | 21486 | 3078 | | | |
| 1 | 5 | 3087 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 66030 | 29494 | 11905 | 21544 | 3087 | | | |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 3 | 121 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2579 | 1152 | 461 | 845 | 121 | | | |
| 2 | 7 | 121 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2579 | 1152 | 461 | 845 | 121 | | | |

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 4 | 157 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3333 | 1491 | 584 | 1101 | 157 | | | |
| 3 | 8 | 158 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3353 | 1500 | 586 | 1109 | 158 | | | |

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | L2 | 248 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1884 | 1173 | 382 | 328 | 1 | | | |
| 4 | l2 | 248 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1884 | 1173 | 382 | 328 | 1 | | | |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | L3 | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3081 | 1956 | 584 | 533 | 8 | | | |
| 5 | l3 | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3081 | 1956 | 584 | 533 | 8 | | | |

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | L4 | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2749 | 1730 | 522 | 494 | 3 | | | |
| 6 | l4 | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2749 | 1730 | 522 | 494 | 3 | | | |

- Molecule 7 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | L5 | 293 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2353 | 1489 | 409 | 453 | 2 | | | |
| 7 | l5 | 294 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2359 | 1489 | 412 | 456 | 2 | | | |

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | L6 | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1239 | 800 | 222 | 216 | 1 | | | |
| 8 | l6 | 157 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1248 | 806 | 224 | 217 | 1 | | | |

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | L7 | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1818 | 1171 | 331 | 315 | 1 | | | |
| 9 | l7 | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1791 | 1155 | 325 | 310 | 1 | | | |

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | L8 | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1793 | 1145 | 321 | 324 | 3 | | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | l8 | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1130 | 316 | 314 | 3 | | | |

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | L9 | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1502 | 953 | 272 | 273 | 4 | | | |
| 11 | l9 | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | | |

- Molecule 12 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | M0 | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1759 | 1114 | 333 | 305 | 7 | | | |
| 12 | m0 | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1773 | 1122 | 336 | 308 | 7 | | | |

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | M1 | 169 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1353 | 847 | 253 | 249 | 4 | | | |
| 13 | m1 | 169 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1353 | 847 | 253 | 249 | 4 | | | |

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | M3 | 193 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1543 | 962 | 315 | 266 | | | |
| 14 | m3 | 194 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1548 | 965 | 316 | 267 | | | |

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | M4 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1053 | 675 | 199 | 177 | 2 | | | |
| 15 | m4 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1059 | 678 | 200 | 179 | 2 | | | |

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | M5 | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1720 | 1077 | 361 | 281 | 1 | | | |
| 16 | m5 | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1720 | 1077 | 361 | 281 | 1 | | | |

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | M6 | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 1003 | 289 | 262 | 1 | | | |
| 17 | m6 | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 1003 | 289 | 262 | 1 | | | |

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | M7 | 175 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1378 | 856 | 273 | 249 | | | |
| 18 | m7 | 155 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1227 | 764 | 238 | 225 | | | |

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | M8 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1441 | 908 | 290 | 241 | 2 | | | |
| 19 | m8 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1441 | 908 | 290 | 241 | 2 | | | |

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | M9 | 185 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1499 | 923 | 323 | 253 | | | |
| 20 | m9 | 188 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1521 | 935 | 326 | 260 | | | |

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | N0 | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 930 | 267 | 244 | 4 | | | |
| 21 | n0 | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 930 | 267 | 244 | 4 | | | |

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | N1 | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1276 | 805 | 246 | 221 | 4 | | | |
| 22 | n1 | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1276 | 805 | 246 | 221 | 4 | | | |

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | N2 | 99 | Total | C | N | O | 0 | 0 | 0 |
| | | | 787 | 511 | 129 | 147 | | | |
| 23 | n2 | 98 | Total | C | N | O | 0 | 0 | 0 |
| | | | 778 | 505 | 127 | 146 | | | |

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | N3 | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 981 | 617 | 184 | 173 | 7 | | | |
| 24 | n3 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | N4 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 521 | 336 | 102 | 82 | 1 | | | |
| 25 | n4 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1038 | 651 | 206 | 180 | 1 | | | |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | N5 | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 946 | 608 | 166 | 170 | 2 | | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | n5 | 120 | Total<br>959 | C<br>617 | N<br>168 | O<br>172 | S<br>2 | 0 | 0 | 0 |

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | N6 | 125 | Total<br>984 | C<br>620 | N<br>191 | O<br>173 | 0 | 0 | 0 |
| 27 | n6 | 123 | Total<br>967 | C<br>608 | N<br>188 | O<br>171 | 0 | 0 | 0 |

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | N7 | 135 | Total<br>1092 | C<br>710 | N<br>202 | O<br>180 | 0 | 0 | 0 |
| 28 | n7 | 135 | Total<br>1092 | C<br>710 | N<br>202 | O<br>180 | 0 | 0 | 0 |

- Molecule 29 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | N8 | 148 | Total<br>1173 | C<br>749 | N<br>231 | O<br>190 | S<br>3 | 0 | 0 | 0 |
| 29 | n8 | 148 | Total<br>1173 | C<br>749 | N<br>231 | O<br>190 | S<br>3 | 0 | 0 | 0 |

- Molecule 30 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | N9 | 56 | Total<br>444 | C<br>277 | N<br>96 | O<br>71 | 0 | 0 | 0 |
| 30 | n9 | 58 | Total<br>462 | C<br>289 | N<br>100 | O<br>73 | 0 | 0 | 0 |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | O0 | 97 | Total<br>743 | C<br>479 | N<br>124 | O<br>139 | S<br>1 | 0 | 0 | 0 |
| 31 | o0 | 100 | Total<br>767 | C<br>492 | N<br>128 | O<br>146 | S<br>1 | 0 | 0 | 0 |

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | O1 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 849 | 541 | 164 | 143 | 1 | | | |
| 32 | o1 | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 559 | 167 | 156 | 1 | | | |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | O2 | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1007 | 638 | 203 | 165 | 1 | | | |
| 33 | o2 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | O3 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |
| 34 | o3 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | O4 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 546 | 179 | 152 | 4 | | | |
| 35 | o4 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 546 | 179 | 152 | 4 | | | |

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | O5 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |
| 36 | o5 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 965 | 612 | 185 | 167 | 1 | | | |

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | O6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 469 | 149 | 130 | 2 | | | |
| 37 | o6 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | O7 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 405 | 145 | 110 | 5 | | | |
| 38 | o7 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | O8 | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |
| 39 | o8 | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 608 | 388 | 114 | 106 | | | |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | O9 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |
| 40 | o9 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | Q0 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |
| 41 | q0 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |

- Molecule 42 is a protein called 60S ribosomal protein L41-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | Q1 | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | q1 | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | Q2 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |
| 43 | q2 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | Q3 | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |
| 44 | q3 | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |

- Molecule 45 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | 2 | 1712 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 36485 | 16312 | 6462 | 11999 | 1712 | | | |
| 45 | 6 | 1683 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 35865 | 16035 | 6355 | 11792 | 1683 | | | |

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | S0 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1017 | 278 | 284 | 2 | | | |
| 46 | s0 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1017 | 278 | 284 | 2 | | | |

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | S1 | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1688 | 1071 | 305 | 308 | 4 | | | |
| 47 | s1 | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1722 | 1091 | 312 | 315 | 4 | | | |

- Molecule 48 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | S2 | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1635 | 1047 | 289 | 297 | 2 | | | |
| 48 | s2 | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1635 | 1047 | 289 | 297 | 2 | | | |

- Molecule 49 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 49 | S3 | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1621 | 1028 | 297 | 290 | 6 | | | |
| 49 | s3 | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1734 | 1101 | 313 | 314 | 6 | | | |

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | S4 | 256 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2044 | 1300 | 385 | 356 | 3 | | | |
| 50 | s4 | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2068 | 1316 | 389 | 360 | 3 | | | |

- Molecule 51 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | S5 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1007 | 300 | 299 | 3 | | | |
| 51 | s5 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1007 | 300 | 299 | 3 | | | |

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | S6 | 200 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1593 | 997 | 313 | 280 | 3 | | | |

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | S7 | 179 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1442 | 926 | 259 | 257 | | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | s7 | 186 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1492 | 957 | 267 | 268 | | | |

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 54 | S8 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1466 | 910 | 293 | 261 | 2 | | | |
| 54 | s8 | 188 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1489 | 925 | 298 | 264 | 2 | | | |

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 55 | S9 | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1418 | 900 | 273 | 244 | 1 | | | |
| 55 | s9 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1494 | 943 | 289 | 261 | 1 | | | |

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 56 | C0 | 90 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 481 | 120 | 139 | 2 | | | |
| 56 | c0 | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 761 | 490 | 125 | 144 | 2 | | | |

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 57 | C1 | 139 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1127 | 724 | 214 | 186 | 3 | | | |
| 57 | c1 | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1168 | 747 | 221 | 197 | 3 | | | |

- Molecule 58 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 58 | C2 | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 764 | 485 | 132 | 145 | 2 | | | |
| 58 | c2 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 156 | 172 | 2 | | | |

- Molecule 59 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 59 | C3 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | | |
| 59 | c3 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | | |

- Molecule 60 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 60 | C4 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 545 | 182 | 163 | 1 | | | |
| 60 | c4 | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 949 | 582 | 188 | 176 | 3 | | | |

- Molecule 61 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 61 | C5 | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 918 | 583 | 171 | 157 | 7 | | | |
| 61 | c5 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1039 | 658 | 196 | 178 | 7 | | | |

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | C6 | 136 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1064 | 682 | 195 | 187 | | | |
| 62 | c6 | 142 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1111 | 711 | 204 | 196 | | | |

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 63 | C7 | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 901 | 562 | 172 | 165 | 2 | | | |
| 63 | c7 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 906 | 563 | 174 | 167 | 2 | | | |

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 64 | C8 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1178 | 734 | 235 | 207 | 2 | | | |
| 64 | c8 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 65 | C9 | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1072 | 669 | 202 | 199 | 2 | | | |
| 65 | c9 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |

- Molecule 66 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 66 | D0 | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 519 | 148 | 150 | 1 | | | |
| 66 | d0 | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 873 | 549 | 159 | 164 | 1 | | | |

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 67 | D1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |
| 67 | d1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 68 | D2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |
| 68 | d2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 69 | D3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 69 | d3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | D4 | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | |
| 70 | d4 | 134 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | |

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | D5 | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 563 | 360 | 104 | 99 | | | |
| 71 | d5 | 69 | Total | C | N | O | 0 | 0 | 0 |
| | | | 558 | 357 | 103 | 98 | | | |

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 72 | D6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |
| 72 | d6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 73 | D7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |
| 73 | d7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 74 | D8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |
| 74 | d8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 75 | D9 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 443 | 275 | 92 | 72 | 4 | | | |
| 75 | d9 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 443 | 275 | 92 | 72 | 4 | | | |

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 76 | E0 | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 475 | 299 | 98 | 77 | 1 | | | |
| 76 | e0 | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 309 | 101 | 80 | 1 | | | |

- Molecule 77 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 77 | SR | 317 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2432 | 1537 | 416 | 471 | 8 | | | |
| 77 | sR | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2437 | 1540 | 417 | 472 | 8 | | | |

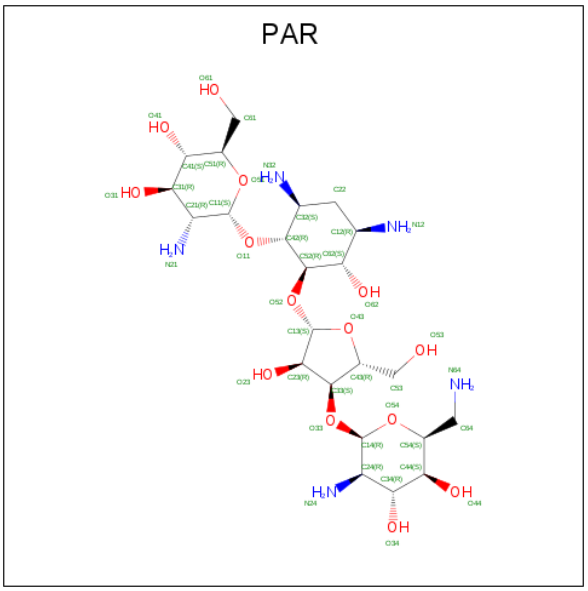
- Molecule 78 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 78 | SM | 147 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1044 | 616 | 209 | 219 | | | |
| 78 | sM | 95 | Total | C | N | O | 0 | 0 | 0 |
| | | | 635 | 376 | 131 | 128 | | | |

- Molecule 79 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 79 | s6 | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1755 | 1102 | 337 | 313 | 3 | | | |

- Molecule 80 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 4 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 4 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 7 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 80 | 7 | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 80 | 8 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 8 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | n3 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | o2 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 6 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 6 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 6 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 6 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 6 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |
| 80 | 6 | 1 | Total C N O<br>42 23 5 14 | 0 | 0 |

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 81 | n8 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 81 | N5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | d2 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | n5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | S9 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | M9 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | q0 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | c1 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | o1 | 3 | Total Mg<br>3 3 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 81 | L4 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | L5 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | O2 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | m9 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 81 | M3 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | n2 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | o2 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | d4 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | 2 | 212 | Total Mg<br>212 212 | 0 | 0 |
| 81 | M6 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 81 | S7 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | n0 | 6 | Total Mg<br>6 6 | 0 | 0 |
| 81 | m6 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 81 | n9 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | M5 | 9 | Total Mg<br>9 9 | 0 | 0 |
| 81 | S2 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | N6 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 81 | Q3 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | m5 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | s4 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | s2 | 1 | Total Mg<br>1 1 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 81 | n6 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 81 | M8 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | q3 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | N3 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 81 | 4 | 35 | Total Mg<br>35 35 | 0 | 0 |
| 81 | L2 | 6 | Total Mg<br>6 6 | 0 | 0 |
| 81 | O1 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | s8 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | m8 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | n3 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | l2 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | N0 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | L7 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | D3 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | 6 | 169 | Total Mg<br>169 169 | 0 | 0 |
| 81 | O4 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | D6 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | S6 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | c9 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | l7 | 6 | Total Mg<br>6 6 | 0 | 0 |
| 81 | L8 | 1 | Total Mg<br>1 1 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 81 | o4 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | O7 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 81 | s6 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | M4 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | 1 | 762 | Total Mg<br>762 762 | 0 | 0 |
| 81 | c4 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | l8 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | Q2 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 81 | o7 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | d6 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | q2 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | Q1 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | L3 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 81 | 8 | 23 | Total Mg<br>23 23 | 0 | 0 |
| 81 | 3 | 15 | Total Mg<br>15 15 | 0 | 0 |
| 81 | O0 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | l3 | 9 | Total Mg<br>9 9 | 0 | 0 |
| 81 | N1 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | C8 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | N7 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | o0 | 3 | Total Mg<br>3 3 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 81 | O3 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | M0 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | 5 | 698 | Total Mg<br>698 698 | 0 | 0 |
| 81 | n1 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | l4 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | L9 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 81 | d3 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 81 | o3 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | O9 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | m0 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | O6 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | M7 | 6 | Total Mg<br>6 6 | 0 | 0 |
| 81 | N8 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 81 | l9 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 81 | C9 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 81 | 7 | 12 | Total Mg<br>12 12 | 0 | 0 |
| 81 | m7 | 9 | Total Mg<br>9 9 | 0 | 0 |

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 82 | o4 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | O7 | 1 | Total Zn<br>1 1 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 82 | q0 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | Q2 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | Q3 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | D9 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | q3 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | Q0 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | d7 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | O4 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | d9 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | D7 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | d6 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | o7 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | D6 | 1 | Total Zn<br>1 1 | 0 | 0 |
| 82 | q2 | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 83 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | 1 | 500 | Total O<br>500 500 | 0 | 0 |
| 83 | 3 | 7 | Total O<br>7 7 | 0 | 0 |
| 83 | 4 | 15 | Total O<br>15 15 | 0 | 0 |
| 83 | L2 | 5 | Total O<br>5 5 | 0 | 0 |
| 83 | L3 | 2 | Total O<br>2 2 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | L4 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | L5 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | L7 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | M5 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | M6 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | M7 | 4 | Total O<br>4 4 | 0 | 0 |
| 83 | N0 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | N1 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | N3 | 3 | Total O<br>3 3 | 0 | 0 |
| 83 | N6 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | N7 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | N8 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | N9 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | O0 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | O2 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | O3 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | O4 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | O7 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | Q2 | 4 | Total O<br>4 4 | 0 | 0 |
| 83 | 2 | 122 | Total O<br>122 122 | 0 | 0 |
| 83 | S1 | 1 | Total O<br>1 1 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | S9 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | C3 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | C6 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | C7 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | C9 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | D3 | 4 | Total O<br>4 4 | 0 | 0 |
| 83 | 5 | 477 | Total O<br>477 477 | 0 | 0 |
| 83 | 7 | 12 | Total O<br>12 12 | 0 | 0 |
| 83 | 8 | 7 | Total O<br>7 7 | 0 | 0 |
| 83 | l2 | 5 | Total O<br>5 5 | 0 | 0 |
| 83 | l3 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | l5 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | l7 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | l9 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | m0 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | m6 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | m7 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | m9 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | n0 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | n1 | 2 | Total O<br>2 2 | 0 | 0 |
| 83 | n3 | 3 | Total O<br>3 3 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

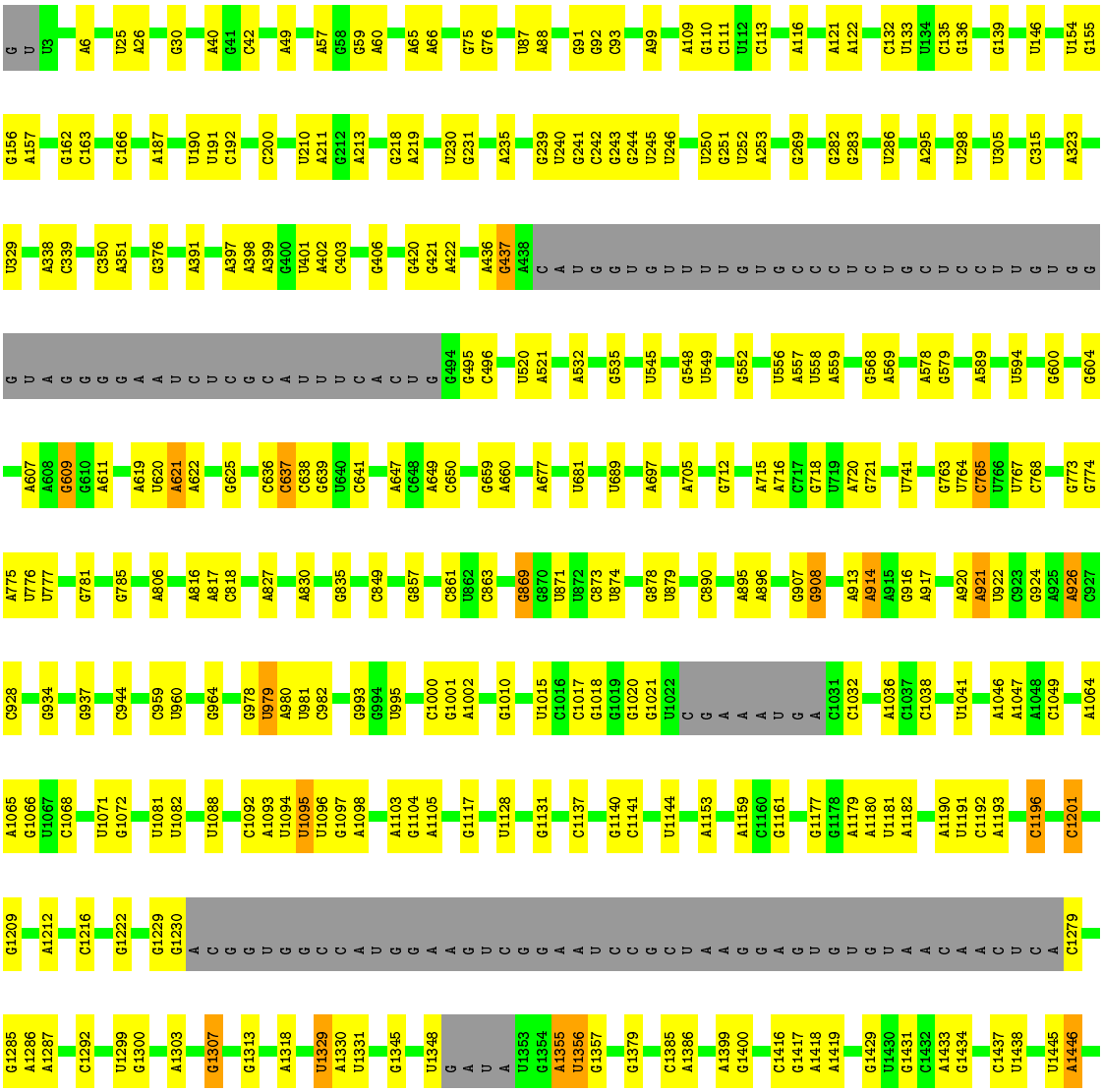
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 83 | n6 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | n7 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | n8 | 3 | Total O<br>3 3 | 0 | 0 |
| 83 | o2 | 3 | Total O<br>3 3 | 0 | 0 |
| 83 | 6 | 113 | Total O<br>113 113 | 0 | 0 |
| 83 | c3 | 4 | Total O<br>4 4 | 0 | 0 |
| 83 | c4 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | c6 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | c9 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | d3 | 1 | Total O<br>1 1 | 0 | 0 |
| 83 | d6 | 1 | Total O<br>1 1 | 0 | 0 |

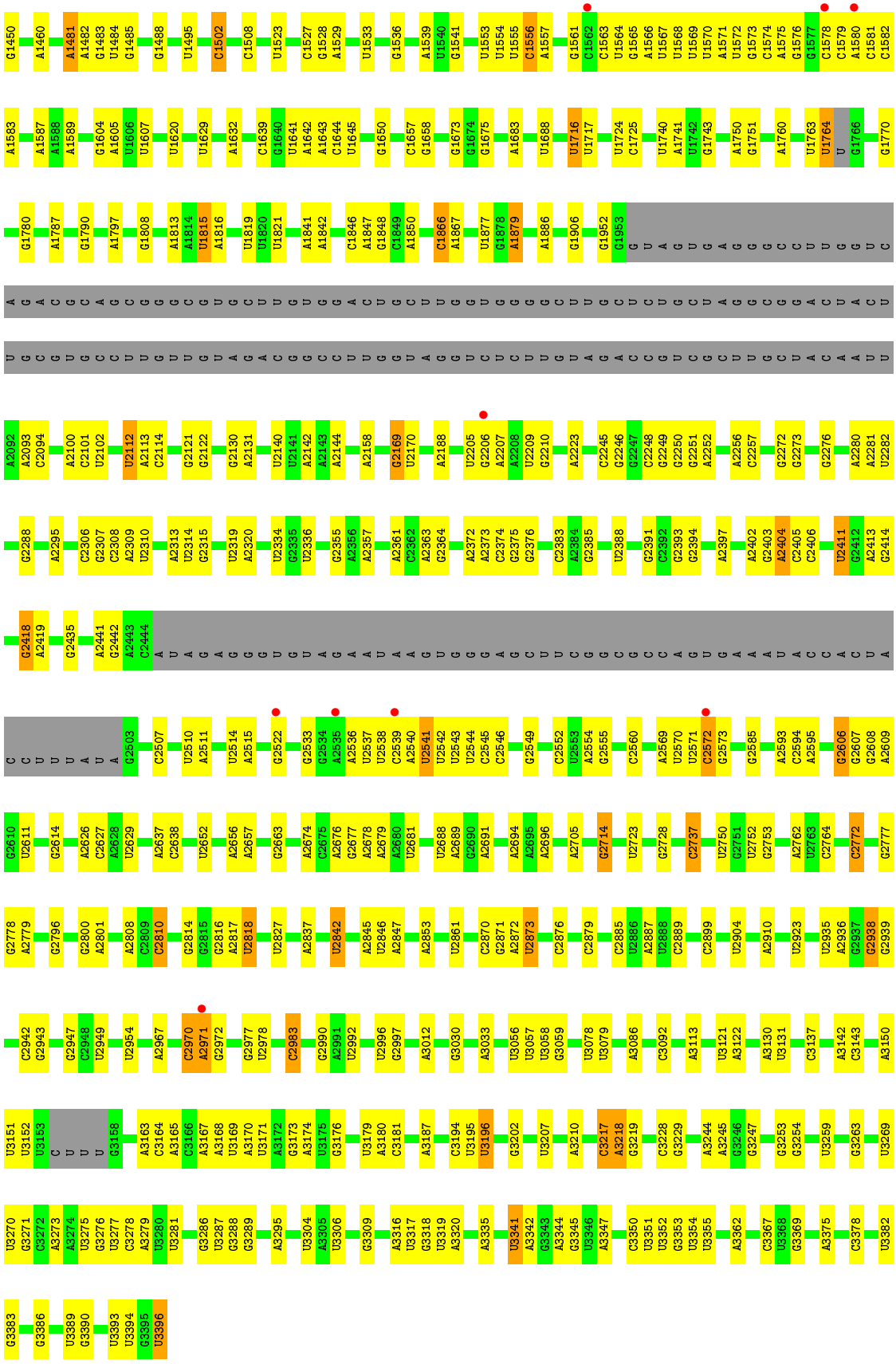
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 25S ribosomal RNA

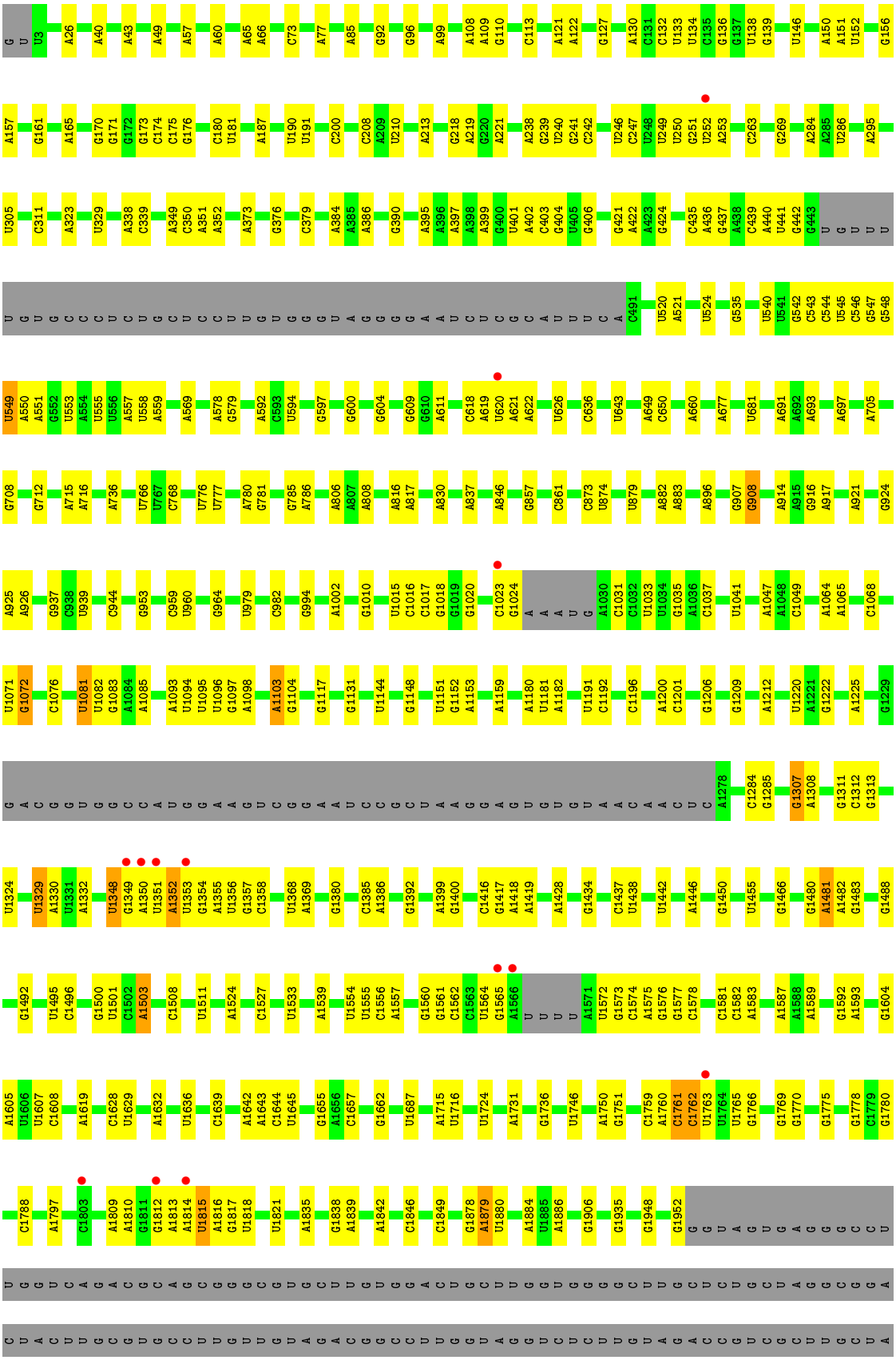
Chain 1:

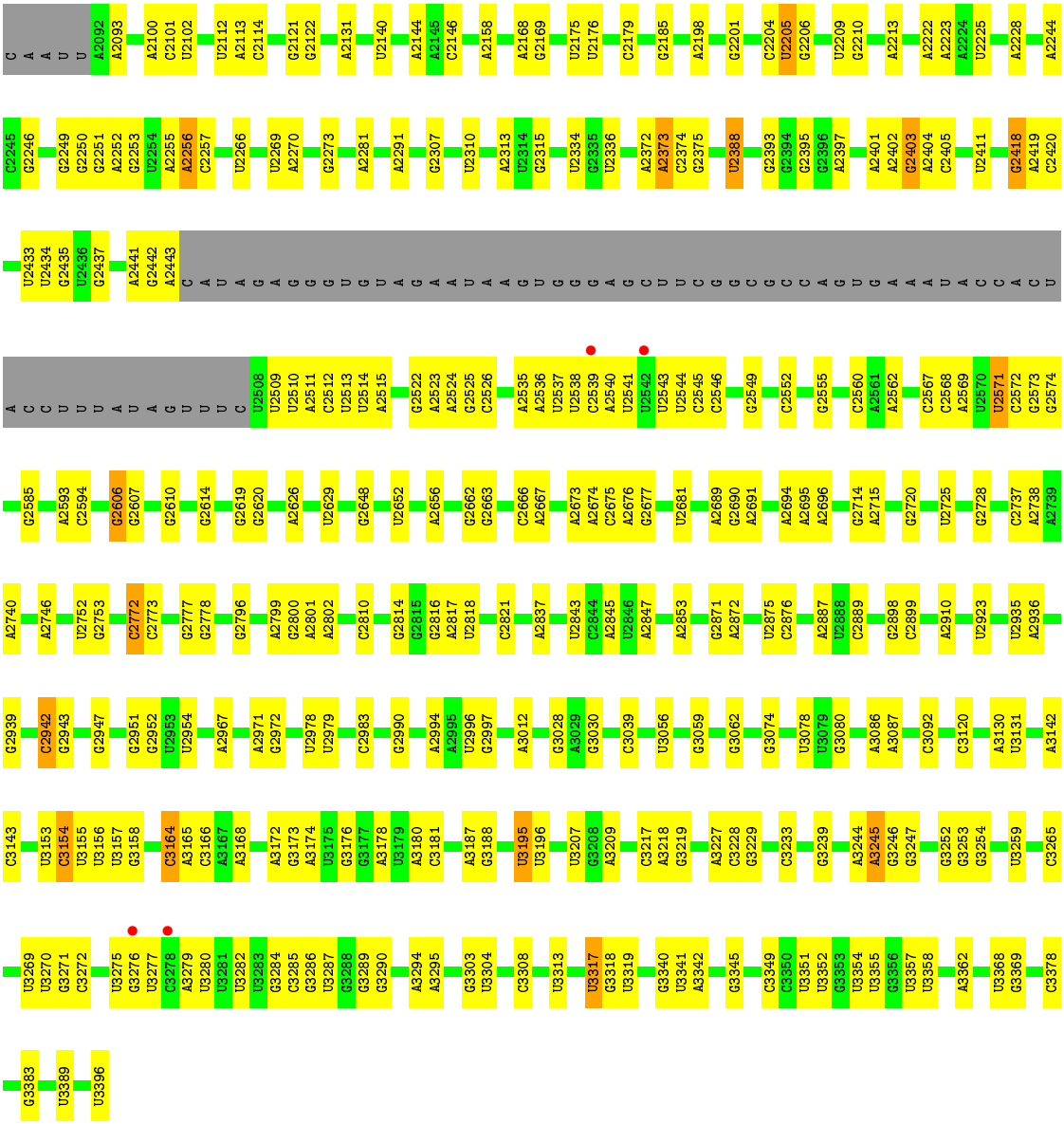




- Molecule 1: 25S ribosomal RNA

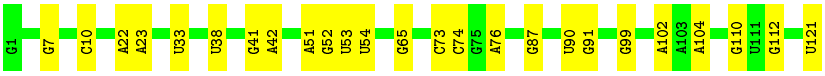
Chain 5:





• Molecule 2: 5S ribosomal RNA

Chain 3:

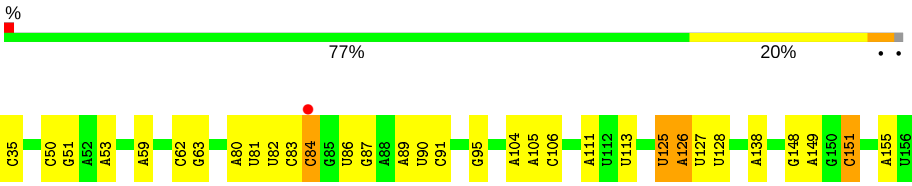


• Molecule 2: 5S ribosomal RNA

Chain 7:

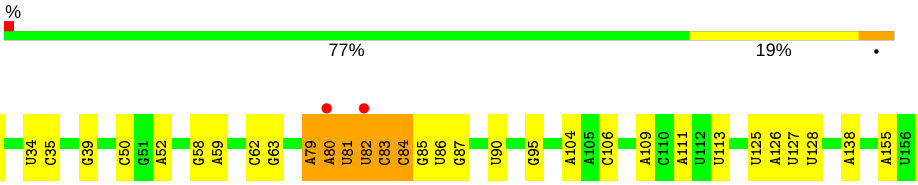
• Molecule 3: 5.8S ribosomal RNA

Chain 4:



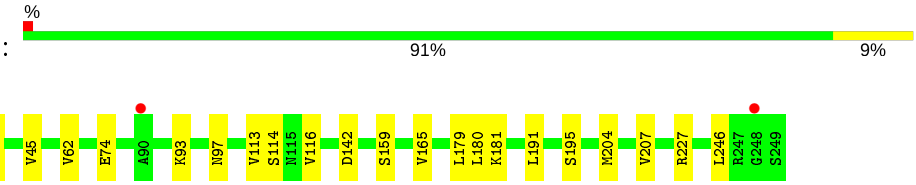

- Molecule 3: 5.8S ribosomal RNA

Chain 8:



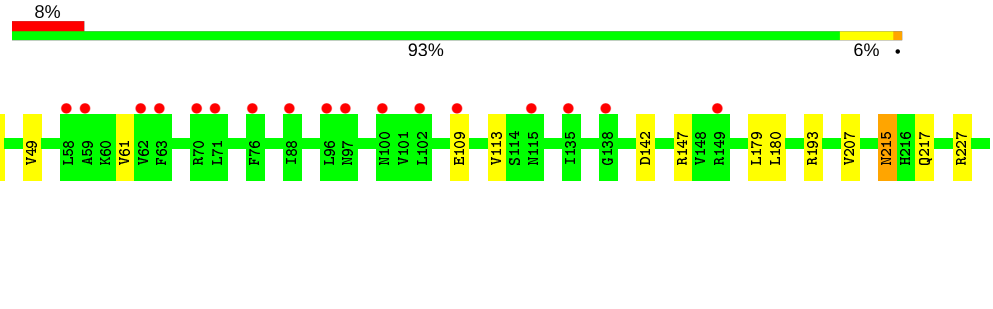

- Molecule 4: 60S ribosomal protein L2-A

Chain L2:



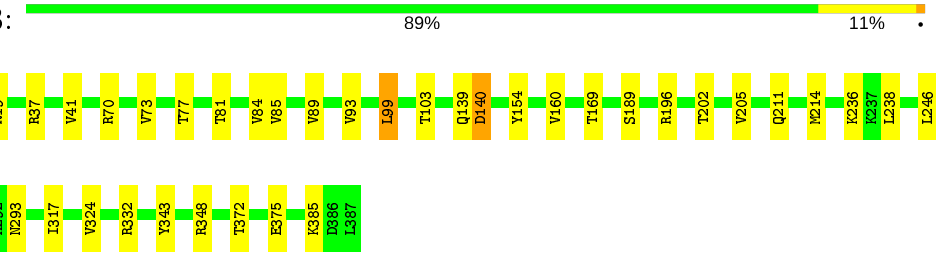

- Molecule 4: 60S ribosomal protein L2-A

Chain l2:



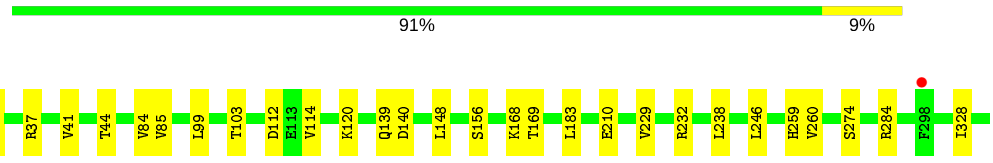

- Molecule 5: 60S ribosomal protein L3

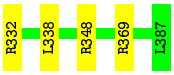
Chain L3:




- Molecule 5: 60S ribosomal protein L3

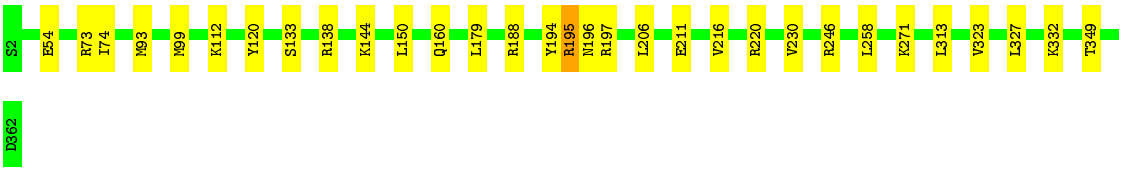
Chain l3:





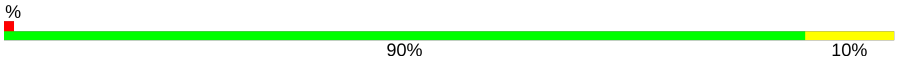

• Molecule 6: 60S ribosomal protein L4-A

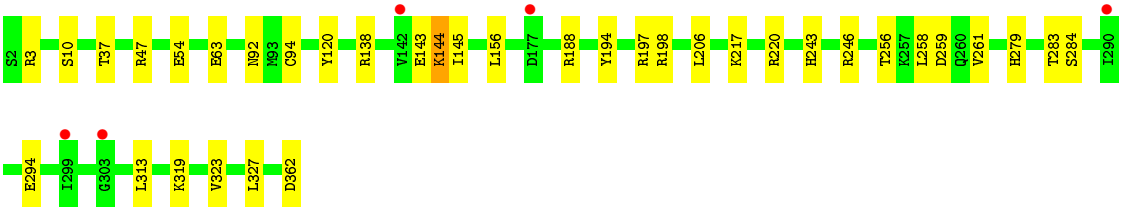
Chain L4:




• Molecule 6: 60S ribosomal protein L4-A

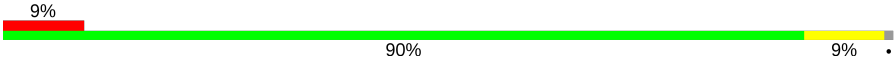
Chain l4:

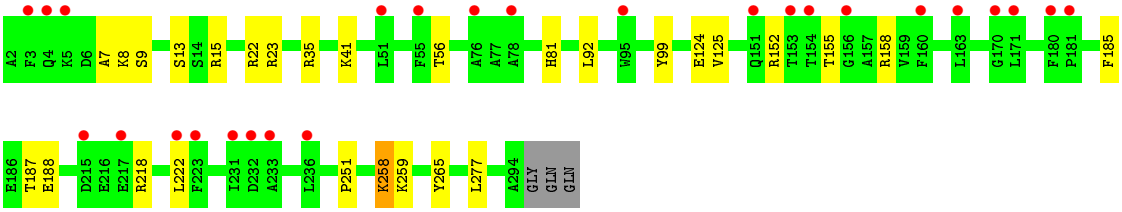



• Molecule 7: 60S ribosomal protein L5

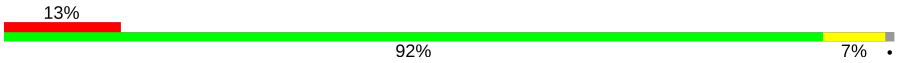
Chain L5:

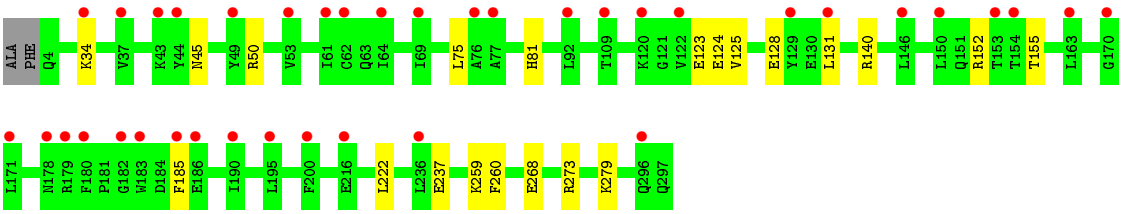



• Molecule 7: 60S ribosomal protein L5

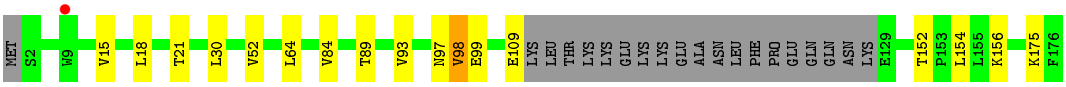
Chain l5:



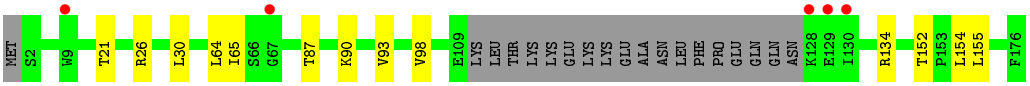

• Molecule 8: 60S ribosomal protein L6-A

Chain L6:



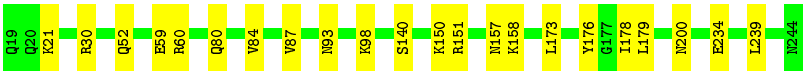

• Molecule 8: 60S ribosomal protein L6-A

Chain l6:




• Molecule 9: 60S ribosomal protein L7-A

Chain L7:

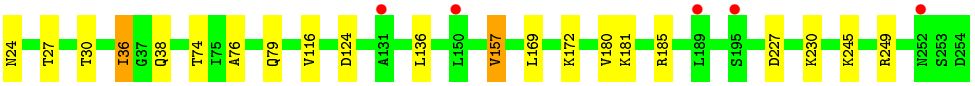



• Molecule 9: 60S ribosomal protein L7-A

Chain l7:

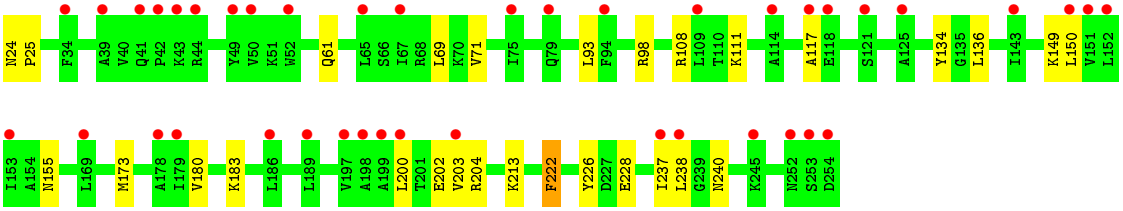
• Molecule 10: 60S ribosomal protein L8-A

Chain L8:



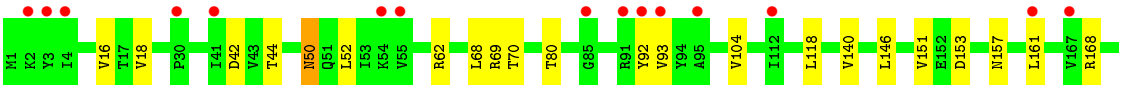

• Molecule 10: 60S ribosomal protein L8-A

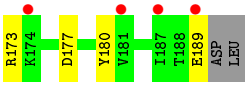
Chain l8:




• Molecule 11: 60S ribosomal protein L9-A

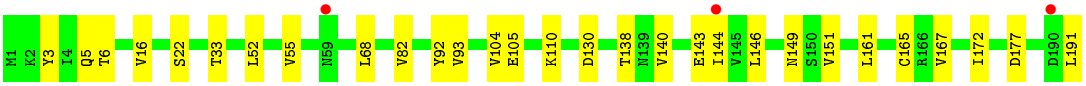
Chain L9:





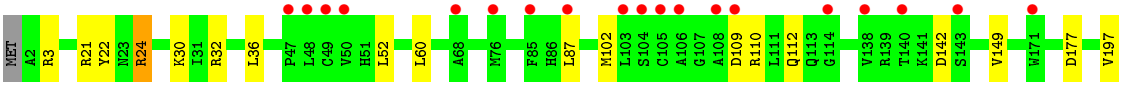

- Molecule 11: 60S ribosomal protein L9-A

Chain l9:



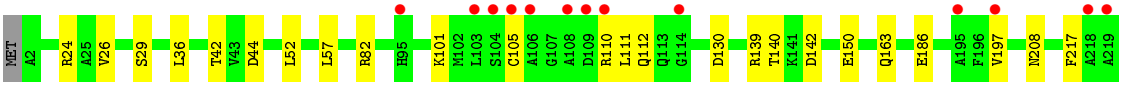

- Molecule 12: 60S ribosomal protein L10

Chain M0:



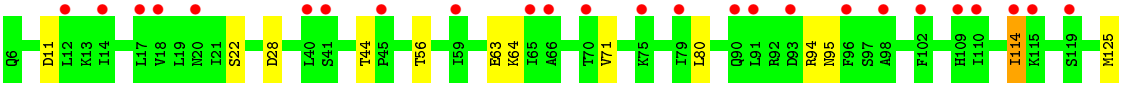
- Molecule 12: 60S ribosomal protein L10

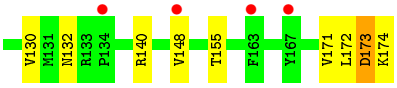
Chain m0:



- Molecule 13: 60S ribosomal protein L11-B

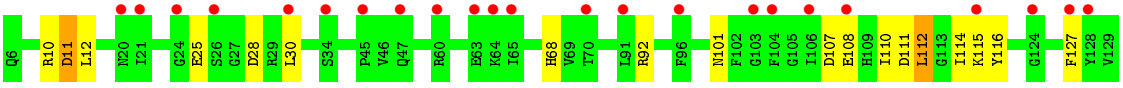
Chain M1:

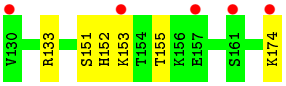



- Molecule 13: 60S ribosomal protein L11-B

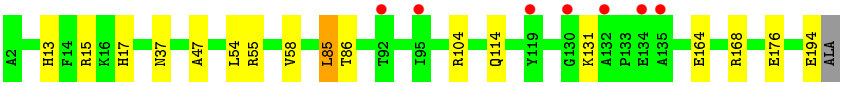
Chain m1:





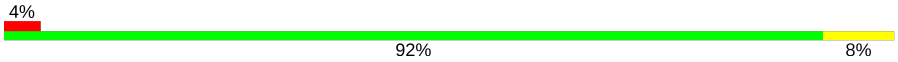

- Molecule 14: 60S ribosomal protein L13-A

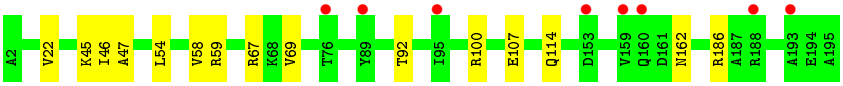
Chain M3:




- Molecule 14: 60S ribosomal protein L13-A

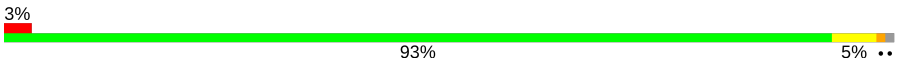
Chain m3:

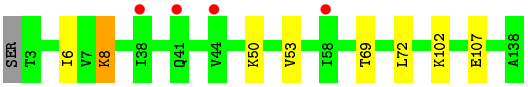



- Molecule 15: 60S ribosomal protein L14-A

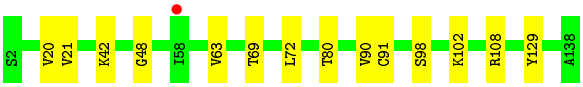
Chain M4:



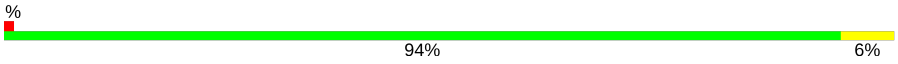

- Molecule 15: 60S ribosomal protein L14-A

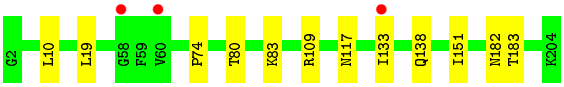
Chain m4:




- Molecule 16: 60S ribosomal protein L15-A

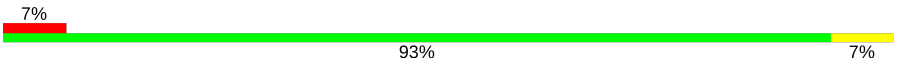
Chain M5:

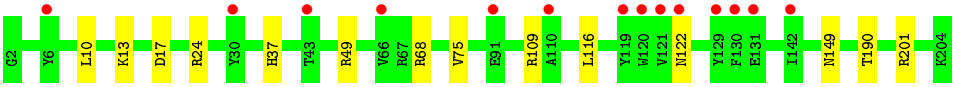



- Molecule 16: 60S ribosomal protein L15-A

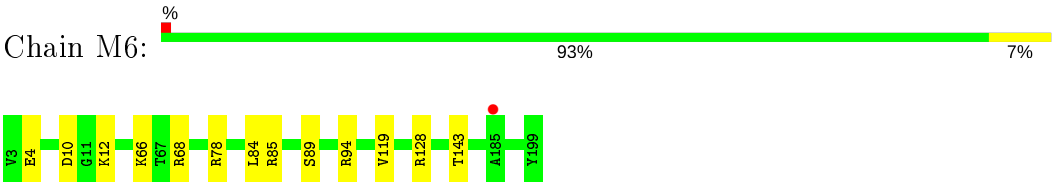
Chain m5:



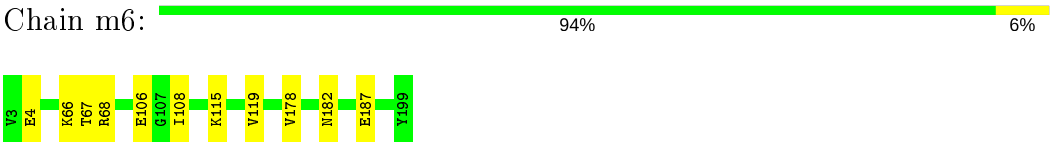

- Molecule 17: 60S ribosomal protein L16-A

Chain M6:



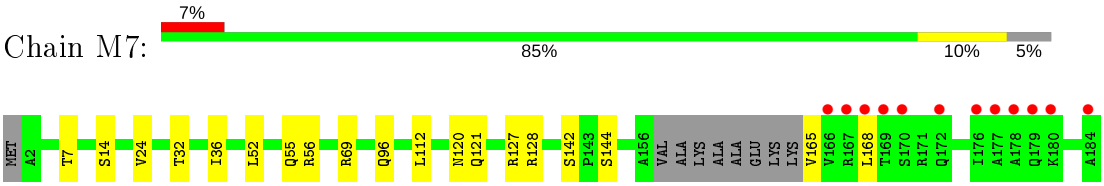

• Molecule 17: 60S ribosomal protein L16-A

Chain m6:



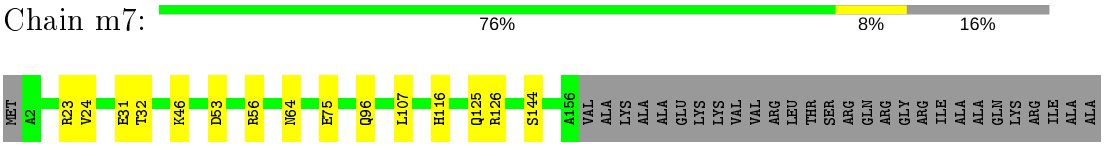

• Molecule 18: 60S ribosomal protein L17-A

Chain M7:



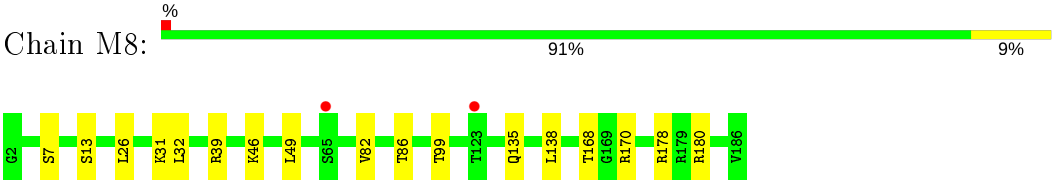

• Molecule 18: 60S ribosomal protein L17-A

Chain m7:



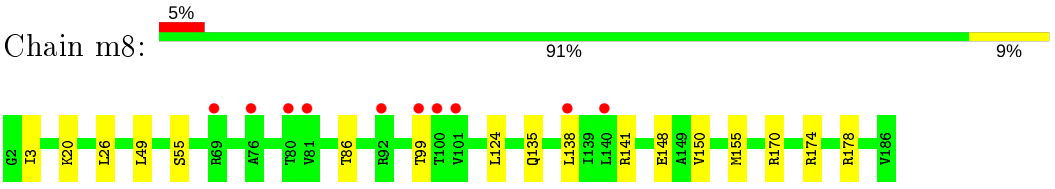

• Molecule 19: 60S ribosomal protein L18-A

Chain M8:



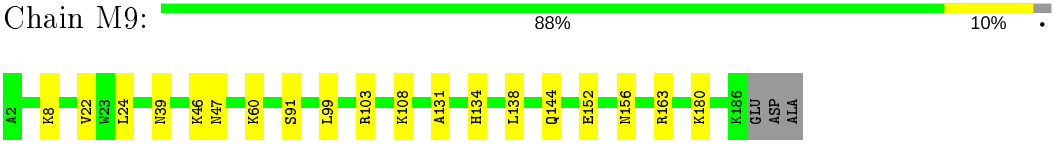

• Molecule 19: 60S ribosomal protein L18-A

Chain m8:



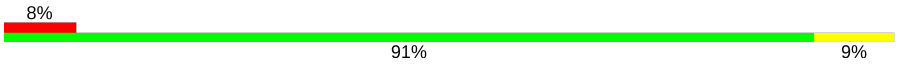

• Molecule 20: 60S ribosomal protein L19-A

Chain M9:



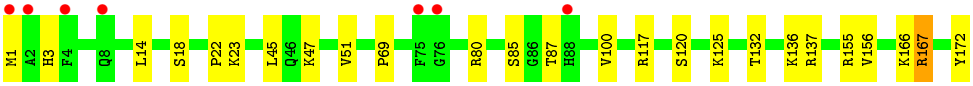

• Molecule 20: 60S ribosomal protein L19-A

Chain m9:



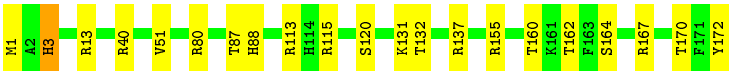
• Molecule 21: 60S ribosomal protein L20-A

Chain N0:



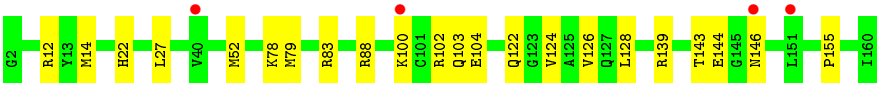

• Molecule 21: 60S ribosomal protein L20-A

Chain n0:



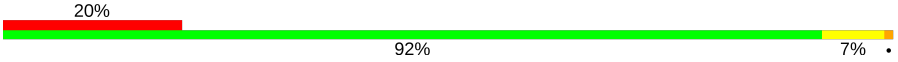

• Molecule 22: 60S ribosomal protein L21-A

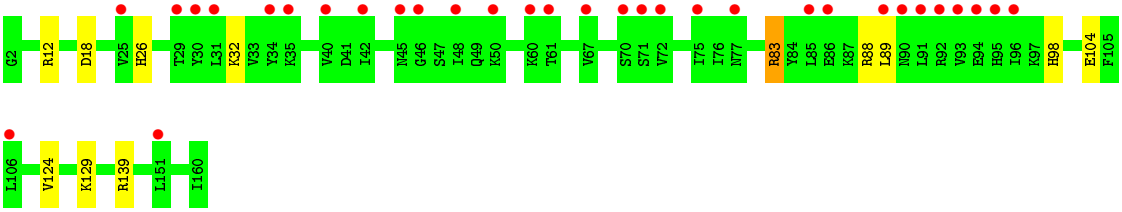
Chain N1:




• Molecule 22: 60S ribosomal protein L21-A

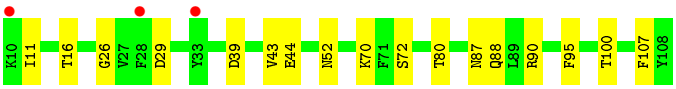
Chain n1:



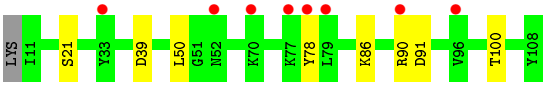

• Molecule 23: 60S ribosomal protein L22-A

Chain N2:



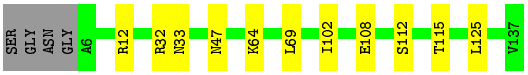

• Molecule 23: 60S ribosomal protein L22-A

Chain n2:



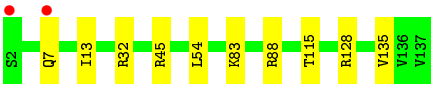

• Molecule 24: 60S ribosomal protein L23-A

Chain N3:



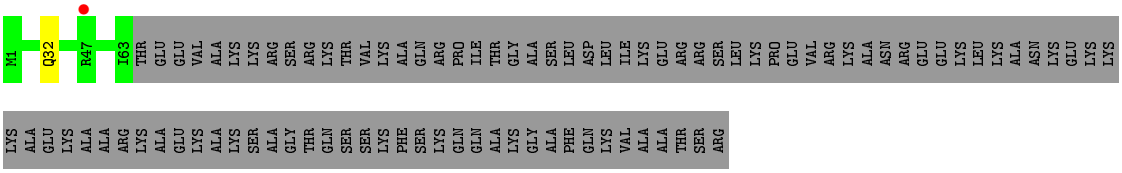

• Molecule 24: 60S ribosomal protein L23-A

Chain n3:



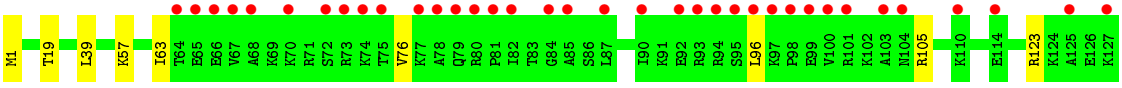

• Molecule 25: 60S ribosomal protein L24-A

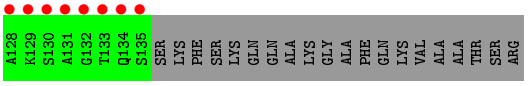
Chain N4:




• Molecule 25: 60S ribosomal protein L24-A

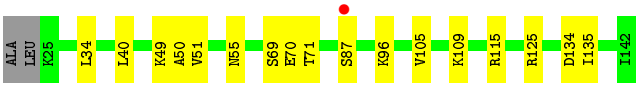
Chain n4:



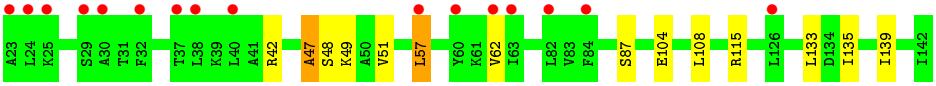

• Molecule 26: 60S ribosomal protein L25

Chain N5:



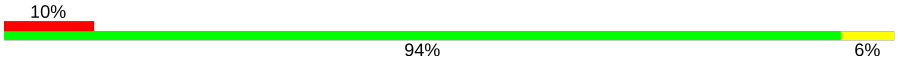

• Molecule 26: 60S ribosomal protein L25

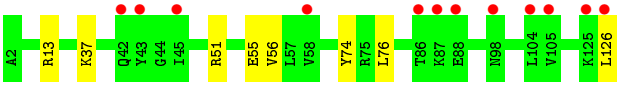
Chain n5:




• Molecule 27: 60S ribosomal protein L26-A

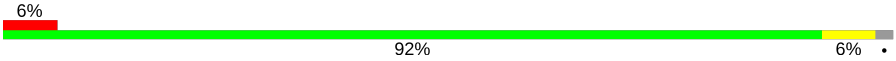
Chain N6:

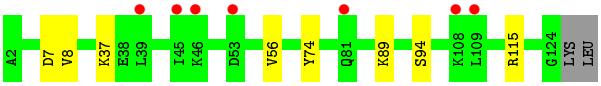



• Molecule 27: 60S ribosomal protein L26-A

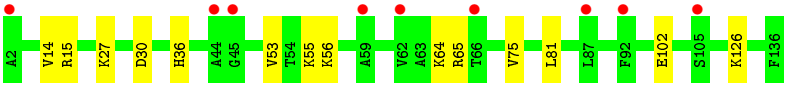
Chain n6:



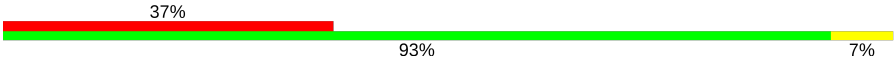

• Molecule 28: 60S ribosomal protein L27-A

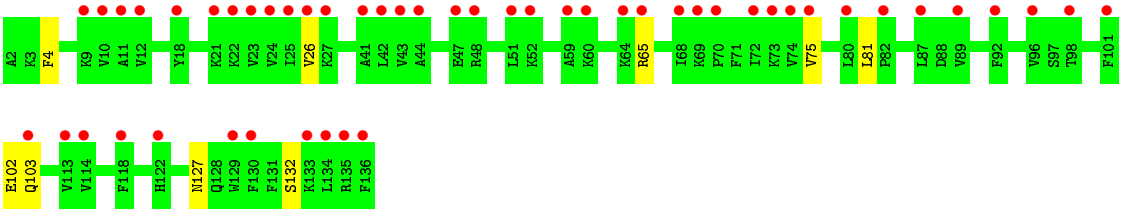
Chain N7:




• Molecule 28: 60S ribosomal protein L27-A

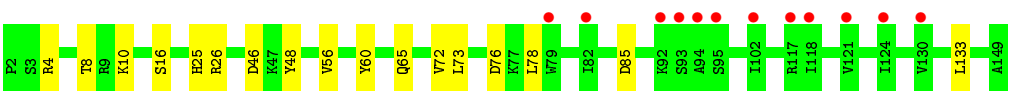
Chain n7:



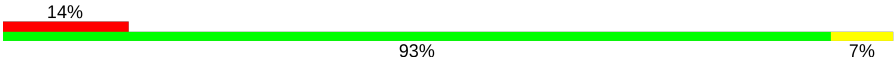

• Molecule 29: 60S ribosomal protein L28

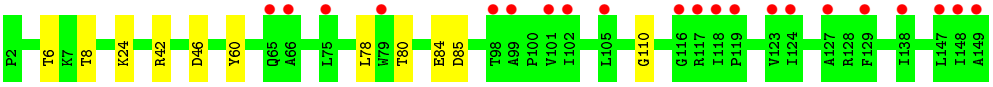
Chain N8:



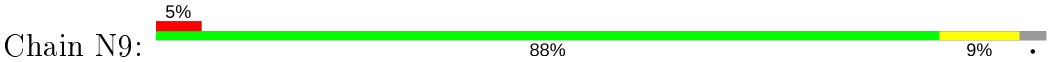

• Molecule 29: 60S ribosomal protein L28

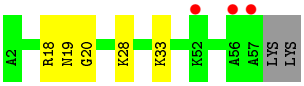
Chain n8:



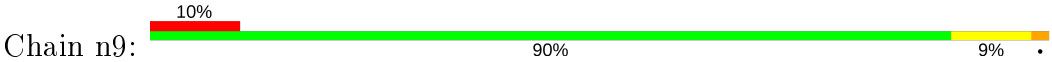


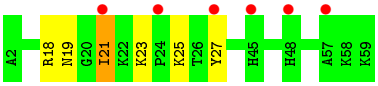

• Molecule 30: 60S ribosomal protein L29



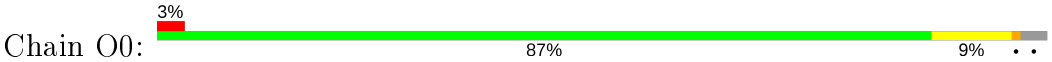



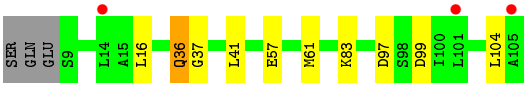

• Molecule 30: 60S ribosomal protein L29



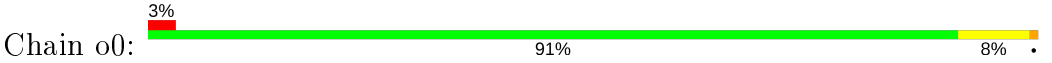



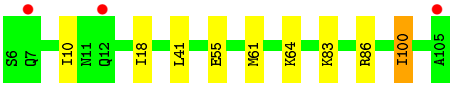

• Molecule 31: 60S ribosomal protein L30



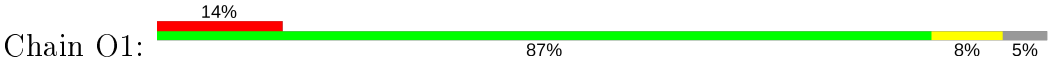



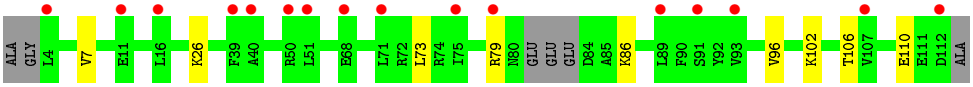

• Molecule 31: 60S ribosomal protein L30



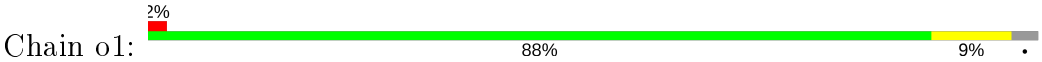



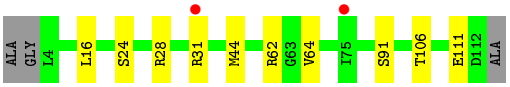

• Molecule 32: 60S ribosomal protein L31-A



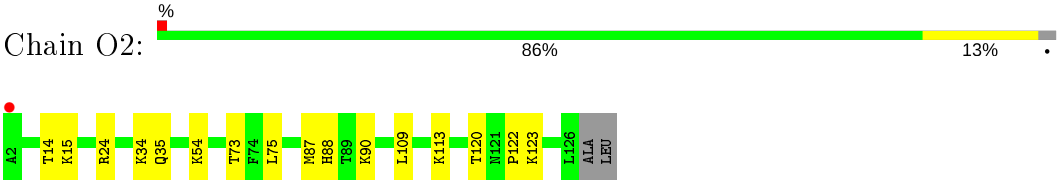

• Molecule 32: 60S ribosomal protein L31-A



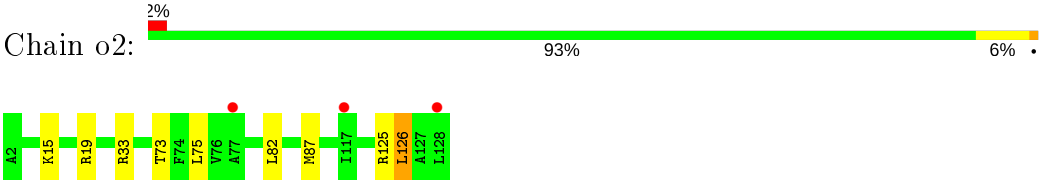

• Molecule 33: 60S ribosomal protein L32

Chain O2:



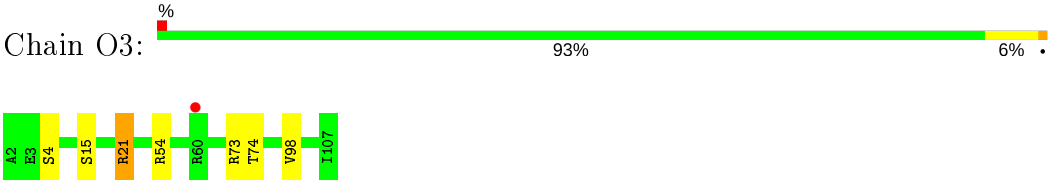

• Molecule 33: 60S ribosomal protein L32

Chain o2:



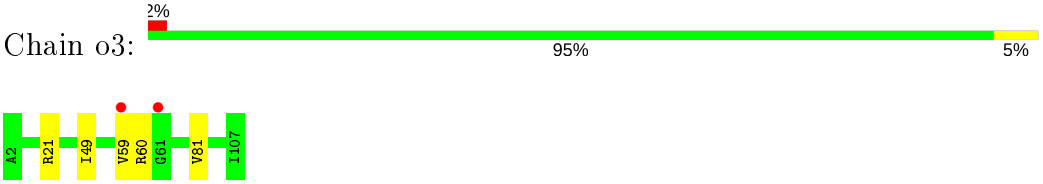

• Molecule 34: 60S ribosomal protein L33-A

Chain O3:



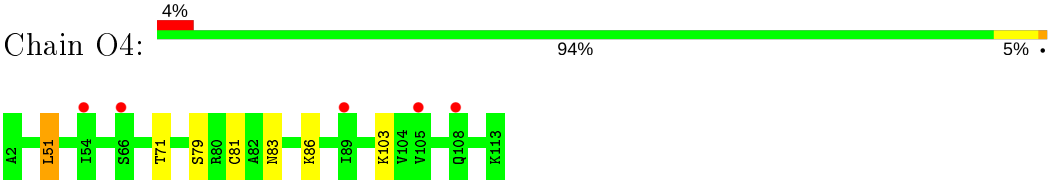

• Molecule 34: 60S ribosomal protein L33-A

Chain o3:



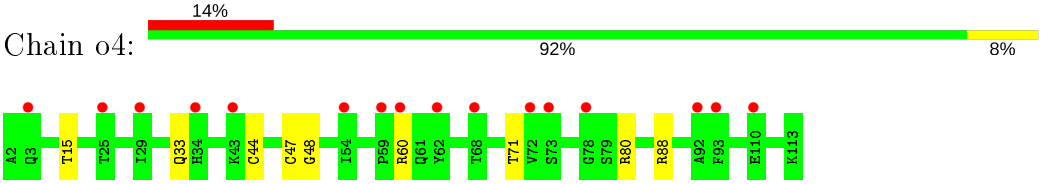

• Molecule 35: 60S ribosomal protein L34-A

Chain O4:



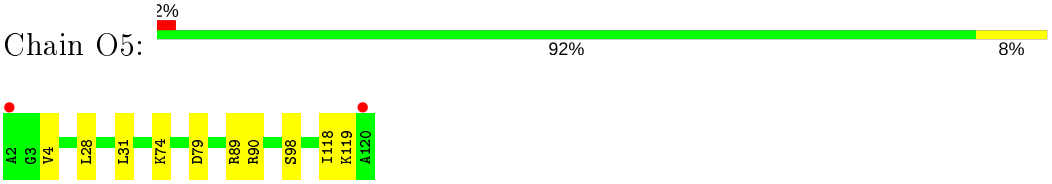

• Molecule 35: 60S ribosomal protein L34-A

Chain o4:



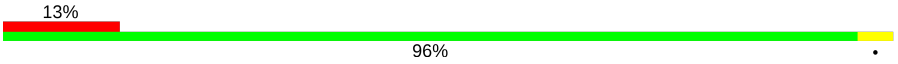

• Molecule 36: 60S ribosomal protein L35-A

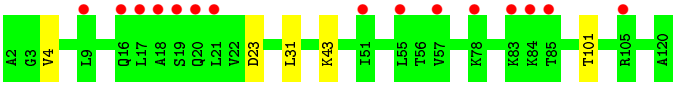
Chain O5:



• Molecule 36: 60S ribosomal protein L35-A

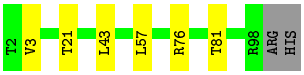
Chain o5:



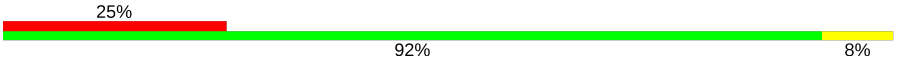

• Molecule 37: 60S ribosomal protein L36-A

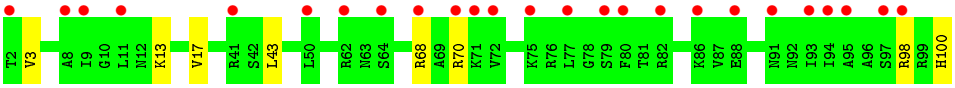
Chain O6:




• Molecule 37: 60S ribosomal protein L36-A

Chain o6:



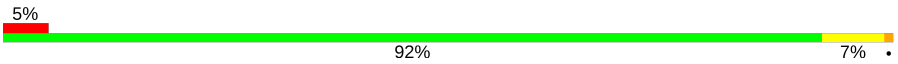




• Molecule 38: 60S ribosomal protein L37-A

Chain O7:

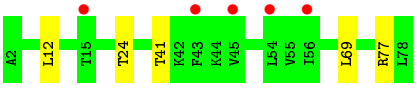
• Molecule 38: 60S ribosomal protein L37-A

Chain o7:



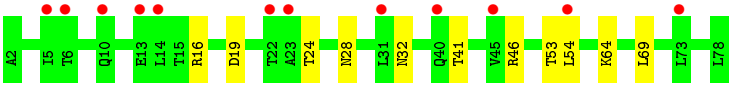
• Molecule 39: 60S ribosomal protein L38

Chain O8:



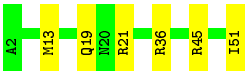

• Molecule 39: 60S ribosomal protein L38

Chain o8:



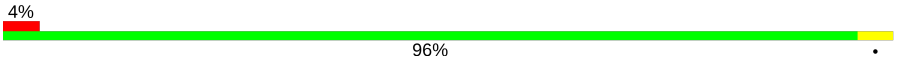
• Molecule 40: 60S ribosomal protein L39

Chain O9:



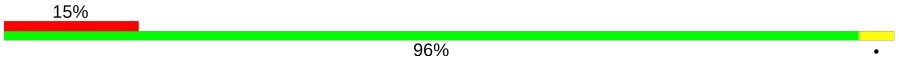

• Molecule 40: 60S ribosomal protein L39

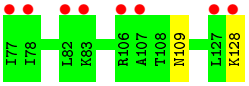
Chain o9:



• Molecule 41: Ubiquitin-60S ribosomal protein L40

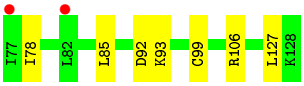
Chain Q0:




• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain q0:

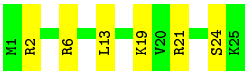



• Molecule 42: 60S ribosomal protein L41-B

Chain Q1:

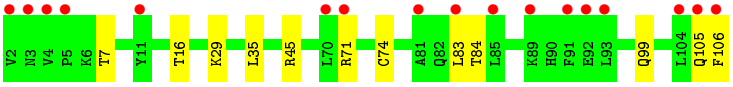
• Molecule 42: 60S ribosomal protein L41-B

Chain q1:



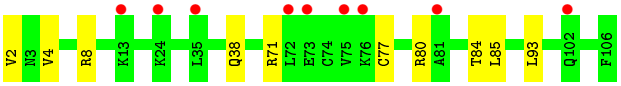

• Molecule 43: 60S ribosomal protein L42-A

Chain Q2:



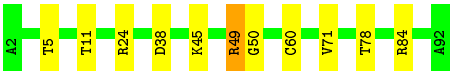

• Molecule 43: 60S ribosomal protein L42-A

Chain q2:



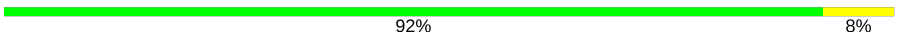

• Molecule 44: 60S ribosomal protein L43-A

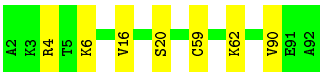
Chain Q3:




• Molecule 44: 60S ribosomal protein L43-A

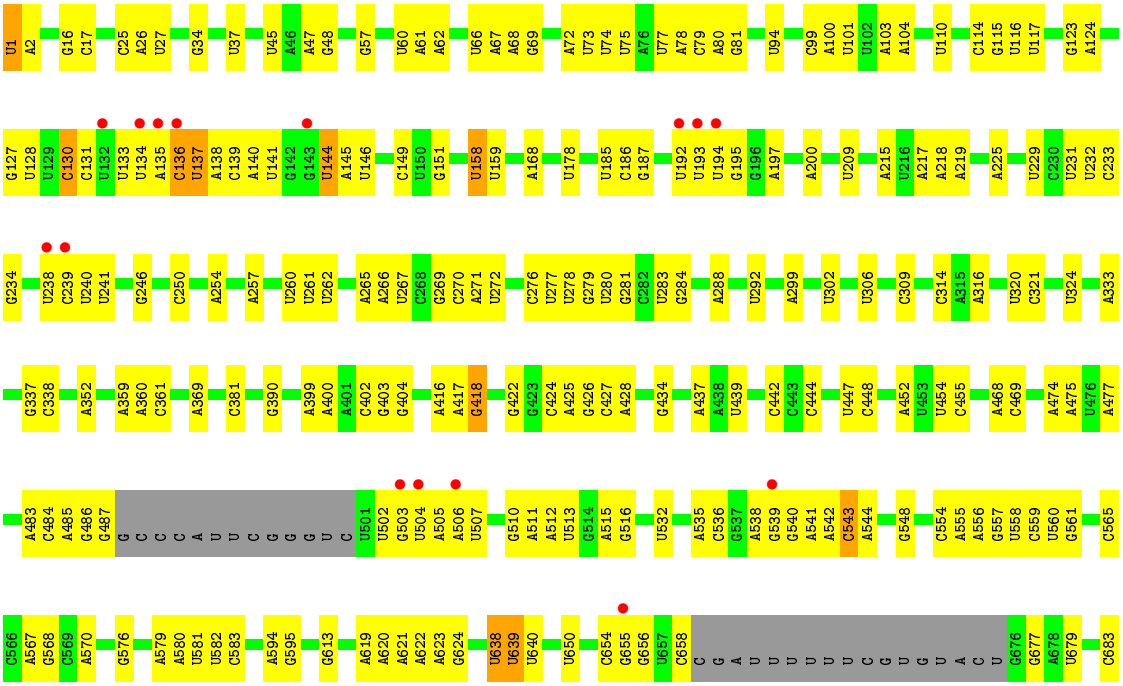
Chain q3:

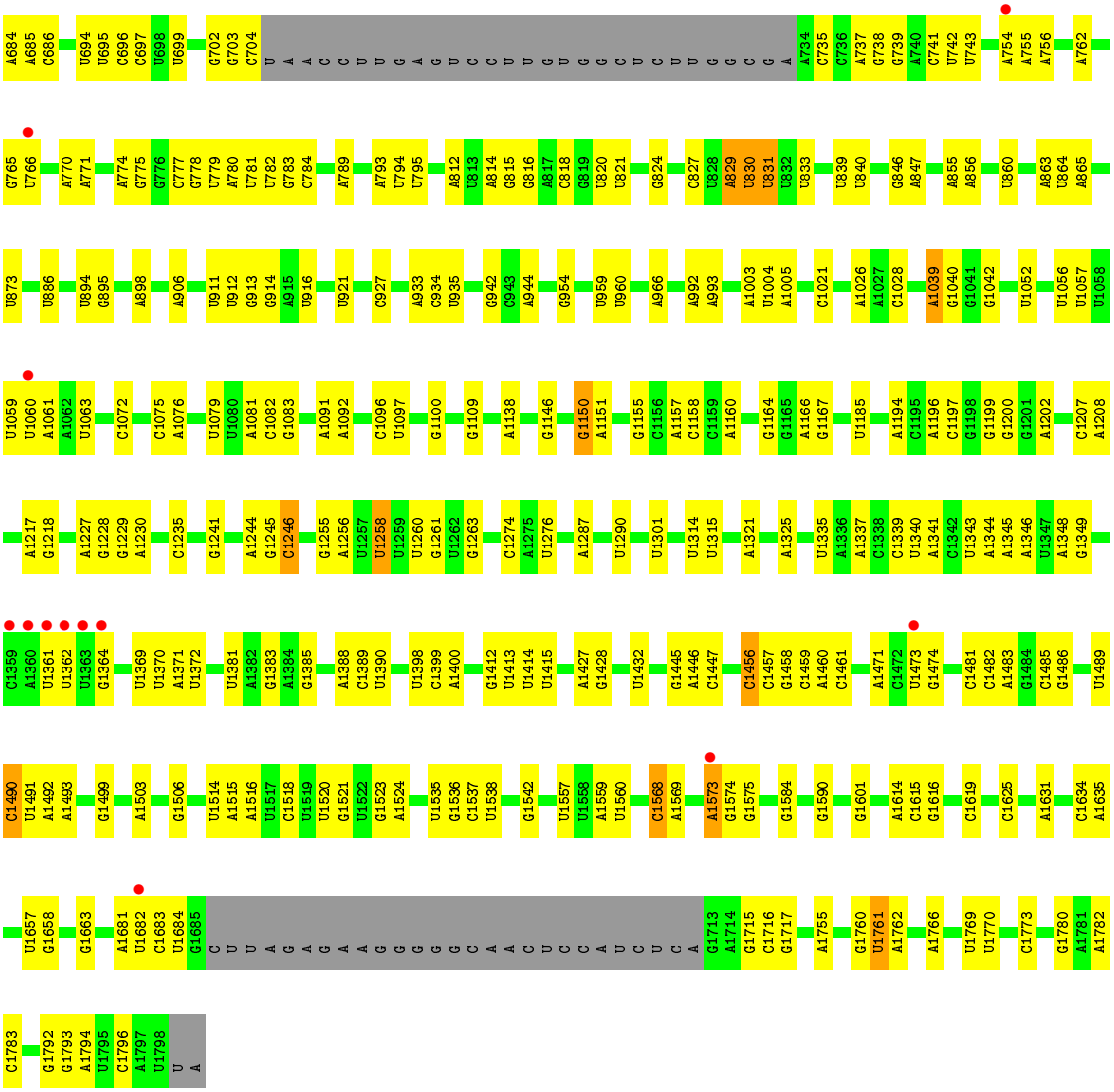



• Molecule 45: 18S ribosomal RNA

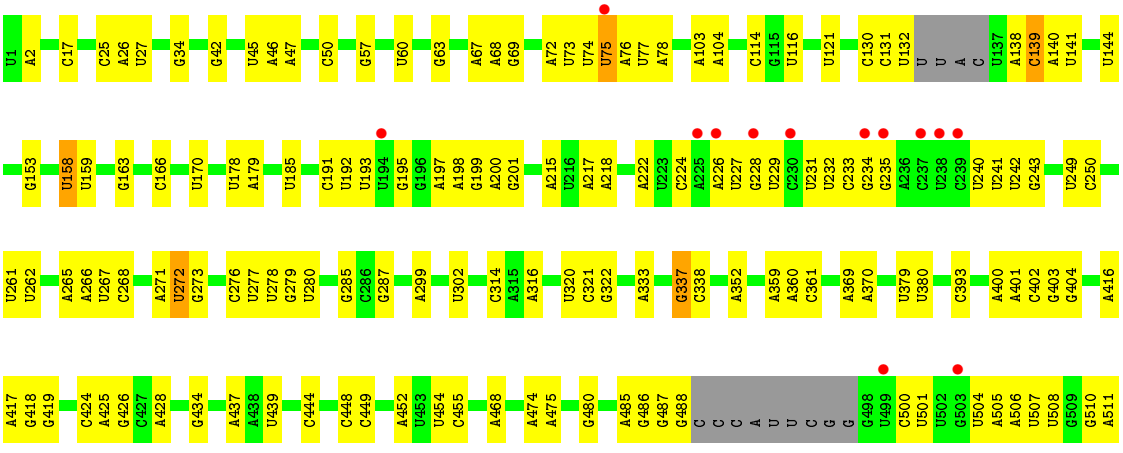
Chain 2:

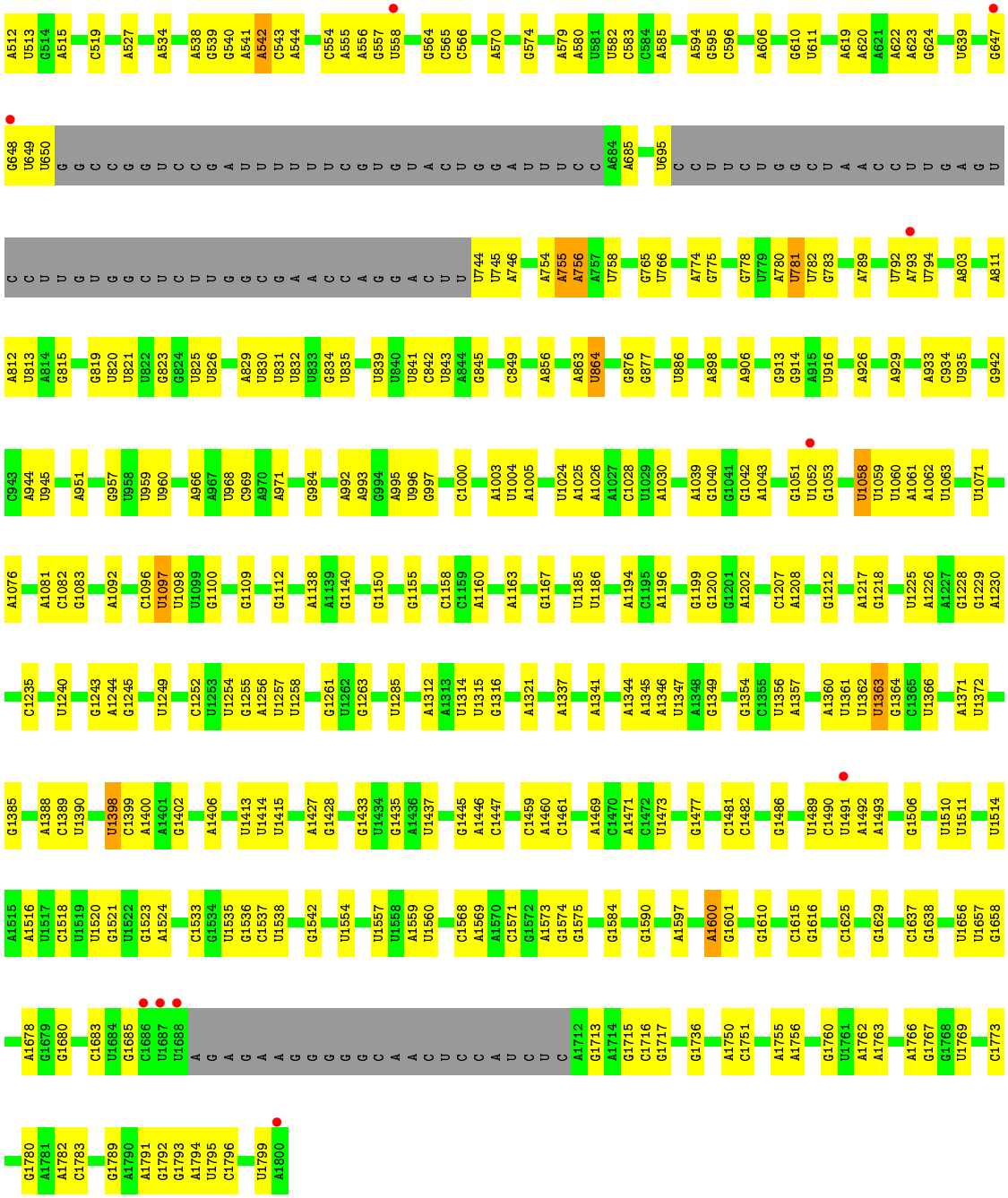




• Molecule 45: 18S ribosomal RNA

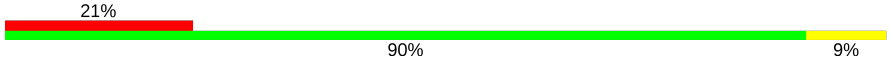
Chain 6:

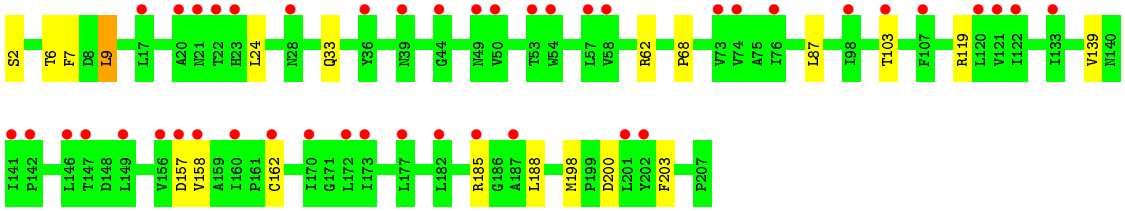




- Molecule 46: 40S ribosomal protein S0-A

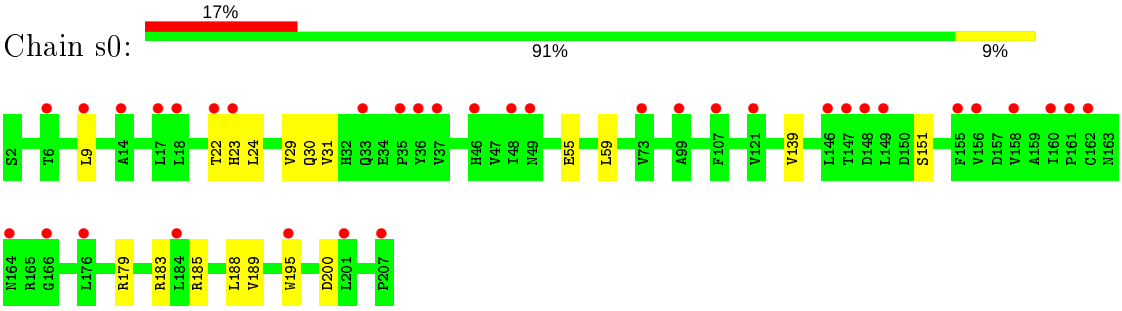
Chain S0:



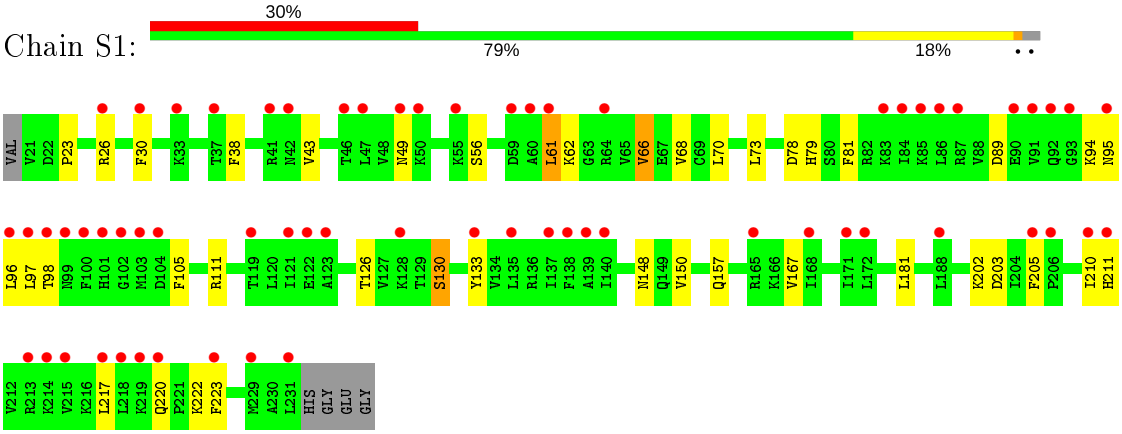
• Molecule 46: 40S ribosomal protein S0-A

Chain s0:



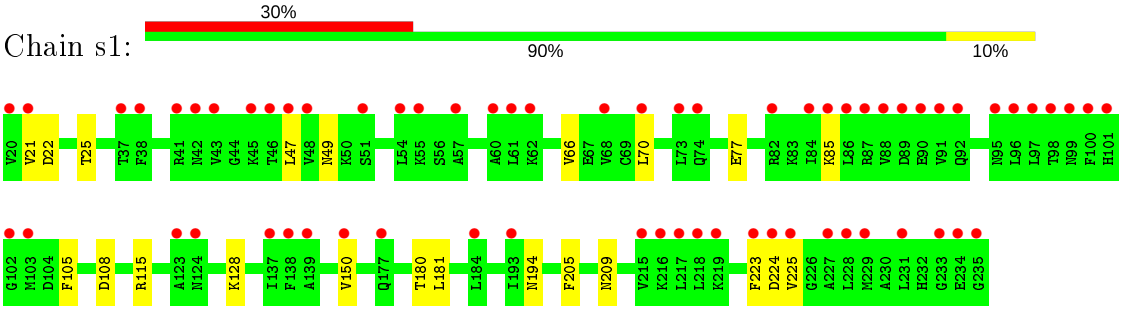

• Molecule 47: 40S ribosomal protein S1-A

Chain S1:



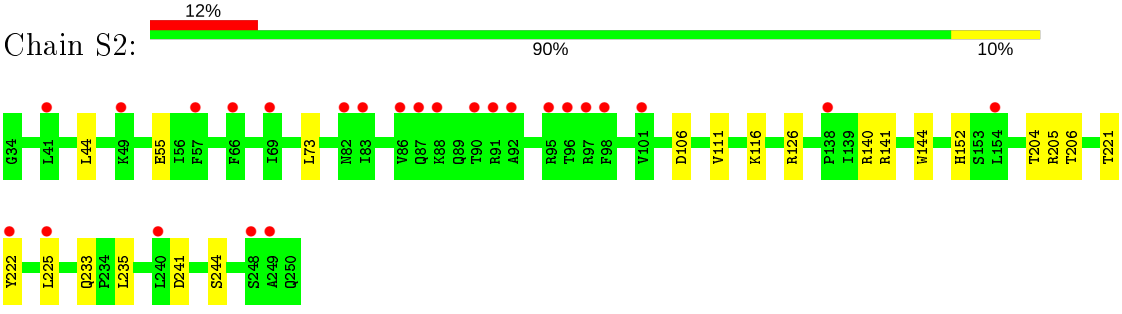

• Molecule 47: 40S ribosomal protein S1-A

Chain s1:



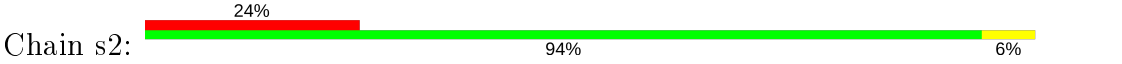

• Molecule 48: 40S ribosomal protein S2

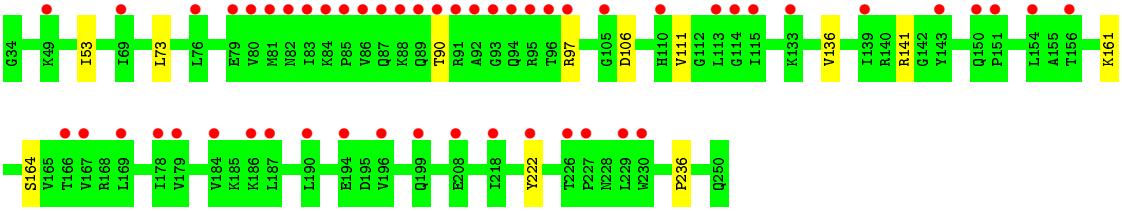
Chain S2:



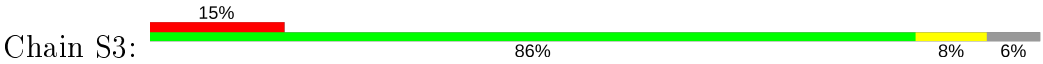

• Molecule 48: 40S ribosomal protein S2

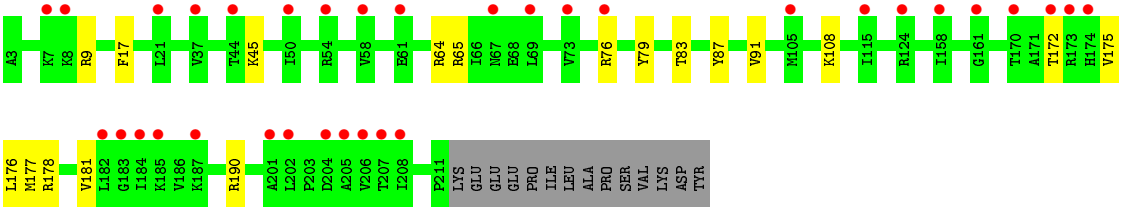
Chain s2:



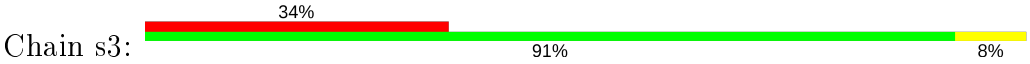


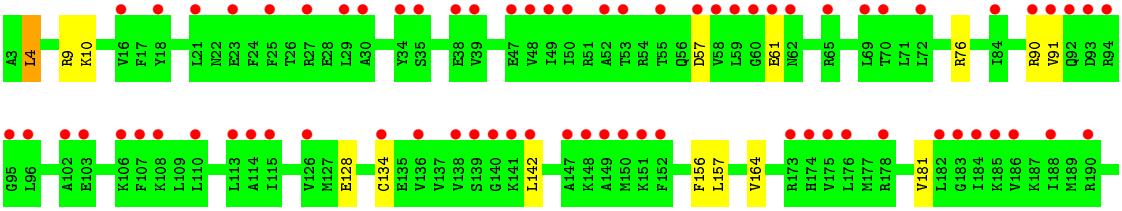

• Molecule 49: 40S ribosomal protein S3



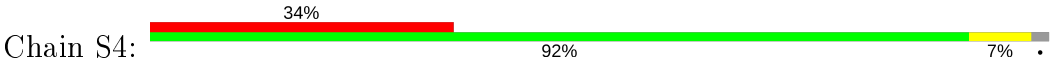



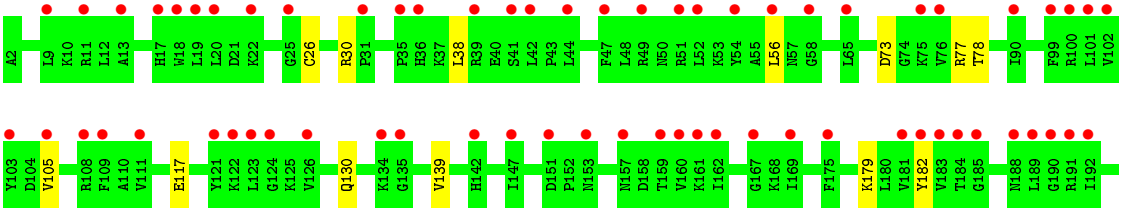

• Molecule 49: 40S ribosomal protein S3



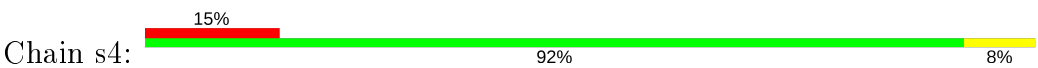



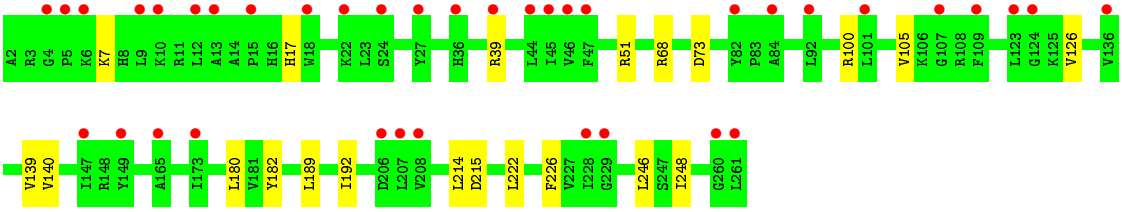

• Molecule 50: 40S ribosomal protein S4-A



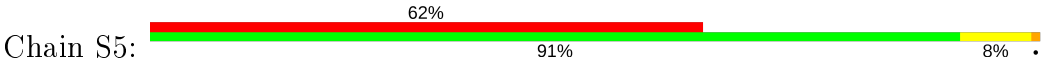



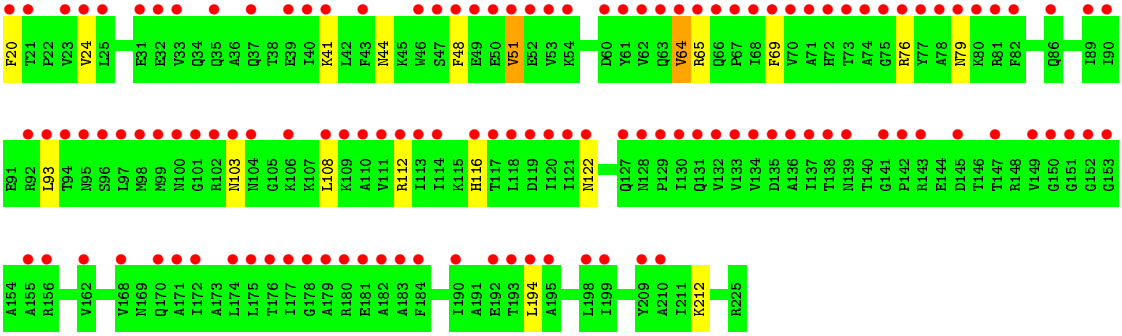

• Molecule 50: 40S ribosomal protein S4-A



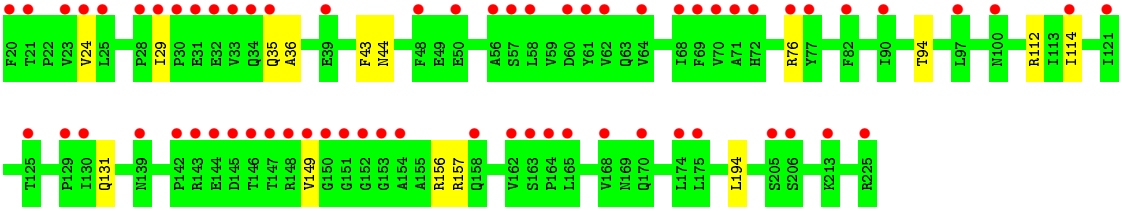



• Molecule 51: 40S ribosomal protein S5

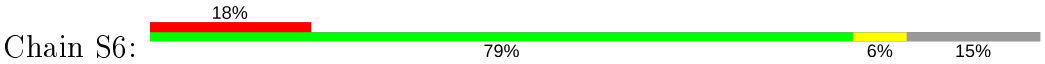


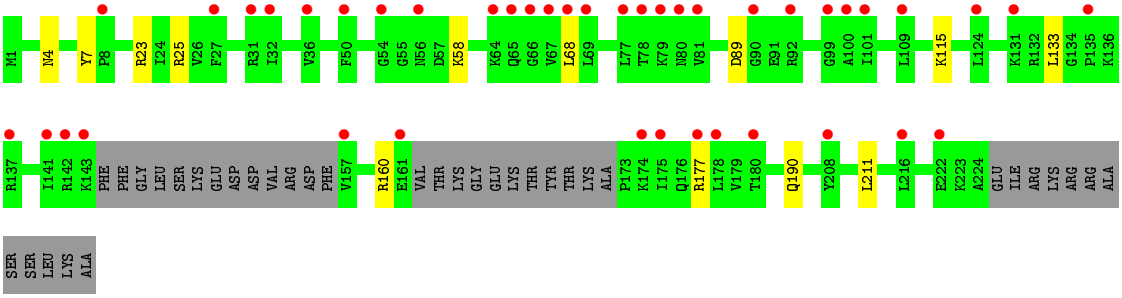




• Molecule 51: 40S ribosomal protein S5

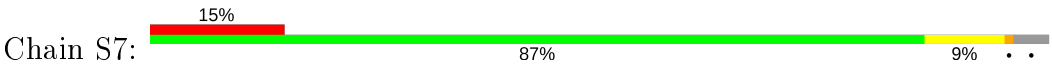


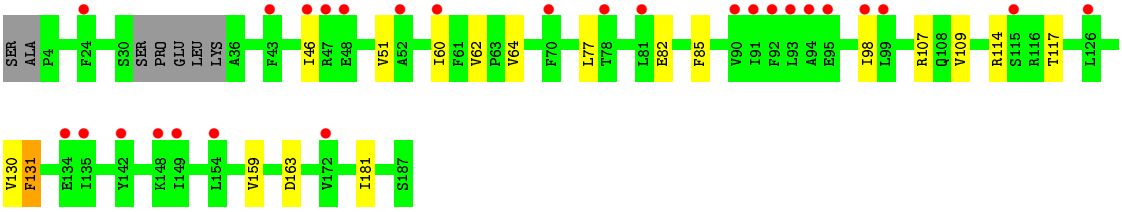

• Molecule 52: 40S ribosomal protein S6-A



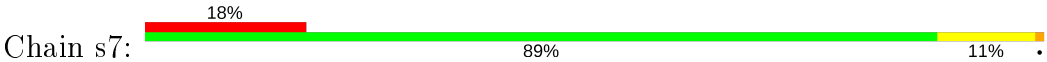



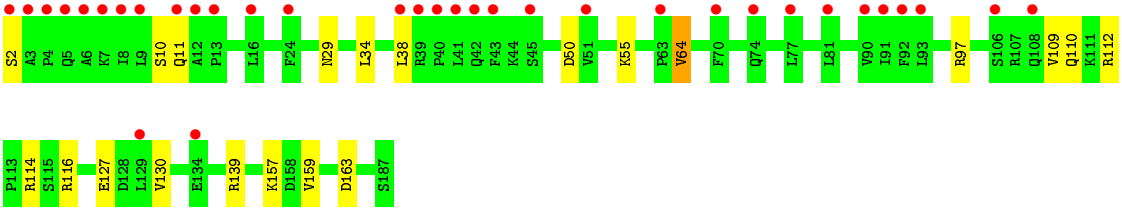

• Molecule 53: 40S ribosomal protein S7-A



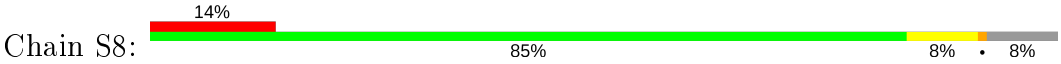


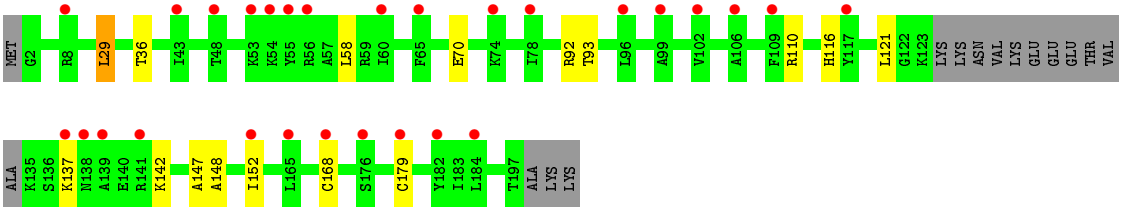

• Molecule 53: 40S ribosomal protein S7-A



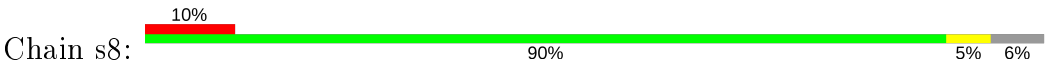



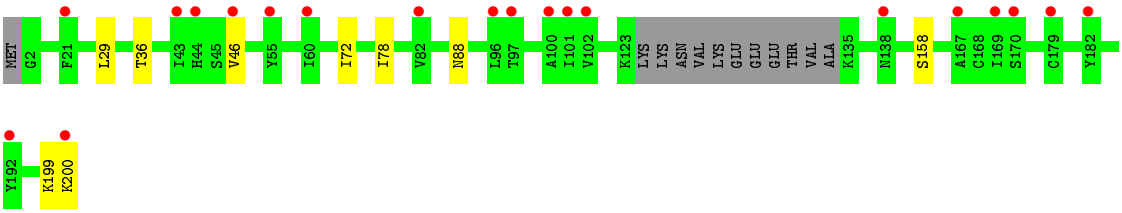

• Molecule 54: 40S ribosomal protein S8-A



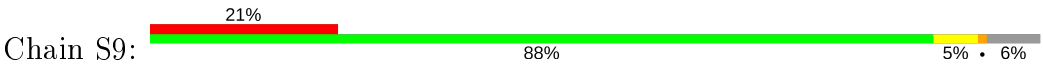



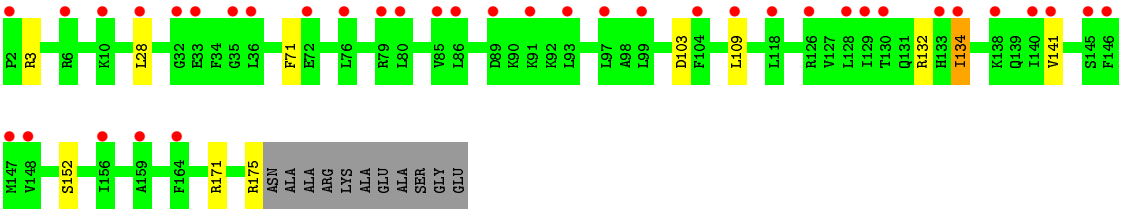

• Molecule 54: 40S ribosomal protein S8-A



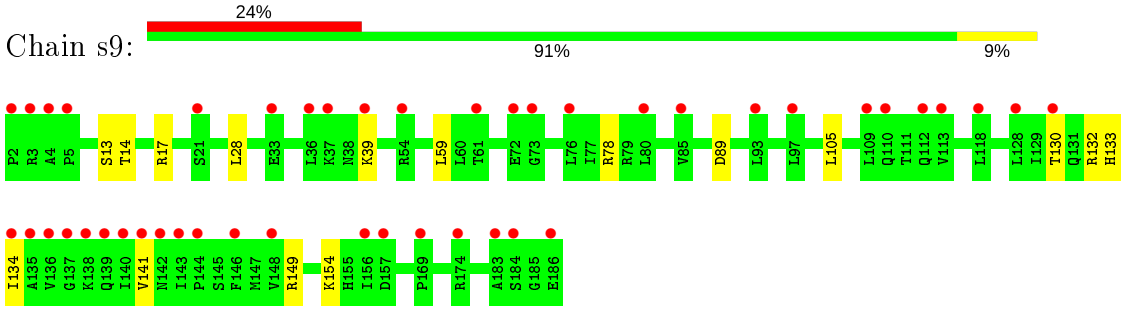

• Molecule 55: 40S ribosomal protein S9-A



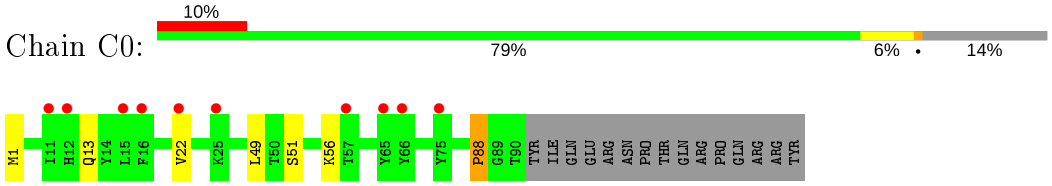
• Molecule 55: 40S ribosomal protein S9-A

Chain s9:



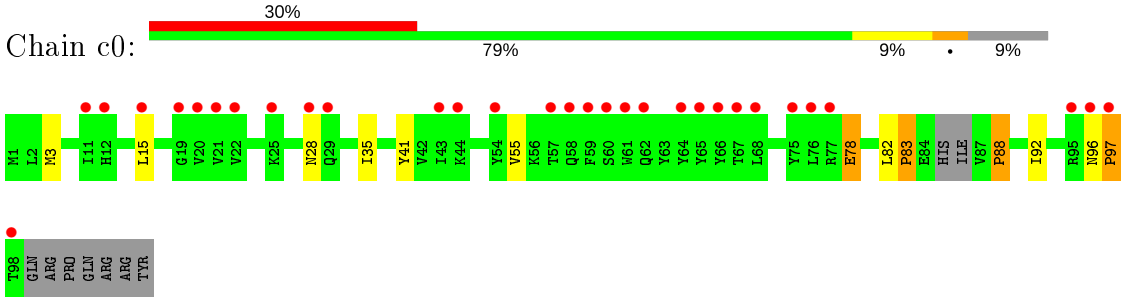

• Molecule 56: 40S ribosomal protein S10-A

Chain C0:



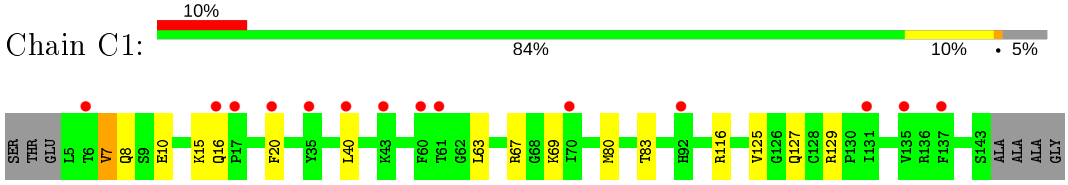

• Molecule 56: 40S ribosomal protein S10-A

Chain c0:



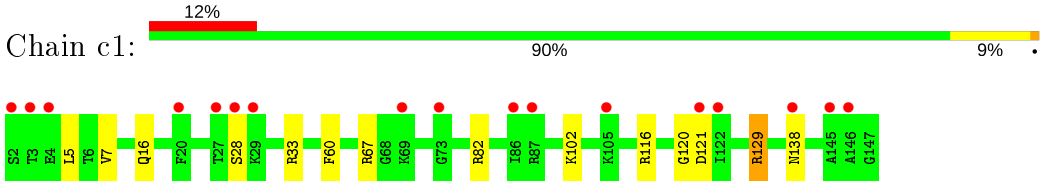

• Molecule 57: 40S ribosomal protein S11-A

Chain C1:



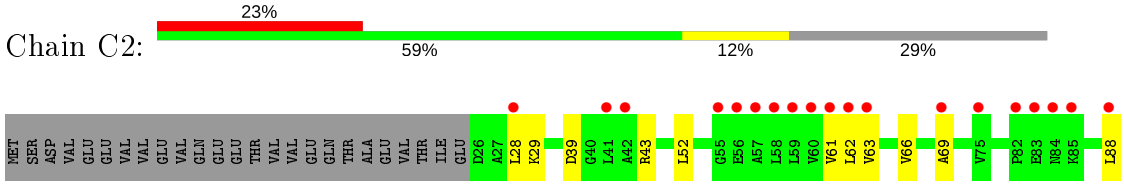

• Molecule 57: 40S ribosomal protein S11-A

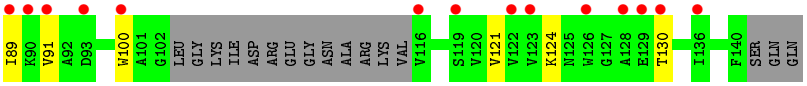
Chain c1:




• Molecule 58: 40S ribosomal protein S12

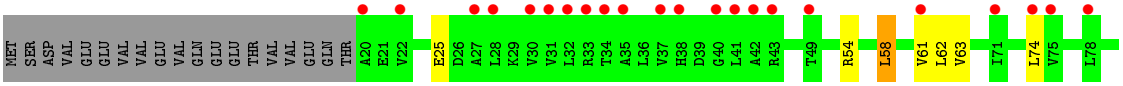
Chain C2:

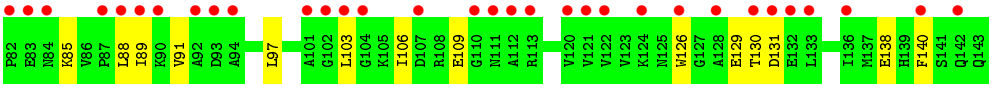





• Molecule 58: 40S ribosomal protein S12

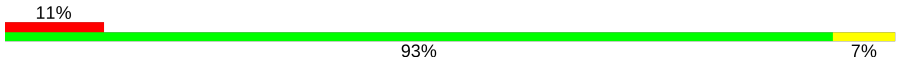
Chain c2:

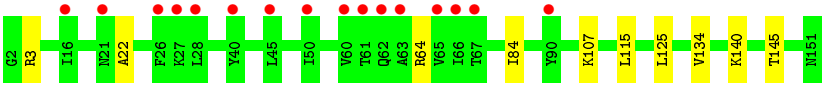



• Molecule 59: 40S ribosomal protein S13

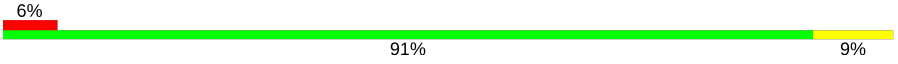
Chain C3:

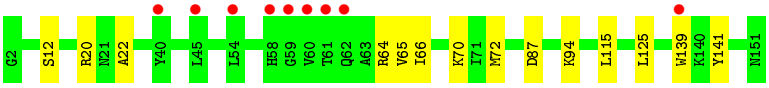



• Molecule 59: 40S ribosomal protein S13

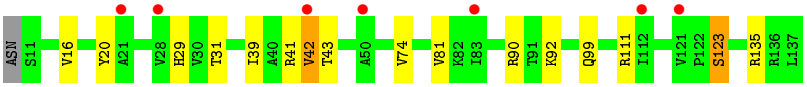
Chain c3:



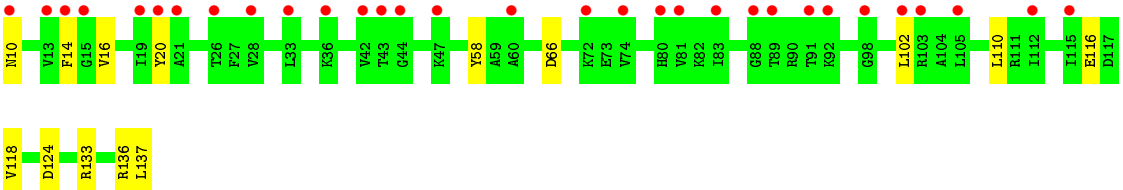

• Molecule 60: 40S ribosomal protein S14-B

Chain C4:



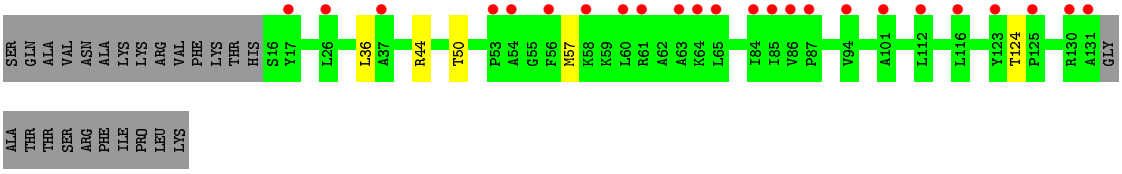

• Molecule 60: 40S ribosomal protein S14-B

Chain c4:



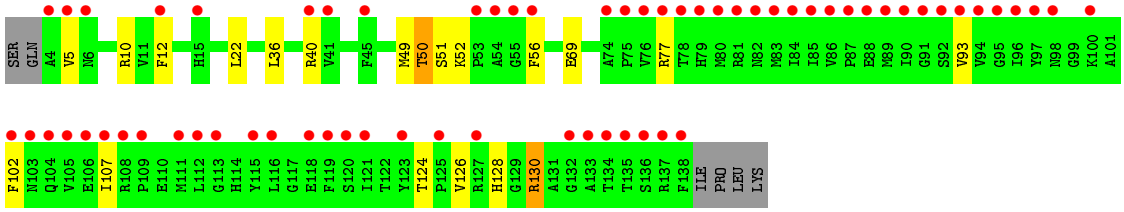

• Molecule 61: 40S ribosomal protein S15

Chain C5:



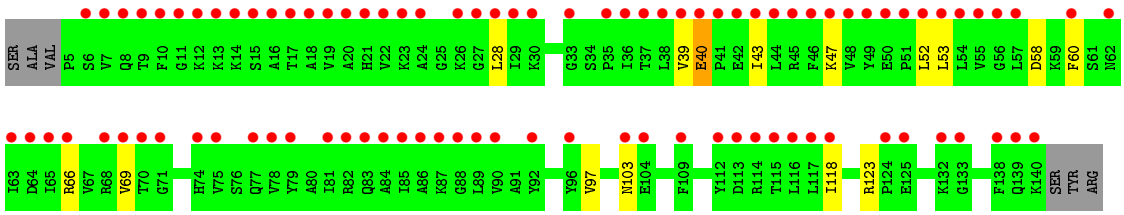

- Molecule 61: 40S ribosomal protein S15

Chain c5:



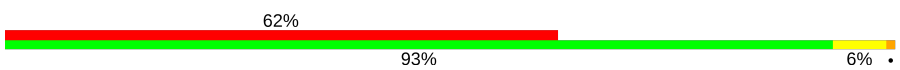

- Molecule 62: 40S ribosomal protein S16-A

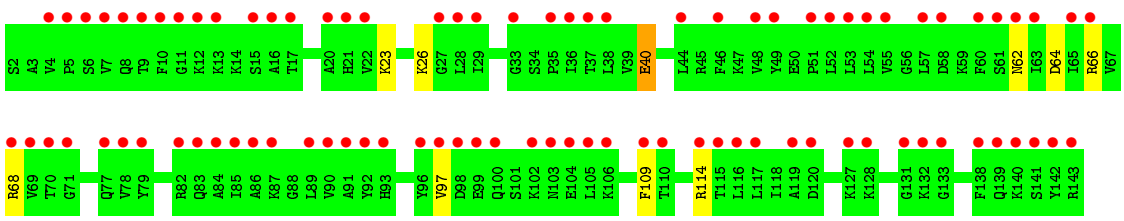
Chain C6:




- Molecule 62: 40S ribosomal protein S16-A

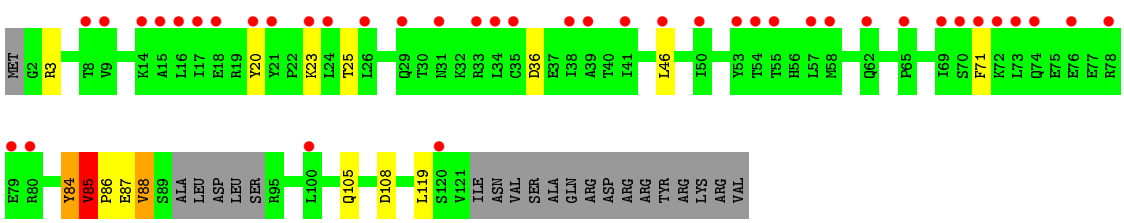
Chain c6:



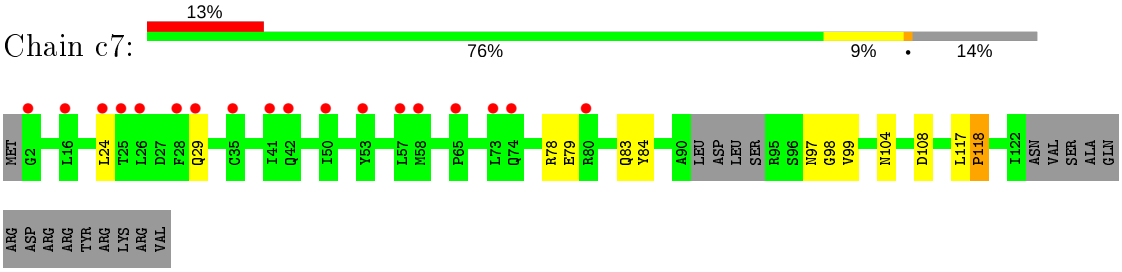

- Molecule 63: 40S ribosomal protein S17-A

Chain C7:



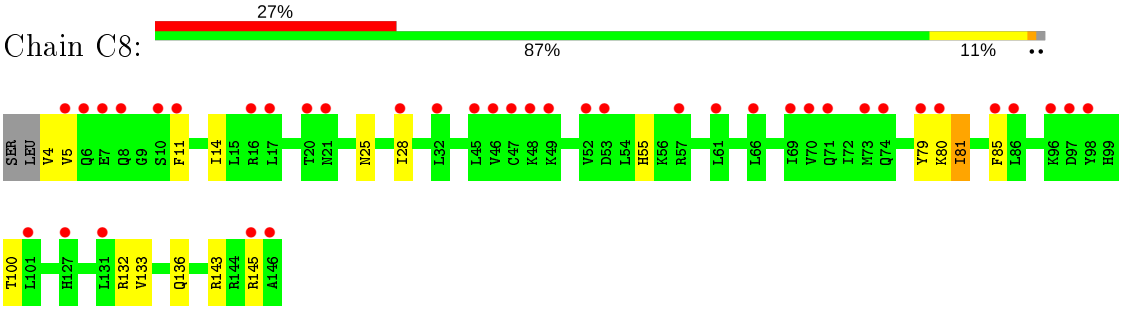
• Molecule 63: 40S ribosomal protein S17-A

Chain c7:



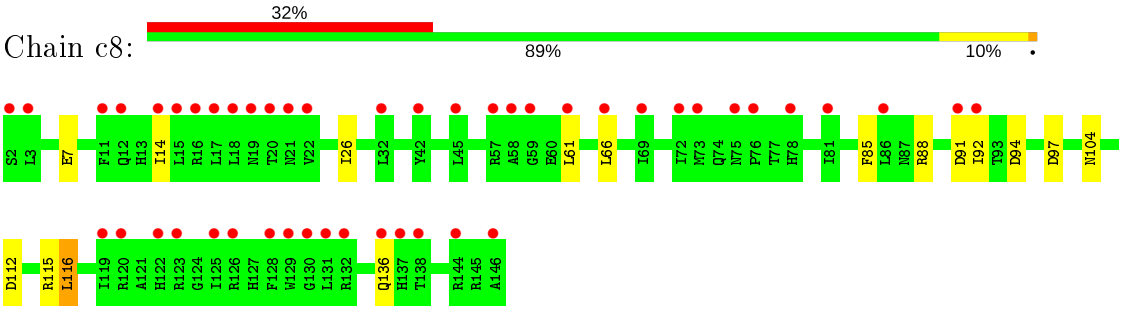

• Molecule 64: 40S ribosomal protein S18-A

Chain C8:



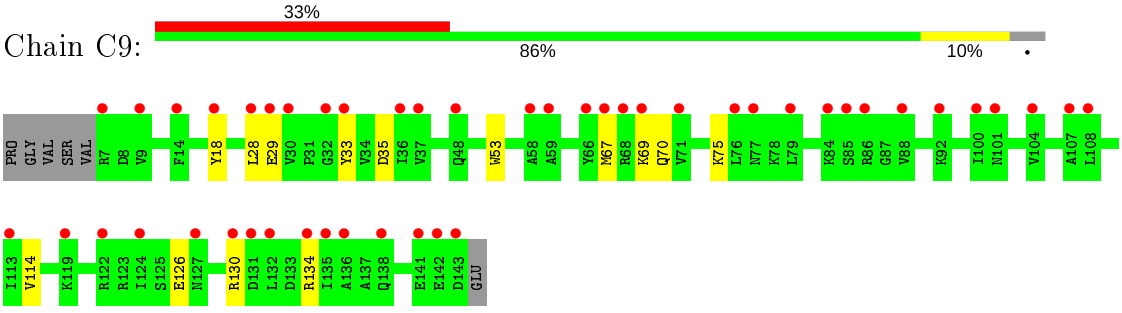

• Molecule 64: 40S ribosomal protein S18-A

Chain c8:



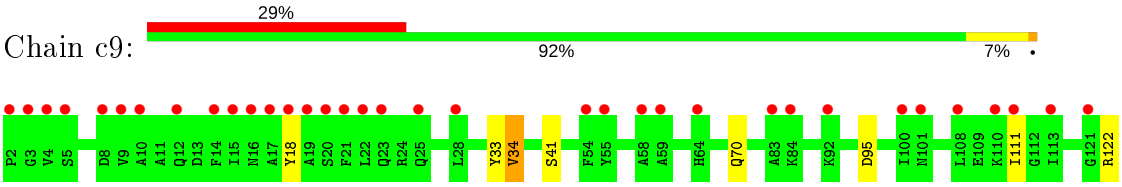

• Molecule 65: 40S ribosomal protein S19-A

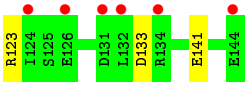
Chain C9:




• Molecule 65: 40S ribosomal protein S19-A

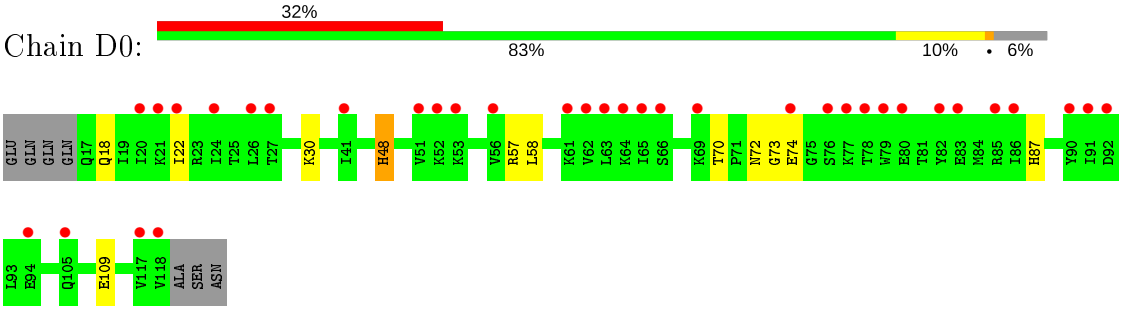
Chain c9:





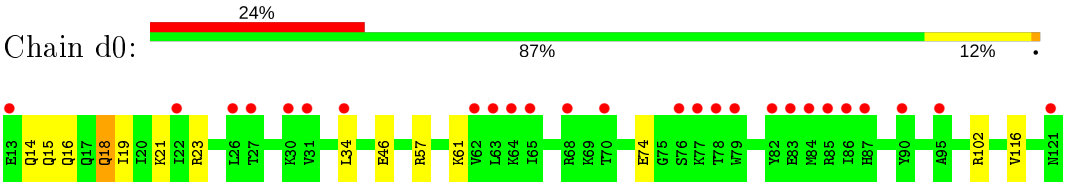

• Molecule 66: 40S ribosomal protein S20

Chain D0:



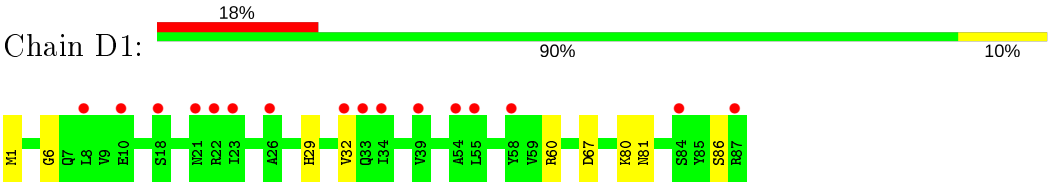

• Molecule 66: 40S ribosomal protein S20

Chain d0:



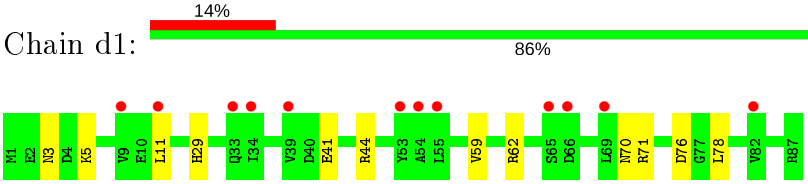

• Molecule 67: 40S ribosomal protein S21-A

Chain D1:



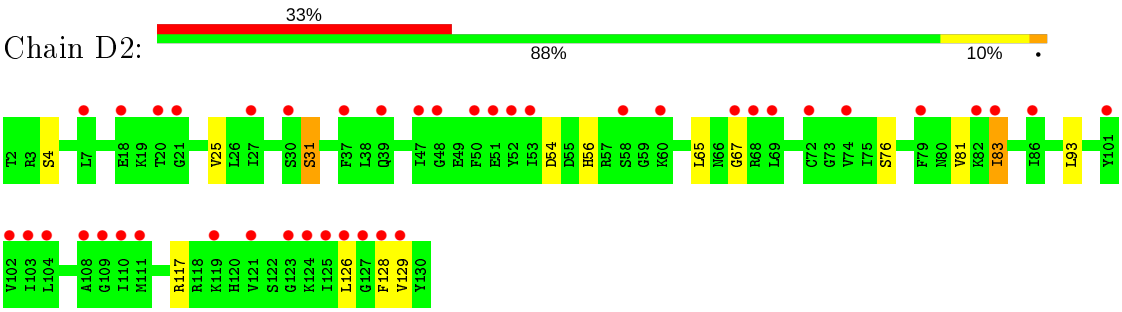

• Molecule 67: 40S ribosomal protein S21-A

Chain d1:



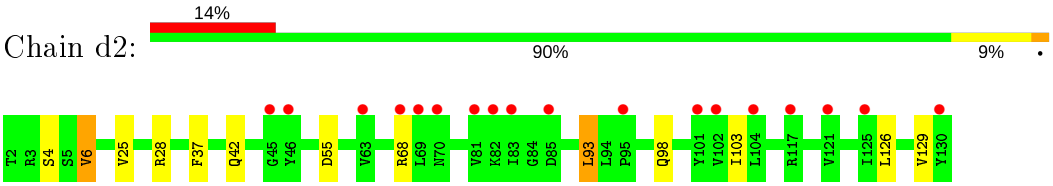

• Molecule 68: 40S ribosomal protein S22-A

Chain D2:



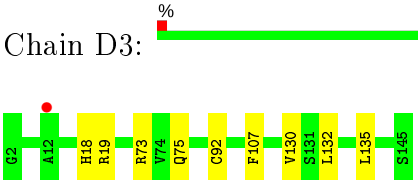

• Molecule 68: 40S ribosomal protein S22-A

Chain d2:



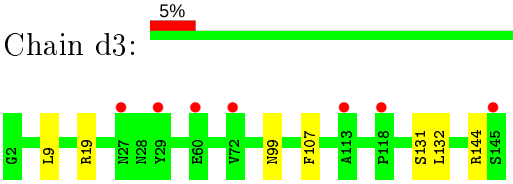

• Molecule 69: 40S ribosomal protein S23-A

Chain D3:



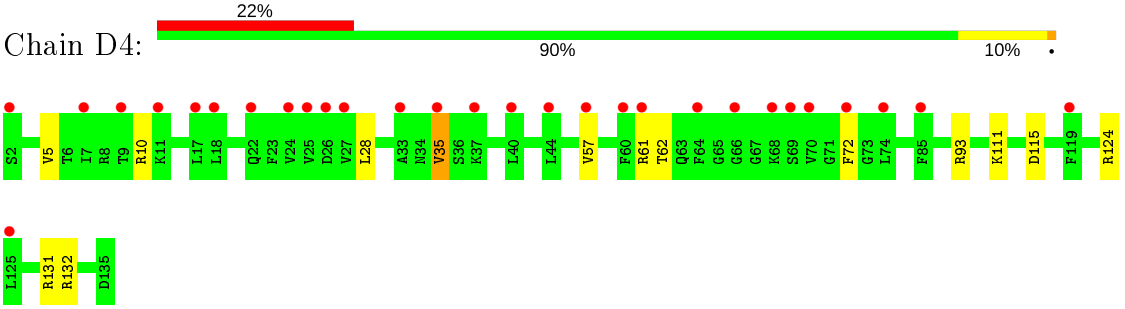

• Molecule 69: 40S ribosomal protein S23-A

Chain d3:



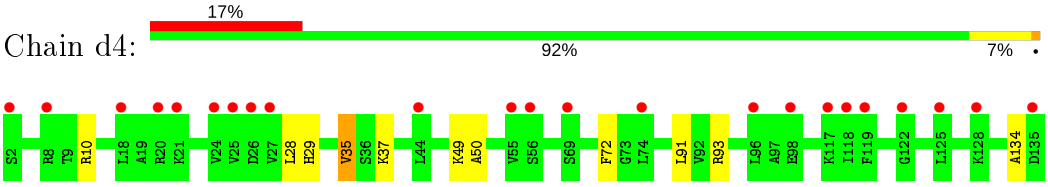

• Molecule 70: 40S ribosomal protein S24-A

Chain D4:



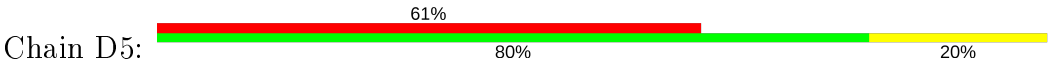

• Molecule 70: 40S ribosomal protein S24-A

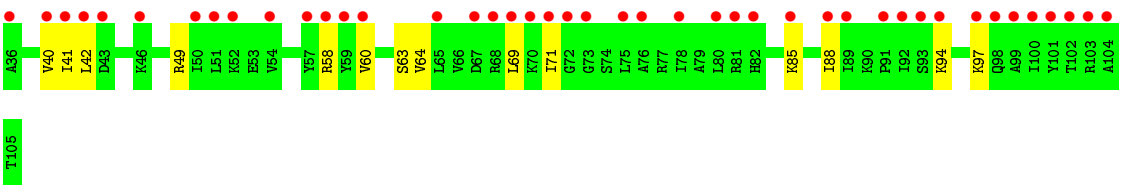
Chain d4:




• Molecule 71: 40S ribosomal protein S25-A

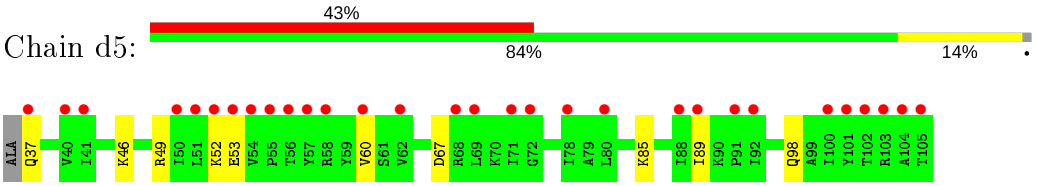
Chain D5:



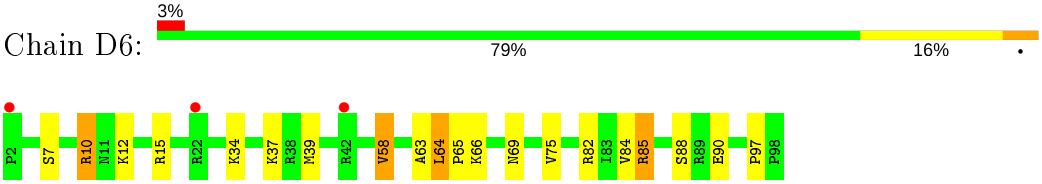

• Molecule 71: 40S ribosomal protein S25-A

Chain d5:



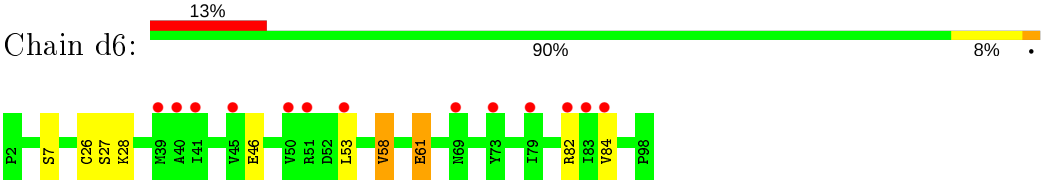

• Molecule 72: 40S ribosomal protein S26-B

Chain D6:



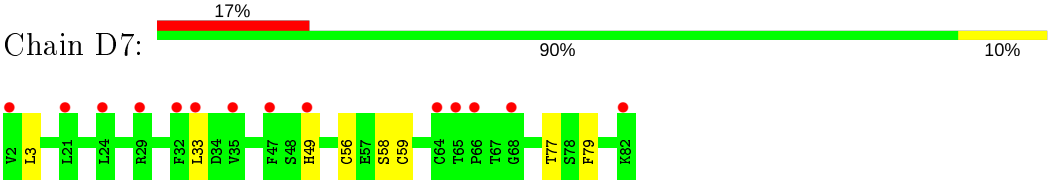

• Molecule 72: 40S ribosomal protein S26-B

Chain d6:



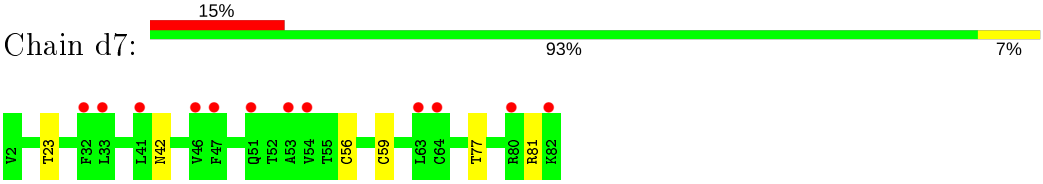

• Molecule 73: 40S ribosomal protein S27-A

Chain D7:



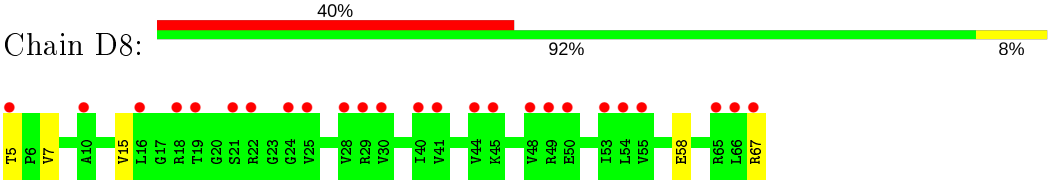

• Molecule 73: 40S ribosomal protein S27-A

Chain d7:



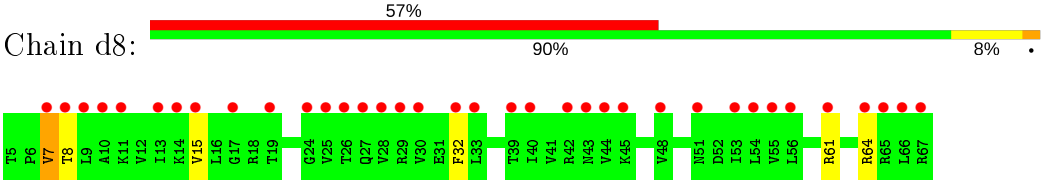

• Molecule 74: 40S ribosomal protein S28-A

Chain D8:



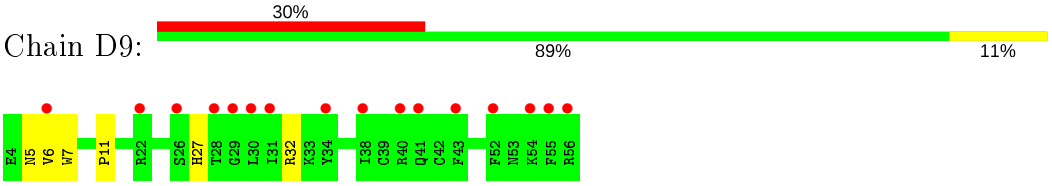

• Molecule 74: 40S ribosomal protein S28-A

Chain d8:



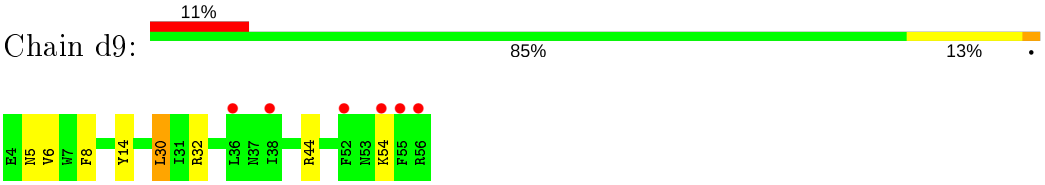
• Molecule 75: 40S ribosomal protein S29-A

Chain D9:



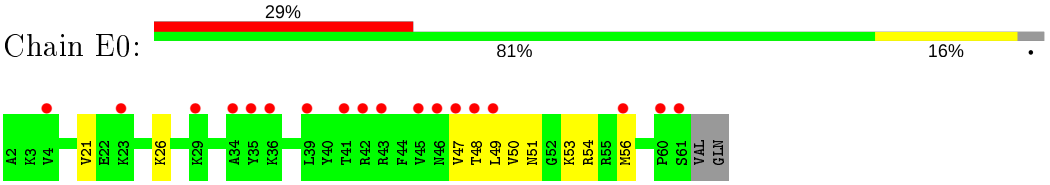

• Molecule 75: 40S ribosomal protein S29-A

Chain d9:



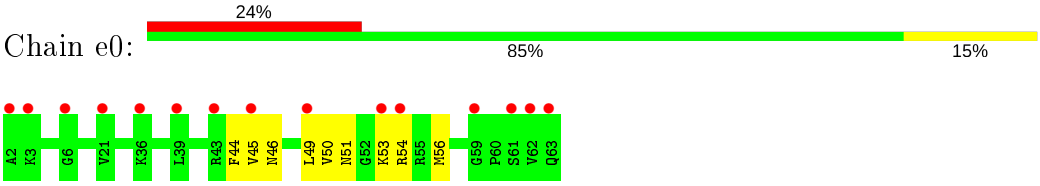

• Molecule 76: 40S ribosomal protein S30-A

Chain E0:



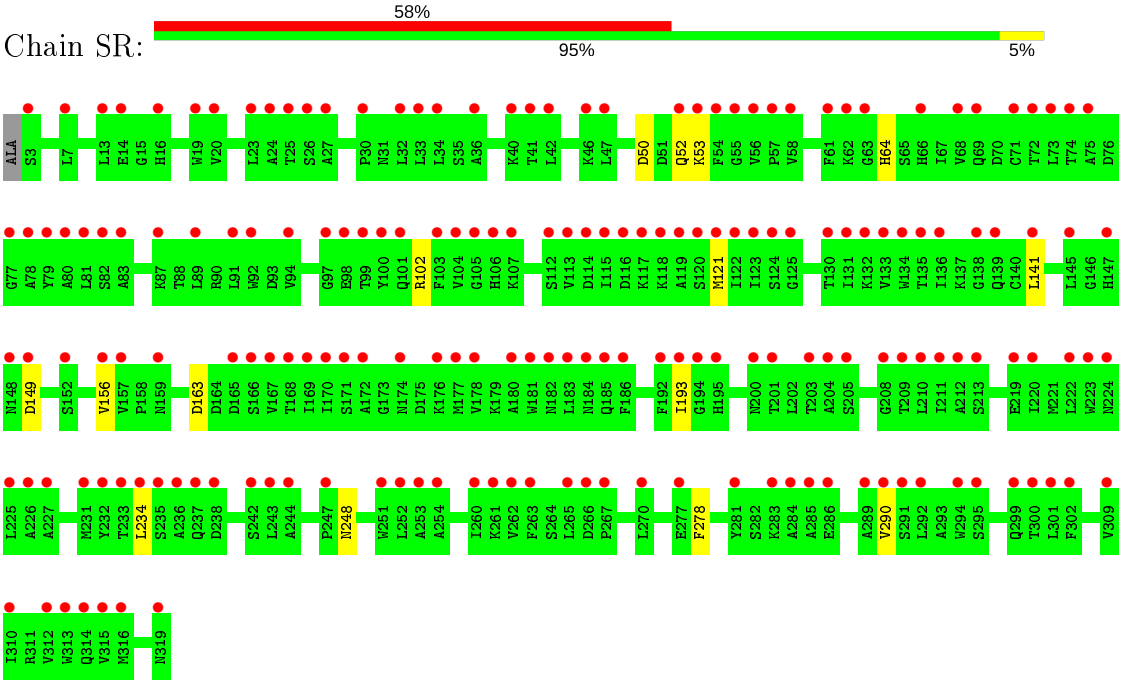

• Molecule 76: 40S ribosomal protein S30-A

Chain e0:



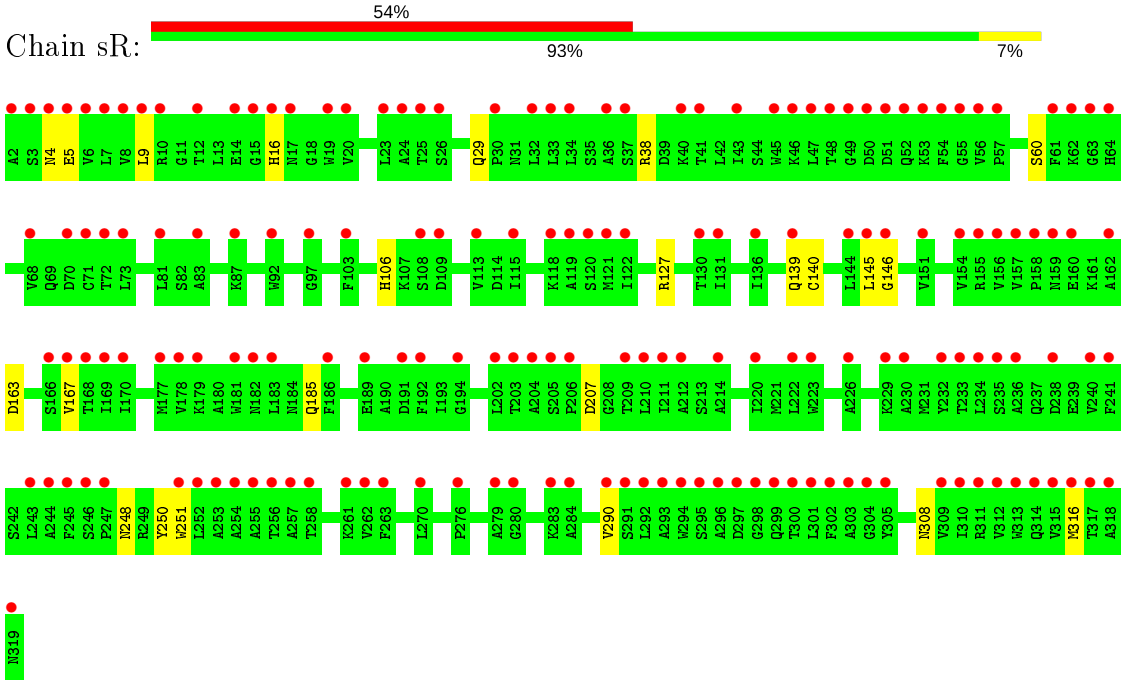

• Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



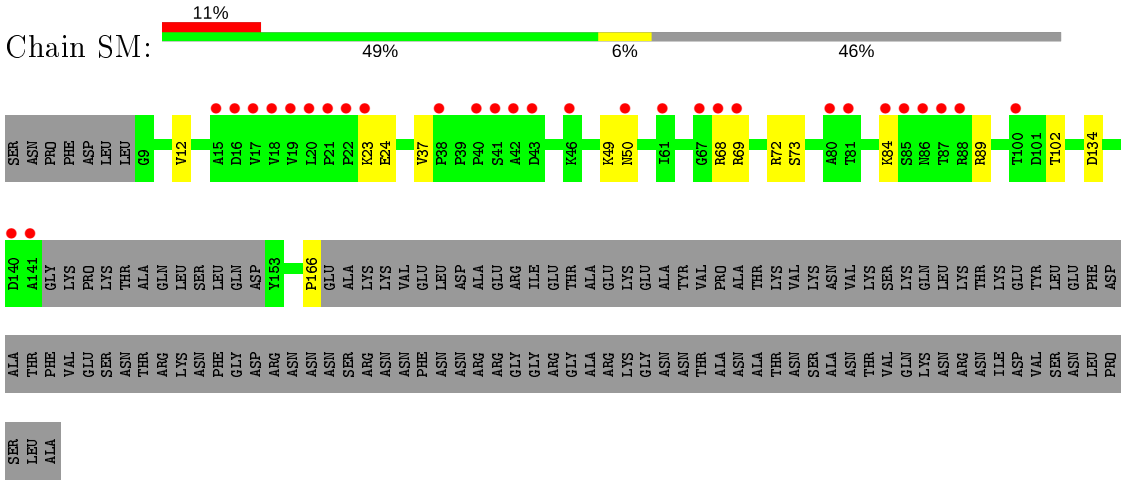
• Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



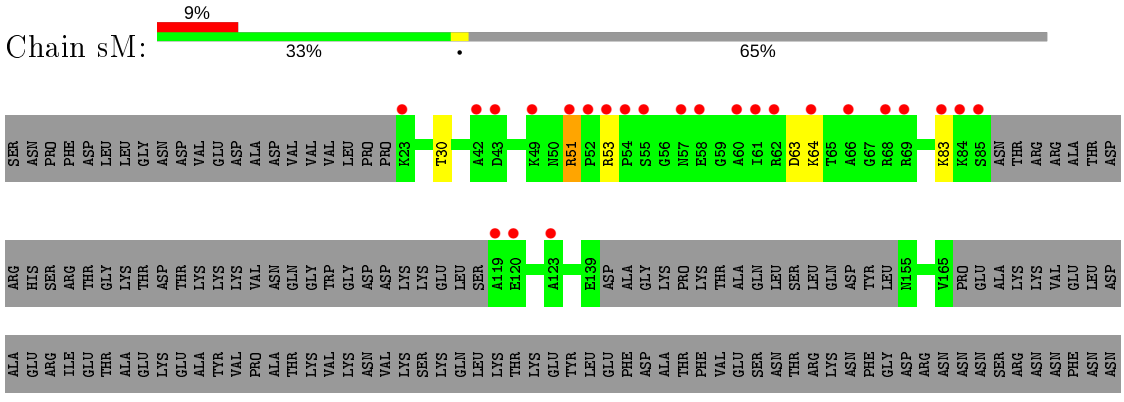

• Molecule 78: Suppressor protein STM1

Chain SM:



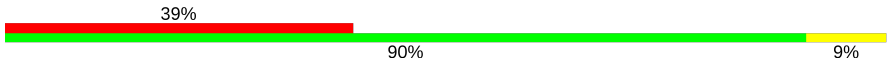

• Molecule 78: Suppressor protein STM1

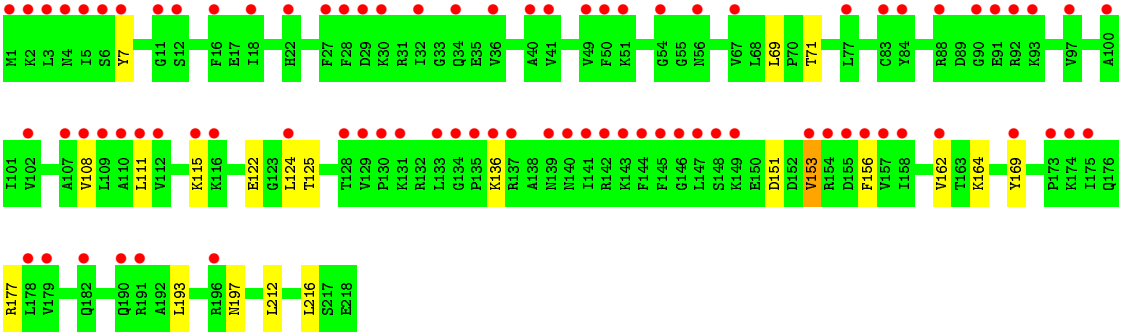
Chain sM:



- Molecule 79: 40S ribosomal protein S6-A

Chain s6:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 434.53Å 293.33Å 295.79Å<br>90.00° 97.40° 90.00° | Depositor |
| Resolution (Å) | 146.66 – 3.30<br>146.66 – 3.30 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.9 (146.66-3.30)<br>91.8 (146.66-3.30) | Depositor<br>EDS |
| $R_{merge}$ | 0.32 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.92 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.203 , 0.250<br>0.203 , 0.250 | Depositor<br>DCC |
| $R_{free}$ test set | 21969 reflections (2.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 77.3 | Xtriage |
| Anisotropy | 0.209 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 92.3 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 397978 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 102.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | 1 | 0.67 | 4/73685 (0.0%) | 1.11 | 189/114868 (0.2%) |
| 1 | 5 | 0.55 | 2/73908 (0.0%) | 1.02 | 101/115221 (0.1%) |
| 2 | 3 | 0.51 | 0/2883 | 0.98 | 2/4491 (0.0%) |
| 2 | 7 | 0.43 | 0/2883 | 0.89 | 0/4491 |
| 3 | 4 | 0.69 | 0/3724 | 1.14 | 14/5798 (0.2%) |
| 3 | 8 | 0.51 | 0/3746 | 1.07 | 21/5832 (0.4%) |
| 4 | L2 | 0.46 | 0/1918 | 0.67 | 2/2577 (0.1%) |
| 4 | l2 | 0.35 | 0/1918 | 0.60 | 1/2577 (0.0%) |
| 5 | L3 | 0.42 | 0/3152 | 0.61 | 1/4239 (0.0%) |
| 5 | l3 | 0.43 | 1/3152 (0.0%) | 0.59 | 0/4239 |
| 6 | L4 | 0.45 | 0/2801 | 0.62 | 0/3792 |
| 6 | l4 | 0.38 | 0/2801 | 0.59 | 0/3792 |
| 7 | L5 | 0.35 | 0/2403 | 0.54 | 0/3242 |
| 7 | l5 | 0.32 | 0/2408 | 0.50 | 0/3248 |
| 8 | L6 | 0.38 | 0/1260 | 0.55 | 0/1694 |
| 8 | l6 | 0.38 | 0/1269 | 0.56 | 0/1705 |
| 9 | L7 | 0.40 | 0/1855 | 0.56 | 0/2496 |
| 9 | l7 | 0.36 | 0/1828 | 0.57 | 0/2461 |
| 10 | L8 | 0.40 | 0/1825 | 0.56 | 0/2466 |
| 10 | l8 | 0.32 | 0/1795 | 0.55 | 1/2429 (0.0%) |
| 11 | L9 | 0.40 | 0/1523 | 0.60 | 0/2051 |
| 11 | l9 | 0.38 | 0/1539 | 0.56 | 0/2073 |
| 12 | M0 | 0.43 | 0/1796 | 0.61 | 0/2409 |
| 12 | m0 | 0.40 | 0/1810 | 0.59 | 1/2428 (0.0%) |
| 13 | M1 | 0.34 | 0/1374 | 0.61 | 0/1842 |
| 13 | m1 | 0.30 | 0/1374 | 0.53 | 1/1842 (0.1%) |
| 14 | M3 | 0.41 | 0/1568 | 0.59 | 1/2106 (0.0%) |
| 14 | m3 | 0.37 | 0/1573 | 0.58 | 0/2113 |
| 15 | M4 | 0.36 | 0/1068 | 0.55 | 0/1438 |
| 15 | m4 | 0.35 | 0/1074 | 0.55 | 0/1446 |
| 16 | M5 | 0.45 | 0/1757 | 0.60 | 0/2354 |
| 16 | m5 | 0.33 | 0/1757 | 0.53 | 0/2354 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | M6 | 0.45 | 0/1585 | 0.56 | 0/2128 |
| 17 | m6 | 0.46 | 0/1585 | 0.60 | 0/2128 |
| 18 | M7 | 0.44 | 0/1400 | 0.62 | 0/1882 |
| 18 | m7 | 0.42 | 0/1250 | 0.60 | 0/1683 |
| 19 | M8 | 0.43 | 0/1465 | 0.61 | 0/1965 |
| 19 | m8 | 0.34 | 0/1465 | 0.57 | 0/1965 |
| 20 | M9 | 0.38 | 0/1516 | 0.56 | 2/2020 (0.1%) |
| 20 | m9 | 0.34 | 0/1538 | 0.49 | 0/2050 |
| 21 | N0 | 0.41 | 0/1481 | 0.59 | 0/1990 |
| 21 | n0 | 0.38 | 0/1481 | 0.53 | 0/1990 |
| 22 | N1 | 0.41 | 0/1300 | 0.58 | 0/1743 |
| 22 | n1 | 0.35 | 0/1300 | 0.54 | 0/1743 |
| 23 | N2 | 0.35 | 0/803 | 0.61 | 0/1087 |
| 23 | n2 | 0.32 | 0/794 | 0.55 | 0/1076 |
| 24 | N3 | 0.45 | 0/996 | 0.62 | 0/1340 |
| 24 | n3 | 0.43 | 0/1018 | 0.59 | 0/1369 |
| 25 | N4 | 0.40 | 0/533 | 0.53 | 0/707 |
| 25 | n4 | 0.33 | 0/1052 | 0.53 | 0/1398 |
| 26 | N5 | 0.44 | 0/961 | 0.61 | 1/1296 (0.1%) |
| 26 | n5 | 0.34 | 0/974 | 0.59 | 1/1314 (0.1%) |
| 27 | N6 | 0.43 | 0/995 | 0.62 | 0/1329 |
| 27 | n6 | 0.38 | 0/978 | 0.58 | 0/1307 |
| 28 | N7 | 0.51 | 2/1118 (0.2%) | 0.58 | 0/1497 |
| 28 | n7 | 0.33 | 0/1118 | 0.52 | 0/1497 |
| 29 | N8 | 0.40 | 0/1204 | 0.66 | 0/1612 |
| 29 | n8 | 0.33 | 0/1204 | 0.59 | 0/1612 |
| 30 | N9 | 0.40 | 0/455 | 0.54 | 0/607 |
| 30 | n9 | 0.34 | 0/473 | 0.55 | 0/629 |
| 31 | O0 | 0.38 | 0/751 | 0.54 | 0/1008 |
| 31 | o0 | 0.31 | 0/775 | 0.54 | 0/1040 |
| 32 | O1 | 0.39 | 0/862 | 0.56 | 0/1157 |
| 32 | o1 | 0.42 | 0/897 | 0.57 | 0/1205 |
| 33 | O2 | 0.45 | 0/1028 | 0.59 | 0/1376 |
| 33 | o2 | 0.41 | 0/1041 | 0.66 | 1/1394 (0.1%) |
| 34 | O3 | 0.46 | 0/868 | 0.65 | 1/1168 (0.1%) |
| 34 | o3 | 0.41 | 0/868 | 0.56 | 0/1168 |
| 35 | O4 | 0.41 | 0/891 | 0.63 | 1/1191 (0.1%) |
| 35 | o4 | 0.34 | 0/891 | 0.55 | 0/1191 |
| 36 | O5 | 0.45 | 0/978 | 0.62 | 1/1301 (0.1%) |
| 36 | o5 | 0.32 | 0/974 | 0.51 | 0/1297 |
| 37 | O6 | 0.41 | 0/756 | 0.58 | 0/1005 |
| 37 | o6 | 0.31 | 0/778 | 0.51 | 0/1034 |
| 38 | O7 | 0.51 | 0/680 | 0.70 | 0/901 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | o7 | 0.40 | 0/696 | 0.64 | 0/923 |
| 39 | O8 | 0.36 | 0/618 | 0.54 | 0/826 |
| 39 | o8 | 0.32 | 0/614 | 0.62 | 0/822 |
| 40 | O9 | 0.49 | 0/443 | 0.67 | 0/588 |
| 40 | o9 | 0.40 | 0/443 | 0.54 | 0/588 |
| 41 | Q0 | 0.44 | 0/423 | 0.62 | 0/562 |
| 41 | q0 | 0.46 | 0/423 | 0.63 | 0/562 |
| 42 | Q1 | 0.36 | 0/234 | 0.45 | 0/300 |
| 42 | q1 | 0.35 | 0/234 | 0.52 | 0/300 |
| 43 | Q2 | 0.43 | 0/860 | 0.62 | 0/1136 |
| 43 | q2 | 0.35 | 0/860 | 0.55 | 0/1136 |
| 44 | Q3 | 0.48 | 0/701 | 0.70 | 2/934 (0.2%) |
| 44 | q3 | 0.35 | 0/701 | 0.58 | 0/934 |
| 45 | 2 | 0.42 | 0/40808 | 0.94 | 54/63582 (0.1%) |
| 45 | 6 | 0.39 | 0/40116 | 0.91 | 42/62502 (0.1%) |
| 46 | S0 | 0.30 | 0/1621 | 0.54 | 1/2220 (0.0%) |
| 46 | s0 | 0.31 | 0/1621 | 0.54 | 1/2220 (0.0%) |
| 47 | S1 | 0.33 | 0/1713 | 0.64 | 1/2305 (0.0%) |
| 47 | s1 | 0.29 | 0/1748 | 0.54 | 0/2352 |
| 48 | S2 | 0.32 | 0/1665 | 0.53 | 0/2263 |
| 48 | s2 | 0.32 | 0/1665 | 0.58 | 0/2263 |
| 49 | S3 | 0.31 | 0/1643 | 0.50 | 0/2210 |
| 49 | s3 | 0.29 | 0/1759 | 0.55 | 1/2368 (0.0%) |
| 50 | S4 | 0.32 | 0/2084 | 0.57 | 0/2804 |
| 50 | s4 | 0.32 | 0/2109 | 0.56 | 0/2839 |
| 51 | S5 | 0.27 | 0/1629 | 0.56 | 0/2202 |
| 51 | s5 | 0.29 | 0/1629 | 0.53 | 0/2202 |
| 52 | S6 | 0.31 | 0/1611 | 0.52 | 0/2151 |
| 53 | S7 | 0.30 | 0/1465 | 0.56 | 0/1971 |
| 53 | s7 | 0.31 | 0/1517 | 0.58 | 0/2044 |
| 54 | S8 | 0.34 | 0/1491 | 0.57 | 1/1992 (0.1%) |
| 54 | s8 | 0.32 | 0/1514 | 0.50 | 0/2021 |
| 55 | S9 | 0.30 | 0/1443 | 0.54 | 0/1934 |
| 55 | s9 | 0.30 | 0/1519 | 0.53 | 0/2035 |
| 56 | C0 | 0.29 | 0/759 | 0.56 | 1/1025 (0.1%) |
| 56 | c0 | 0.29 | 0/776 | 0.73 | 4/1047 (0.4%) |
| 57 | C1 | 0.37 | 0/1153 | 0.57 | 0/1554 |
| 57 | c1 | 0.34 | 0/1194 | 0.57 | 0/1610 |
| 58 | C2 | 0.33 | 0/771 | 0.64 | 0/1044 |
| 58 | c2 | 0.30 | 0/898 | 0.66 | 1/1220 (0.1%) |
| 59 | C3 | 0.32 | 0/1215 | 0.51 | 0/1638 |
| 59 | c3 | 0.29 | 0/1215 | 0.50 | 0/1638 |
| 60 | C4 | 0.31 | 0/901 | 0.60 | 0/1217 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 60 | c4 | 0.30 | 0/960 | 0.58 | 0/1290 |
| 61 | C5 | 0.30 | 0/937 | 0.52 | 0/1258 |
| 61 | c5 | 0.35 | 0/1060 | 0.64 | 0/1426 |
| 62 | C6 | 0.29 | 0/1083 | 0.55 | 1/1452 (0.1%) |
| 62 | c6 | 0.29 | 0/1131 | 0.52 | 0/1518 |
| 63 | C7 | 0.31 | 0/910 | 0.70 | 3/1219 (0.2%) |
| 63 | c7 | 0.30 | 0/914 | 0.64 | 1/1224 (0.1%) |
| 64 | C8 | 0.38 | 1/1197 (0.1%) | 0.51 | 0/1609 |
| 64 | c8 | 0.29 | 0/1211 | 0.58 | 1/1628 (0.1%) |
| 65 | C9 | 0.29 | 0/1089 | 0.50 | 0/1461 |
| 65 | c9 | 0.29 | 0/1130 | 0.47 | 0/1517 |
| 66 | D0 | 0.29 | 0/828 | 0.51 | 0/1119 |
| 66 | d0 | 0.31 | 0/883 | 0.58 | 0/1193 |
| 67 | D1 | 0.29 | 0/693 | 0.54 | 0/935 |
| 67 | d1 | 0.30 | 0/693 | 0.59 | 0/935 |
| 68 | D2 | 0.32 | 0/1038 | 0.56 | 0/1395 |
| 68 | d2 | 0.31 | 0/1038 | 0.55 | 1/1395 (0.1%) |
| 69 | D3 | 0.40 | 0/1139 | 0.56 | 0/1518 |
| 69 | d3 | 0.36 | 0/1139 | 0.54 | 0/1518 |
| 70 | D4 | 0.31 | 0/1087 | 0.54 | 0/1449 |
| 70 | d4 | 0.34 | 0/1087 | 0.57 | 1/1449 (0.1%) |
| 71 | D5 | 0.28 | 0/571 | 0.60 | 0/768 |
| 71 | d5 | 0.26 | 0/566 | 0.45 | 0/761 |
| 72 | D6 | 0.43 | 0/782 | 0.73 | 3/1047 (0.3%) |
| 72 | d6 | 0.32 | 0/782 | 0.59 | 0/1047 |
| 73 | D7 | 0.30 | 0/620 | 0.58 | 0/838 |
| 73 | d7 | 0.29 | 0/620 | 0.55 | 0/838 |
| 74 | D8 | 0.29 | 0/499 | 0.57 | 0/670 |
| 74 | d8 | 0.29 | 0/499 | 0.58 | 0/670 |
| 75 | D9 | 0.40 | 0/453 | 0.62 | 0/602 |
| 75 | d9 | 0.39 | 0/453 | 0.63 | 1/602 (0.2%) |
| 76 | E0 | 0.33 | 0/483 | 0.56 | 0/643 |
| 76 | e0 | 0.34 | 0/499 | 0.61 | 0/665 |
| 77 | SR | 0.26 | 0/2485 | 0.51 | 0/3383 |
| 77 | sR | 0.27 | 0/2490 | 0.53 | 0/3390 |
| 78 | SM | 0.32 | 0/1053 | 0.57 | 1/1418 (0.1%) |
| 78 | sM | 0.67 | 1/638 (0.2%) | 0.51 | 0/860 |
| 79 | s6 | 0.31 | 0/1779 | 0.51 | 0/2379 |
| All | All | 0.48 | 11/419528 (0.0%) | 0.87 | 465/615687 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 4 | l2 | 0 | 1 |
| 6 | L4 | 0 | 1 |
| 7 | L5 | 0 | 5 |
| 10 | L8 | 0 | 3 |
| 10 | l8 | 0 | 3 |
| 13 | M1 | 0 | 1 |
| 13 | m1 | 0 | 1 |
| 14 | M3 | 0 | 1 |
| 15 | m4 | 0 | 1 |
| 16 | M5 | 0 | 1 |
| 20 | M9 | 0 | 1 |
| 21 | N0 | 0 | 3 |
| 21 | n0 | 0 | 2 |
| 23 | N2 | 0 | 2 |
| 26 | n5 | 0 | 1 |
| 28 | n7 | 0 | 1 |
| 29 | n8 | 0 | 1 |
| 30 | N9 | 0 | 1 |
| 30 | n9 | 0 | 1 |
| 31 | O0 | 0 | 1 |
| 33 | O2 | 0 | 1 |
| 33 | o2 | 0 | 1 |
| 35 | o4 | 0 | 1 |
| 38 | o7 | 0 | 1 |
| 43 | Q2 | 0 | 1 |
| 47 | S1 | 0 | 2 |
| 48 | S2 | 0 | 1 |
| 48 | s2 | 0 | 2 |
| 49 | s3 | 0 | 1 |
| 51 | S5 | 0 | 1 |
| 51 | s5 | 0 | 1 |
| 53 | S7 | 0 | 2 |
| 53 | s7 | 0 | 5 |
| 54 | S8 | 0 | 1 |
| 55 | s9 | 0 | 4 |
| 57 | c1 | 0 | 1 |
| 58 | C2 | 0 | 1 |
| 58 | c2 | 0 | 2 |
| 60 | C4 | 0 | 3 |
| 61 | c5 | 0 | 1 |
| 62 | C6 | 0 | 1 |
| 62 | c6 | 0 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 63 | C7 | 0 | 2 |
| 63 | c7 | 0 | 1 |
| 65 | C9 | 0 | 1 |
| 66 | D0 | 0 | 2 |
| 68 | D2 | 0 | 3 |
| 70 | d4 | 0 | 3 |
| 71 | D5 | 0 | 1 |
| 72 | D6 | 0 | 3 |
| 73 | D7 | 0 | 1 |
| 75 | D9 | 0 | 2 |
| 75 | d9 | 0 | 1 |
| 77 | SR | 0 | 2 |
| 77 | sR | 0 | 1 |
| 78 | SM | 0 | 1 |
| 78 | sM | 0 | 1 |
| All | All | 0 | 92 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 78 | sM | 51 | ARG | C-N | 14.96 | 1.62 | 1.34 |
| 28 | N7 | 36 | HIS | C-N | 9.18 | 1.51 | 1.34 |
| 64 | C8 | 81 | ILE | C-N | -9.18 | 1.16 | 1.34 |
| 1 | 5 | 1152 | G | N9-C4 | -8.15 | 1.31 | 1.38 |
| 1 | 1 | 2606 | G | N9-C4 | -7.56 | 1.31 | 1.38 |
| 5 | l3 | 168 | LYS | C-N | -7.45 | 1.17 | 1.34 |
| 1 | 1 | 2971 | A | N9-C4 | 7.10 | 1.42 | 1.37 |
| 1 | 5 | 1103 | A | N9-C4 | 6.08 | 1.41 | 1.37 |
| 1 | 1 | 2971 | A | N3-C4 | 5.63 | 1.38 | 1.34 |
| 28 | N7 | 27 | LYS | C-N | -5.44 | 1.24 | 1.34 |
| 1 | 1 | 2418 | G | C6-N1 | 5.24 | 1.43 | 1.39 |

All (465) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 5 | 1152 | G | N3-C4-N9 | -14.66 | 117.20 | 126.00 |
| 1 | 5 | 1152 | G | N3-C4-C5 | 12.74 | 134.97 | 128.60 |
| 3 | 8 | 84 | C | N1-C2-O2 | 12.54 | 126.42 | 118.90 |
| 1 | 1 | 2606 | G | C5-N7-C8 | -12.29 | 98.15 | 104.30 |
| 1 | 1 | 2606 | G | N3-C4-C5 | 12.25 | 134.72 | 128.60 |
| 1 | 1 | 2606 | G | N3-C4-N9 | -10.16 | 119.91 | 126.00 |
| 3 | 8 | 84 | C | C5-C6-N1 | 9.89 | 125.94 | 121.00 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 2606 | G | C4-C5-N7 | 9.69 | 114.68 | 110.80 |
| 1 | 1 | 2808 | A | N1-C6-N6 | 9.40 | 124.24 | 118.60 |
| 1 | 1 | 1866 | C | N1-C2-O2 | 9.38 | 124.53 | 118.90 |
| 3 | 8 | 84 | C | C2-N1-C1' | 9.22 | 128.94 | 118.80 |
| 1 | 1 | 1866 | C | N3-C2-O2 | -9.17 | 115.48 | 121.90 |
| 1 | 1 | 2606 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 45 | 2 | 1274 | C | N1-C2-O2 | 8.89 | 124.24 | 118.90 |
| 1 | 1 | 1866 | C | C2-N1-C1' | 8.79 | 128.47 | 118.80 |
| 3 | 8 | 84 | C | C6-N1-C2 | -8.62 | 116.85 | 120.30 |
| 3 | 4 | 126 | A | O5'-P-OP1 | -8.53 | 98.03 | 105.70 |
| 45 | 6 | 542 | A | O4'-C1'-N9 | 8.43 | 114.95 | 108.20 |
| 1 | 1 | 2772 | C | C6-N1-C1' | -8.26 | 110.89 | 120.80 |
| 1 | 1 | 1495 | U | C5-C6-N1 | -8.24 | 118.58 | 122.70 |
| 3 | 4 | 84 | C | C2-N1-C1' | 8.23 | 127.85 | 118.80 |
| 1 | 1 | 3217 | C | N1-C2-O2 | 8.19 | 123.81 | 118.90 |
| 3 | 8 | 84 | C | N3-C2-O2 | -8.18 | 116.18 | 121.90 |
| 45 | 6 | 163 | G | N3-C4-N9 | -8.13 | 121.12 | 126.00 |
| 1 | 5 | 2205 | U | N1-C2-O2 | 8.08 | 128.45 | 122.80 |
| 1 | 5 | 549 | U | C2-N1-C1' | 8.06 | 127.37 | 117.70 |
| 45 | 2 | 1274 | C | C2-N1-C1' | 8.05 | 127.65 | 118.80 |
| 1 | 5 | 437 | G | N7-C8-N9 | 8.02 | 117.11 | 113.10 |
| 1 | 5 | 2256 | A | O4'-C1'-N9 | 7.99 | 114.59 | 108.20 |
| 3 | 4 | 151 | C | N3-C2-O2 | -7.98 | 116.32 | 121.90 |
| 1 | 5 | 2205 | U | N3-C2-O2 | -7.96 | 116.63 | 122.20 |
| 3 | 4 | 84 | C | C6-N1-C2 | -7.93 | 117.13 | 120.30 |
| 45 | 2 | 1490 | C | C2-N1-C1' | 7.89 | 127.48 | 118.80 |
| 3 | 4 | 125 | U | N1-C2-O2 | 7.86 | 128.30 | 122.80 |
| 1 | 1 | 2606 | G | N7-C8-N9 | 7.86 | 117.03 | 113.10 |
| 44 | Q3 | 49 | ARG | C-N-CA | 7.80 | 138.67 | 122.30 |
| 45 | 2 | 1490 | C | N1-C2-O2 | 7.79 | 123.58 | 118.90 |
| 1 | 1 | 2772 | C | C2-N1-C1' | 7.73 | 127.30 | 118.80 |
| 1 | 1 | 2842 | U | C2-N1-C1' | 7.60 | 126.82 | 117.70 |
| 45 | 6 | 132 | U | C2-N1-C1' | 7.59 | 126.80 | 117.70 |
| 2 | 3 | 73 | C | N1-C2-O2 | 7.57 | 123.44 | 118.90 |
| 3 | 8 | 84 | C | C2-N3-C4 | 7.52 | 123.66 | 119.90 |
| 3 | 4 | 84 | C | O5'-P-OP2 | -7.47 | 98.97 | 105.70 |
| 1 | 1 | 895 | A | N7-C8-N9 | 7.46 | 117.53 | 113.80 |
| 3 | 8 | 83 | C | N1-C2-O2 | 7.42 | 123.35 | 118.90 |
| 3 | 8 | 83 | C | N3-C2-O2 | -7.41 | 116.71 | 121.90 |
| 1 | 5 | 1152 | G | C5-N7-C8 | -7.36 | 100.62 | 104.30 |
| 63 | C7 | 85 | VAL | C-N-CD | -7.36 | 104.41 | 120.60 |
| 1 | 1 | 895 | A | C8-N9-C4 | -7.33 | 102.87 | 105.80 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 2 | 934 | C | C2-N1-C1' | 7.32 | 126.85 | 118.80 |
| 1 | 1 | 2595 | A | C5-N7-C8 | -7.26 | 100.27 | 103.90 |
| 1 | 5 | 2205 | U | C2-N1-C1' | 7.26 | 126.41 | 117.70 |
| 1 | 1 | 1764 | U | C2-N1-C1' | 7.24 | 126.39 | 117.70 |
| 46 | S0 | 9 | LEU | CA-CB-CG | 7.22 | 131.92 | 115.30 |
| 1 | 5 | 1200 | A | N1-C6-N6 | 7.22 | 122.94 | 118.60 |
| 1 | 1 | 979 | U | C5-C6-N1 | 7.21 | 126.31 | 122.70 |
| 1 | 5 | 1307 | G | P-O3'-C3' | 7.21 | 128.35 | 119.70 |
| 56 | c0 | 88 | PRO | N-CA-CB | 7.20 | 111.94 | 103.30 |
| 1 | 1 | 2873 | U | C5-C4-O4 | 7.17 | 130.20 | 125.90 |
| 45 | 2 | 137 | U | C2-N1-C1' | 7.15 | 126.28 | 117.70 |
| 1 | 1 | 1495 | U | N1-C2-N3 | 7.15 | 119.19 | 114.90 |
| 1 | 5 | 3362 | A | O4'-C1'-N9 | 7.09 | 113.88 | 108.20 |
| 1 | 1 | 895 | A | C5-N7-C8 | -7.05 | 100.38 | 103.90 |
| 1 | 1 | 3217 | C | C2-N1-C1' | 7.05 | 126.56 | 118.80 |
| 56 | c0 | 97 | PRO | N-CA-CB | 7.03 | 111.73 | 103.30 |
| 3 | 4 | 151 | C | N1-C2-O2 | 7.01 | 123.11 | 118.90 |
| 1 | 5 | 424 | G | N1-C6-O6 | 7.01 | 124.11 | 119.90 |
| 3 | 4 | 84 | C | N1-C2-O2 | 6.97 | 123.08 | 118.90 |
| 63 | c7 | 118 | PRO | N-CA-CB | 6.96 | 111.66 | 103.30 |
| 45 | 2 | 137 | U | N1-C2-O2 | 6.92 | 127.64 | 122.80 |
| 1 | 1 | 2971 | A | C2-N3-C4 | 6.92 | 114.06 | 110.60 |
| 1 | 1 | 3341 | U | N1-C2-O2 | 6.91 | 127.63 | 122.80 |
| 45 | 2 | 1274 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 1 | 5 | 1838 | G | C8-N9-C4 | 6.89 | 109.16 | 106.40 |
| 1 | 5 | 3245 | A | N7-C8-N9 | 6.88 | 117.24 | 113.80 |
| 45 | 2 | 934 | C | N1-C2-O2 | 6.83 | 123.00 | 118.90 |
| 1 | 5 | 1072 | G | N3-C4-N9 | 6.83 | 130.10 | 126.00 |
| 1 | 1 | 2870 | C | N3-C4-C5 | 6.82 | 124.63 | 121.90 |
| 1 | 1 | 2606 | G | C5-C6-O6 | -6.81 | 124.51 | 128.60 |
| 45 | 2 | 830 | U | N3-C2-O2 | -6.80 | 117.44 | 122.20 |
| 1 | 1 | 895 | A | C2-N3-C4 | -6.79 | 107.20 | 110.60 |
| 1 | 1 | 2355 | G | N1-C6-O6 | 6.73 | 123.94 | 119.90 |
| 45 | 6 | 163 | G | N3-C4-C5 | 6.71 | 131.95 | 128.60 |
| 1 | 5 | 549 | U | N1-C2-O2 | 6.70 | 127.49 | 122.80 |
| 3 | 4 | 125 | U | C2-N1-C1' | 6.68 | 125.72 | 117.70 |
| 1 | 5 | 2175 | U | N1-C2-O2 | -6.68 | 118.12 | 122.80 |
| 1 | 5 | 3245 | A | C2-N3-C4 | -6.67 | 107.26 | 110.60 |
| 1 | 1 | 2391 | G | N1-C6-O6 | -6.67 | 115.90 | 119.90 |
| 1 | 1 | 2772 | C | N1-C2-O2 | 6.66 | 122.89 | 118.90 |
| 56 | C0 | 88 | PRO | N-CA-CB | 6.66 | 111.29 | 103.30 |
| 1 | 1 | 3278 | C | C2-N1-C1' | 6.65 | 126.12 | 118.80 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | O3 | 21 | ARG | NE-CZ-NH1 | 6.65 | 123.63 | 120.30 |
| 45 | 2 | 959 | U | C2-N1-C1' | 6.64 | 125.67 | 117.70 |
| 1 | 1 | 1495 | U | C5-C4-O4 | 6.62 | 129.87 | 125.90 |
| 1 | 5 | 650 | C | N1-C2-O2 | -6.62 | 114.93 | 118.90 |
| 1 | 1 | 1604 | G | C4-N9-C1' | 6.60 | 135.08 | 126.50 |
| 1 | 1 | 3217 | C | N3-C2-O2 | -6.60 | 117.28 | 121.90 |
| 3 | 8 | 81 | U | OP1-P-OP2 | -6.59 | 109.72 | 119.60 |
| 45 | 6 | 1473 | U | C2-N1-C1' | 6.58 | 125.60 | 117.70 |
| 45 | 6 | 337 | G | C4-C5-N7 | 6.56 | 113.42 | 110.80 |
| 45 | 2 | 959 | U | N3-C2-O2 | -6.56 | 117.61 | 122.20 |
| 45 | 6 | 1473 | U | N1-C2-O2 | 6.55 | 127.39 | 122.80 |
| 1 | 1 | 765 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 1 | 5 | 3308 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 1 | 1 | 2879 | C | C6-N1-C2 | 6.52 | 122.91 | 120.30 |
| 3 | 8 | 81 | U | OP2-P-O3' | 6.52 | 119.55 | 105.20 |
| 45 | 6 | 1389 | C | C2-N1-C1' | 6.52 | 125.97 | 118.80 |
| 1 | 1 | 913 | A | N1-C6-N6 | -6.48 | 114.71 | 118.60 |
| 1 | 1 | 1741 | A | O4'-C1'-N9 | 6.48 | 113.39 | 108.20 |
| 45 | 2 | 581 | U | C2-N1-C1' | 6.47 | 125.47 | 117.70 |
| 1 | 5 | 1879 | A | C5-N7-C8 | -6.46 | 100.67 | 103.90 |
| 1 | 1 | 2808 | A | N9-C4-C5 | -6.44 | 103.22 | 105.80 |
| 45 | 6 | 132 | U | N1-C2-O2 | 6.42 | 127.29 | 122.80 |
| 1 | 1 | 2364 | G | N1-C6-O6 | -6.42 | 116.05 | 119.90 |
| 1 | 1 | 621 | A | O4'-C1'-N9 | 6.42 | 113.33 | 108.20 |
| 3 | 4 | 151 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 1 | 1 | 621 | A | C8-N9-C4 | 6.41 | 108.36 | 105.80 |
| 1 | 1 | 979 | U | C2-N1-C1' | 6.40 | 125.38 | 117.70 |
| 1 | 1 | 2873 | U | N3-C4-O4 | -6.38 | 114.93 | 119.40 |
| 54 | S8 | 29 | LEU | CA-CB-CG | 6.38 | 129.98 | 115.30 |
| 1 | 1 | 621 | A | C4-N9-C1' | -6.37 | 114.83 | 126.30 |
| 4 | l2 | 246 | LEU | CA-CB-CG | 6.35 | 129.90 | 115.30 |
| 3 | 4 | 125 | U | N3-C2-O2 | -6.34 | 117.76 | 122.20 |
| 45 | 2 | 959 | U | N1-C2-O2 | 6.33 | 127.23 | 122.80 |
| 1 | 5 | 406 | G | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 1 | 5 | 1762 | C | C2-N1-C1' | 6.32 | 125.75 | 118.80 |
| 1 | 1 | 3278 | C | N1-C2-O2 | 6.31 | 122.69 | 118.90 |
| 1 | 5 | 3362 | A | N7-C8-N9 | 6.31 | 116.95 | 113.80 |
| 1 | 1 | 869 | G | C2-N3-C4 | -6.30 | 108.75 | 111.90 |
| 45 | 2 | 1082 | C | C2-N1-C1' | 6.30 | 125.73 | 118.80 |
| 1 | 1 | 2846 | U | N3-C2-O2 | -6.29 | 117.80 | 122.20 |
| 3 | 4 | 84 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 3 | 8 | 82 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 926 | A | N1-C6-N6 | 6.26 | 122.36 | 118.60 |
| 1 | 1 | 2142 | A | N1-C6-N6 | -6.26 | 114.84 | 118.60 |
| 1 | 1 | 908 | G | C4-N9-C1' | 6.25 | 134.62 | 126.50 |
| 1 | 5 | 549 | U | N3-C2-O2 | -6.23 | 117.84 | 122.20 |
| 1 | 1 | 3382 | U | N1-C2-O2 | 6.22 | 127.15 | 122.80 |
| 1 | 1 | 2943 | G | N1-C6-O6 | 6.22 | 123.63 | 119.90 |
| 1 | 1 | 1604 | G | N3-C4-C5 | -6.21 | 125.50 | 128.60 |
| 1 | 5 | 1148 | G | C8-N9-C4 | 6.19 | 108.88 | 106.40 |
| 47 | S1 | 61 | LEU | CA-CB-CG | 6.19 | 129.53 | 115.30 |
| 64 | c8 | 116 | LEU | CA-CB-CG | 6.19 | 129.53 | 115.30 |
| 1 | 1 | 1556 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 1 | 1 | 1866 | C | C6-N1-C1' | -6.18 | 113.39 | 120.80 |
| 1 | 5 | 1152 | G | C8-N9-C1' | 6.18 | 135.03 | 127.00 |
| 1 | 1 | 1495 | U | N1-C2-O2 | -6.17 | 118.48 | 122.80 |
| 45 | 2 | 144 | U | N1-C2-O2 | 6.17 | 127.12 | 122.80 |
| 45 | 2 | 1274 | C | C6-N1-C1' | -6.14 | 113.44 | 120.80 |
| 1 | 1 | 1495 | U | C4-C5-C6 | 6.12 | 123.38 | 119.70 |
| 72 | D6 | 85 | ARG | N-CA-C | -6.11 | 94.50 | 111.00 |
| 1 | 5 | 1762 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 1 | 5 | 2373 | A | O5'-P-OP1 | -6.10 | 100.21 | 105.70 |
| 1 | 1 | 2818 | U | O5'-P-OP2 | -6.09 | 100.22 | 105.70 |
| 45 | 2 | 830 | U | N1-C2-O2 | 6.09 | 127.06 | 122.80 |
| 1 | 1 | 2320 | A | N1-C2-N3 | 6.09 | 132.34 | 129.30 |
| 1 | 5 | 1152 | G | N9-C4-C5 | 6.06 | 107.83 | 105.40 |
| 1 | 1 | 1848 | G | C5-C6-O6 | -6.06 | 124.97 | 128.60 |
| 1 | 1 | 765 | C | C2-N1-C1' | 6.04 | 125.44 | 118.80 |
| 1 | 5 | 1879 | A | N7-C8-N9 | 6.04 | 116.82 | 113.80 |
| 1 | 1 | 1848 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 1 | 5 | 437 | G | C6-C5-N7 | -6.03 | 126.78 | 130.40 |
| 45 | 2 | 137 | U | N3-C2-O2 | -6.02 | 117.98 | 122.20 |
| 1 | 5 | 2954 | U | N1-C2-O2 | 6.01 | 127.01 | 122.80 |
| 45 | 2 | 1082 | C | N1-C2-O2 | 6.01 | 122.51 | 118.90 |
| 5 | L3 | 99 | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 45 | 6 | 1058 | U | OP1-P-O3' | 6.01 | 118.41 | 105.20 |
| 45 | 2 | 1456 | C | C2-N1-C1' | 6.00 | 125.39 | 118.80 |
| 1 | 1 | 2827 | U | N1-C2-N3 | 5.99 | 118.49 | 114.90 |
| 1 | 5 | 3317 | U | N3-C2-O2 | -5.98 | 118.01 | 122.20 |
| 3 | 8 | 83 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 1 | 1 | 2816 | G | C4-N9-C1' | -5.97 | 118.74 | 126.50 |
| 1 | 5 | 3245 | A | N1-C6-N6 | 5.97 | 122.18 | 118.60 |
| 1 | 1 | 857 | G | C8-N9-C4 | 5.96 | 108.79 | 106.40 |
| 45 | 6 | 1363 | U | P-O3'-C3' | 5.96 | 126.85 | 119.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 406 | G | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 1 | 1 | 3396 | U | N1-C2-O2 | 5.96 | 126.97 | 122.80 |
| 1 | 1 | 2595 | A | N1-C6-N6 | 5.95 | 122.17 | 118.60 |
| 13 | m1 | 112 | LEU | CA-CB-CG | 5.94 | 128.97 | 115.30 |
| 1 | 1 | 3382 | U | C2-N1-C1' | 5.94 | 124.83 | 117.70 |
| 72 | D6 | 64 | LEU | CA-CB-CG | 5.94 | 128.96 | 115.30 |
| 45 | 2 | 1490 | C | N3-C2-O2 | -5.94 | 117.74 | 121.90 |
| 45 | 6 | 163 | G | N3-C2-N2 | -5.94 | 115.75 | 119.90 |
| 45 | 6 | 1097 | U | P-O3'-C3' | 5.93 | 126.82 | 119.70 |
| 1 | 1 | 3344 | A | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 45 | 6 | 132 | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 1 | 1 | 1279 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 78 | SM | 166 | PRO | N-CA-CB | 5.92 | 110.40 | 103.30 |
| 1 | 5 | 1495 | U | C2-N1-C1' | 5.92 | 124.80 | 117.70 |
| 45 | 2 | 1761 | U | C5-C4-O4 | 5.92 | 129.45 | 125.90 |
| 1 | 1 | 3341 | U | N3-C2-O2 | -5.92 | 118.06 | 122.20 |
| 45 | 6 | 158 | U | P-O3'-C3' | 5.91 | 126.80 | 119.70 |
| 1 | 5 | 437 | G | C5-N7-C8 | -5.91 | 101.34 | 104.30 |
| 1 | 5 | 424 | G | C5-C6-O6 | -5.90 | 125.06 | 128.60 |
| 1 | 1 | 2627 | C | C4-C5-C6 | 5.89 | 120.35 | 117.40 |
| 1 | 1 | 2810 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 45 | 2 | 442 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 1 | 5 | 1200 | A | C5-C6-N6 | -5.88 | 119.00 | 123.70 |
| 1 | 1 | 650 | C | N1-C2-O2 | -5.87 | 115.38 | 118.90 |
| 45 | 2 | 144 | U | C2-N1-C1' | 5.87 | 124.74 | 117.70 |
| 1 | 5 | 3245 | A | C5-N7-C8 | -5.87 | 100.97 | 103.90 |
| 1 | 1 | 922 | U | C2-N1-C1' | 5.86 | 124.74 | 117.70 |
| 1 | 5 | 3245 | A | C6-C5-N7 | -5.86 | 128.20 | 132.30 |
| 58 | c2 | 58 | LEU | CA-CB-CG | 5.85 | 128.76 | 115.30 |
| 1 | 1 | 2967 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 1 | 5 | 693 | A | O5'-P-OP1 | -5.84 | 100.44 | 105.70 |
| 1 | 1 | 1604 | G | C8-N9-C1' | -5.84 | 119.41 | 127.00 |
| 1 | 5 | 1503 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 36 | O5 | 118 | ILE | C-N-CA | 5.82 | 136.25 | 121.70 |
| 1 | 5 | 1072 | G | C8-N9-C1' | -5.82 | 119.44 | 127.00 |
| 1 | 1 | 2714 | G | N3-C4-C5 | 5.80 | 131.50 | 128.60 |
| 1 | 1 | 2411 | U | C6-N1-C2 | 5.80 | 124.48 | 121.00 |
| 1 | 1 | 3344 | A | N7-C8-N9 | 5.78 | 116.69 | 113.80 |
| 1 | 1 | 3277 | U | N3-C2-O2 | -5.78 | 118.16 | 122.20 |
| 1 | 5 | 2571 | U | C2-N1-C1' | 5.77 | 124.63 | 117.70 |
| 1 | 5 | 2388 | U | C5-C6-N1 | -5.77 | 119.81 | 122.70 |
| 1 | 5 | 2821 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 6 | 1473 | U | N3-C2-O2 | -5.76 | 118.17 | 122.20 |
| 1 | 1 | 1741 | A | N7-C8-N9 | 5.76 | 116.68 | 113.80 |
| 1 | 1 | 2679 | A | O4'-C1'-N9 | 5.74 | 112.79 | 108.20 |
| 1 | 5 | 1352 | A | P-O3'-C3' | 5.73 | 126.57 | 119.70 |
| 56 | c0 | 83 | PRO | N-CA-CB | 5.73 | 110.17 | 103.30 |
| 1 | 1 | 895 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 1 | 5 | 437 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 45 | 2 | 934 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 45 | 2 | 1761 | U | N3-C2-O2 | -5.71 | 118.20 | 122.20 |
| 45 | 6 | 1000 | C | C2-N1-C1' | 5.71 | 125.08 | 118.80 |
| 1 | 5 | 1492 | G | C8-N9-C4 | 5.71 | 108.68 | 106.40 |
| 45 | 6 | 337 | G | C5-N7-C8 | -5.71 | 101.45 | 104.30 |
| 1 | 1 | 2595 | A | C4-C5-N7 | 5.70 | 113.55 | 110.70 |
| 1 | 1 | 2827 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 1 | 5 | 2291 | A | N1-C6-N6 | -5.70 | 115.18 | 118.60 |
| 45 | 6 | 542 | A | C4-N9-C1' | 5.70 | 136.56 | 126.30 |
| 1 | 5 | 3164 | C | O4'-C1'-N1 | 5.69 | 112.75 | 108.20 |
| 1 | 5 | 424 | G | C6-C5-N7 | -5.69 | 126.98 | 130.40 |
| 1 | 1 | 2827 | U | C5-C6-N1 | -5.69 | 119.86 | 122.70 |
| 1 | 1 | 609 | G | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 1 | 1 | 3057 | U | N3-C2-O2 | -5.68 | 118.22 | 122.20 |
| 1 | 5 | 1592 | G | C5-C6-N1 | -5.68 | 108.66 | 111.50 |
| 1 | 1 | 2376 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 1 | 1 | 3196 | U | O5'-P-OP2 | -5.68 | 100.59 | 105.70 |
| 3 | 8 | 82 | U | N1-C2-O2 | 5.68 | 126.78 | 122.80 |
| 1 | 1 | 2609 | A | O5'-P-OP2 | -5.68 | 100.59 | 105.70 |
| 1 | 1 | 1137 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 1 | 1 | 2404 | A | O4'-C1'-N9 | -5.67 | 103.66 | 108.20 |
| 3 | 8 | 83 | C | C2-N1-C1' | 5.67 | 125.04 | 118.80 |
| 45 | 2 | 1560 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 1 | 1 | 2808 | A | C4-C5-N7 | 5.65 | 113.53 | 110.70 |
| 45 | 2 | 1490 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 1 | 5 | 1072 | G | N9-C4-C5 | -5.64 | 103.14 | 105.40 |
| 1 | 5 | 1352 | A | OP1-P-O3' | 5.63 | 117.60 | 105.20 |
| 45 | 6 | 1560 | U | C2-N1-C1' | 5.63 | 124.46 | 117.70 |
| 3 | 4 | 84 | C | C5-C6-N1 | 5.63 | 123.81 | 121.00 |
| 3 | 8 | 81 | U | P-O3'-C3' | 5.61 | 126.44 | 119.70 |
| 1 | 1 | 921 | A | N1-C6-N6 | -5.61 | 115.23 | 118.60 |
| 1 | 5 | 3362 | A | C6-C5-N7 | -5.60 | 128.38 | 132.30 |
| 45 | 2 | 1258 | U | N3-C2-O2 | -5.59 | 118.29 | 122.20 |
| 1 | 1 | 1502 | C | N1-C2-O2 | -5.58 | 115.55 | 118.90 |
| 45 | 2 | 1573 | A | P-O3'-C3' | 5.58 | 126.39 | 119.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 70 | d4 | 134 | ALA | CB-CA-C | 5.58 | 118.46 | 110.10 |
| 1 | 1 | 1329 | U | P-O3'-C3' | 5.57 | 126.39 | 119.70 |
| 1 | 1 | 3362 | A | C2-N3-C4 | -5.57 | 107.81 | 110.60 |
| 1 | 1 | 1741 | A | C8-N9-C4 | -5.56 | 103.58 | 105.80 |
| 1 | 1 | 2842 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 1 | 1 | 641 | C | O4'-C1'-N1 | 5.56 | 112.64 | 108.20 |
| 1 | 1 | 1866 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 1 | 5 | 2978 | U | C5-C6-N1 | -5.55 | 119.92 | 122.70 |
| 1 | 5 | 3154 | C | OP1-P-O3' | 5.55 | 117.41 | 105.20 |
| 3 | 8 | 84 | C | C6-N1-C1' | -5.55 | 114.14 | 120.80 |
| 3 | 4 | 151 | C | C2-N1-C1' | 5.55 | 124.90 | 118.80 |
| 1 | 1 | 2816 | G | C5-C6-O6 | -5.54 | 125.27 | 128.60 |
| 10 | l8 | 69 | LEU | CA-CB-CG | 5.54 | 128.04 | 115.30 |
| 1 | 5 | 1329 | U | P-O3'-C3' | 5.54 | 126.34 | 119.70 |
| 1 | 1 | 1433 | A | N1-C2-N3 | 5.53 | 132.07 | 129.30 |
| 49 | s3 | 4 | LEU | CA-CB-CG | 5.53 | 128.03 | 115.30 |
| 1 | 1 | 835 | G | O4'-C1'-N9 | 5.53 | 112.62 | 108.20 |
| 1 | 1 | 2606 | G | C2-N3-C4 | -5.53 | 109.14 | 111.90 |
| 45 | 6 | 864 | U | N3-C2-O2 | -5.53 | 118.33 | 122.20 |
| 1 | 5 | 1604 | G | C4-N9-C1' | 5.53 | 133.69 | 126.50 |
| 3 | 8 | 11 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 1 | 1 | 1879 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 45 | 2 | 1389 | C | C2-N1-C1' | 5.50 | 124.86 | 118.80 |
| 4 | L2 | 180 | LEU | CA-CB-CG | 5.50 | 127.96 | 115.30 |
| 45 | 2 | 1039 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 1 | 1 | 2939 | G | C8-N9-C4 | 5.50 | 108.60 | 106.40 |
| 1 | 1 | 75 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 1 | 1 | 3396 | U | C2-N1-C1' | 5.49 | 124.29 | 117.70 |
| 2 | 3 | 87 | G | N9-C4-C5 | -5.49 | 103.20 | 105.40 |
| 1 | 5 | 1081 | U | P-O3'-C3' | 5.49 | 126.28 | 119.70 |
| 1 | 1 | 283 | G | O4'-C1'-N9 | -5.48 | 103.82 | 108.20 |
| 45 | 2 | 418 | G | C4-N9-C1' | 5.48 | 133.62 | 126.50 |
| 1 | 1 | 437 | G | C5-C6-O6 | -5.48 | 125.31 | 128.60 |
| 45 | 2 | 934 | C | N3-C2-O2 | -5.47 | 118.07 | 121.90 |
| 45 | 2 | 1456 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 1 | 1 | 1307 | G | C4-N9-C1' | -5.46 | 119.40 | 126.50 |
| 12 | m0 | 57 | LEU | CA-CB-CG | 5.46 | 127.86 | 115.30 |
| 1 | 1 | 2245 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 1 | 1 | 1299 | U | C5-C6-N1 | -5.45 | 119.97 | 122.70 |
| 1 | 1 | 1815 | U | P-O3'-C3' | 5.45 | 126.24 | 119.70 |
| 1 | 1 | 2816 | G | C8-N9-C1' | 5.44 | 134.07 | 127.00 |
| 1 | 1 | 2885 | C | C6-N1-C2 | 5.44 | 122.47 | 120.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 2 | 1246 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |
| 1 | 1 | 827 | A | C8-N9-C4 | 5.41 | 107.97 | 105.80 |
| 1 | 5 | 424 | G | C4-C5-N7 | 5.40 | 112.96 | 110.80 |
| 1 | 5 | 3362 | A | C5-N7-C8 | -5.40 | 101.20 | 103.90 |
| 1 | 1 | 1556 | C | N3-C2-O2 | -5.39 | 118.13 | 121.90 |
| 1 | 1 | 2983 | C | C4-C5-C6 | 5.39 | 120.09 | 117.40 |
| 45 | 2 | 638 | U | C2-N1-C1' | 5.39 | 124.17 | 117.70 |
| 45 | 2 | 1773 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 1 | 5 | 2666 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 45 | 6 | 755 | A | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 |
| 1 | 1 | 621 | A | C4-C5-C6 | -5.38 | 114.31 | 117.00 |
| 1 | 1 | 2970 | C | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 45 | 2 | 1150 | G | C2-N3-C4 | -5.36 | 109.22 | 111.90 |
| 1 | 5 | 1496 | C | C2-N1-C1' | 5.36 | 124.70 | 118.80 |
| 1 | 1 | 91 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 45 | 6 | 934 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 1 | 5 | 1152 | G | C8-N9-C4 | -5.35 | 104.26 | 106.40 |
| 1 | 1 | 2541 | U | P-O3'-C3' | 5.35 | 126.11 | 119.70 |
| 20 | M9 | 24 | LEU | CA-CB-CG | 5.34 | 127.59 | 115.30 |
| 1 | 5 | 1481 | A | C8-N9-C4 | -5.34 | 103.66 | 105.80 |
| 1 | 1 | 2606 | G | N1-C2-N2 | 5.34 | 121.00 | 116.20 |
| 45 | 2 | 1560 | U | C2-N1-C1' | 5.33 | 124.10 | 117.70 |
| 1 | 5 | 1072 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 45 | 2 | 1490 | C | C6-N1-C1' | -5.33 | 114.41 | 120.80 |
| 1 | 5 | 549 | U | C5-C6-N1 | 5.33 | 125.36 | 122.70 |
| 1 | 1 | 2842 | U | C6-N1-C1' | -5.32 | 113.75 | 121.20 |
| 33 | o2 | 126 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 1 | 1 | 914 | A | N1-C6-N6 | -5.32 | 115.41 | 118.60 |
| 46 | s0 | 9 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 45 | 6 | 1058 | U | P-O3'-C3' | 5.31 | 126.07 | 119.70 |
| 3 | 8 | 80 | A | C8-N9-C4 | 5.31 | 107.92 | 105.80 |
| 45 | 6 | 864 | U | C2-N1-C1' | 5.31 | 124.07 | 117.70 |
| 56 | c0 | 78 | GLU | N-CA-C | -5.31 | 96.67 | 111.00 |
| 45 | 6 | 1773 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 1 | 5 | 1152 | G | N1-C2-N2 | 5.30 | 120.97 | 116.20 |
| 1 | 1 | 2572 | C | C2-N1-C1' | 5.30 | 124.63 | 118.80 |
| 1 | 1 | 2595 | A | N7-C8-N9 | 5.29 | 116.45 | 113.80 |
| 1 | 1 | 2663 | G | N1-C6-O6 | 5.29 | 123.08 | 119.90 |
| 1 | 1 | 1141 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 26 | n5 | 57 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 68 | d2 | 93 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 1 | 5 | 1815 | U | P-O3'-C3' | 5.28 | 126.03 | 119.70 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 5 | 437 | G | C4-N9-C1' | 5.28 | 133.36 | 126.50 |
| 1 | 5 | 1481 | A | P-O3'-C3' | 5.28 | 126.03 | 119.70 |
| 1 | 5 | 2978 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 1 | 1 | 3218 | A | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 45 | 2 | 1456 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 45 | 6 | 864 | U | N1-C2-O2 | 5.27 | 126.49 | 122.80 |
| 72 | D6 | 63 | ALA | C-N-CA | 5.26 | 134.86 | 121.70 |
| 45 | 6 | 272 | U | P-O3'-C3' | 5.26 | 126.02 | 119.70 |
| 1 | 1 | 2560 | C | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 1 | 5 | 1348 | U | O4'-C1'-N1 | 5.26 | 112.41 | 108.20 |
| 45 | 6 | 756 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 45 | 6 | 781 | U | N1-C2-O2 | 5.25 | 126.47 | 122.80 |
| 1 | 1 | 1092 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 1 | 5 | 2725 | U | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 45 | 2 | 829 | A | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 45 | 6 | 934 | C | C2-N1-C1' | 5.24 | 124.56 | 118.80 |
| 1 | 1 | 1196 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 1 | 1 | 3278 | C | C5-C6-N1 | 5.23 | 123.62 | 121.00 |
| 45 | 2 | 158 | U | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 75 | d9 | 30 | LEU | CA-CB-CG | 5.23 | 127.34 | 115.30 |
| 4 | L2 | 191 | LEU | CA-CB-CG | -5.23 | 103.28 | 115.30 |
| 1 | 5 | 2526 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 1 | 1 | 155 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 1 | 1 | 3137 | C | C5-C6-N1 | -5.22 | 118.39 | 121.00 |
| 1 | 5 | 2606 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 1 | 1 | 2357 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 1 | 1 | 1095 | U | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 1 | 5 | 2942 | C | O5'-P-OP2 | -5.21 | 101.01 | 105.70 |
| 1 | 1 | 3278 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 45 | 6 | 139 | C | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 14 | M3 | 85 | LEU | CA-CB-CG | 5.21 | 127.27 | 115.30 |
| 45 | 2 | 543 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 1 | 5 | 2939 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 1 | 1 | 3362 | A | C5-N7-C8 | -5.21 | 101.30 | 103.90 |
| 1 | 5 | 908 | G | O4'-C1'-N9 | -5.20 | 104.04 | 108.20 |
| 1 | 1 | 1303 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 1 | 1 | 113 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 1 | 1 | 1379 | G | N9-C4-C5 | -5.20 | 103.32 | 105.40 |
| 1 | 5 | 2418 | G | OP1-P-O3' | 5.20 | 116.63 | 105.20 |
| 1 | 1 | 928 | C | N3-C2-O2 | -5.20 | 118.26 | 121.90 |
| 1 | 5 | 3195 | U | N1-C2-O2 | 5.19 | 126.44 | 122.80 |
| 44 | Q3 | 50 | GLY | N-CA-C | -5.19 | 100.12 | 113.10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | 2 | 1 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 1 | 1 | 1764 | U | N1-C2-O2 | 5.19 | 126.43 | 122.80 |
| 1 | 1 | 1819 | U | N3-C2-O2 | -5.19 | 118.57 | 122.20 |
| 1 | 1 | 637 | C | P-O3'-C3' | 5.19 | 125.93 | 119.70 |
| 1 | 5 | 437 | G | C5-C6-O6 | -5.19 | 125.49 | 128.60 |
| 45 | 6 | 792 | U | N1-C2-O2 | 5.19 | 126.43 | 122.80 |
| 45 | 6 | 1398 | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 1 | 5 | 1879 | A | C4-C5-N7 | 5.18 | 113.29 | 110.70 |
| 1 | 1 | 2764 | C | N1-C2-O2 | -5.17 | 115.80 | 118.90 |
| 1 | 1 | 1356 | U | C2-N1-C1' | -5.17 | 111.49 | 117.70 |
| 45 | 6 | 1600 | A | OP1-P-O3' | 5.17 | 116.58 | 105.20 |
| 26 | N5 | 34 | LEU | CA-CB-CG | 5.16 | 127.18 | 115.30 |
| 45 | 2 | 1568 | C | P-O3'-C3' | 5.16 | 125.90 | 119.70 |
| 45 | 6 | 695 | U | N3-C2-O2 | -5.16 | 118.58 | 122.20 |
| 45 | 6 | 792 | U | C2-N1-C1' | 5.16 | 123.89 | 117.70 |
| 1 | 1 | 639 | G | N1-C6-O6 | 5.16 | 122.99 | 119.90 |
| 3 | 8 | 79 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 1 | 1 | 2611 | U | N3-C4-O4 | -5.15 | 115.79 | 119.40 |
| 3 | 8 | 80 | A | O4'-C1'-N9 | -5.14 | 104.08 | 108.20 |
| 1 | 1 | 1355 | A | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 1 | 1 | 878 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |
| 1 | 1 | 1446 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 45 | 6 | 1097 | U | OP2-P-O3' | 5.14 | 116.50 | 105.20 |
| 1 | 1 | 3306 | U | N3-C2-O2 | -5.13 | 118.61 | 122.20 |
| 1 | 1 | 1201 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 1 | 5 | 1442 | U | C6-N1-C2 | 5.12 | 124.07 | 121.00 |
| 45 | 6 | 75 | U | C2-N1-C1' | 5.12 | 123.84 | 117.70 |
| 1 | 1 | 2169 | G | C2-N3-C4 | 5.12 | 114.46 | 111.90 |
| 1 | 1 | 2978 | U | O4'-C1'-N1 | 5.12 | 112.29 | 108.20 |
| 1 | 1 | 659 | G | C8-N9-C4 | 5.11 | 108.44 | 106.40 |
| 3 | 8 | 83 | C | OP2-P-O3' | 5.11 | 116.44 | 105.20 |
| 1 | 5 | 3362 | A | C8-N9-C4 | -5.11 | 103.76 | 105.80 |
| 63 | C7 | 86 | PRO | N-CA-C | 5.11 | 125.37 | 112.10 |
| 1 | 1 | 647 | A | N1-C6-N6 | 5.10 | 121.66 | 118.60 |
| 1 | 1 | 1095 | U | OP2-P-O3' | 5.10 | 116.42 | 105.20 |
| 1 | 1 | 1650 | G | N1-C6-O6 | 5.10 | 122.96 | 119.90 |
| 1 | 1 | 2938 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 45 | 2 | 639 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 1 | 1 | 1716 | U | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 1 | 5 | 1761 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 45 | 6 | 695 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 1 | 1 | 1141 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 5 | 3154 | C | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 1 | 1 | 1137 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 1 | 1 | 2737 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 63 | C7 | 85 | VAL | C-N-CA | 5.08 | 143.35 | 122.00 |
| 1 | 5 | 1480 | G | C8-N9-C4 | 5.08 | 108.43 | 106.40 |
| 1 | 1 | 2363 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 1 | 1 | 1495 | U | C2-N1-C1' | -5.07 | 111.62 | 117.70 |
| 1 | 5 | 1152 | G | C2-N3-C4 | -5.07 | 109.37 | 111.90 |
| 1 | 5 | 208 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 45 | 6 | 1751 | C | C6-N1-C2 | 5.06 | 122.33 | 120.30 |
| 20 | M9 | 99 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 45 | 2 | 831 | U | C5-C6-N1 | 5.05 | 125.23 | 122.70 |
| 1 | 5 | 386 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 35 | O4 | 51 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 45 | 2 | 130 | C | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 62 | C6 | 40 | GLU | C-N-CD | -5.05 | 109.50 | 120.60 |
| 1 | 5 | 1481 | A | C4-C5-C6 | 5.05 | 119.52 | 117.00 |
| 1 | 1 | 908 | G | C8-N9-C1' | -5.05 | 120.44 | 127.00 |
| 45 | 2 | 1150 | G | N3-C4-N9 | -5.04 | 122.97 | 126.00 |
| 1 | 1 | 1429 | G | C8-N9-C4 | 5.03 | 108.41 | 106.40 |
| 1 | 5 | 1072 | G | C6-C5-N7 | -5.03 | 127.38 | 130.40 |
| 1 | 5 | 1838 | G | N7-C8-N9 | -5.03 | 110.58 | 113.10 |
| 1 | 5 | 437 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 1 | 1 | 1604 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 1 | 1 | 1445 | U | N1-C2-O2 | -5.03 | 119.28 | 122.80 |
| 45 | 6 | 1389 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 1 | 1 | 1481 | A | P-O3'-C3' | 5.02 | 125.73 | 119.70 |
| 1 | 1 | 1650 | G | C5-C6-O6 | -5.02 | 125.59 | 128.60 |
| 1 | 5 | 2772 | C | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 1 | 1 | 2608 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 1 | 5 | 2403 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 1 | 1 | 621 | A | C8-N9-C1' | 5.01 | 136.72 | 127.70 |
| 1 | 1 | 2750 | U | C5-C6-N1 | -5.01 | 120.19 | 122.70 |
| 45 | 2 | 136 | C | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 1 | 1 | 869 | G | C6-C5-N7 | -5.01 | 127.40 | 130.40 |
| 1 | 1 | 2112 | U | P-O3'-C3' | 5.00 | 125.71 | 119.70 |
| 1 | 1 | 2595 | A | C2-N3-C4 | -5.00 | 108.10 | 110.60 |
| 45 | 2 | 1241 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |

There are no chirality outliers.

All (92) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 58 | C2 | 39 | ASP | Peptide |
| 60 | C4 | 123 | SER | Peptide |
| 60 | C4 | 74 | VAL | Peptide |
| 60 | C4 | 90 | ARG | Peptide |
| 62 | C6 | 40 | GLU | Peptide |
| 63 | C7 | 20 | TYR | Peptide |
| 63 | C7 | 85 | VAL | Peptide |
| 65 | C9 | 28 | LEU | Peptide |
| 66 | D0 | 48 | HIS | Peptide |
| 66 | D0 | 73 | GLY | Peptide |
| 68 | D2 | 54 | ASP | Peptide |
| 68 | D2 | 67 | GLY | Peptide |
| 68 | D2 | 83 | ILE | Peptide |
| 71 | D5 | 94 | LYS | Peptide |
| 72 | D6 | 10 | ARG | Peptide |
| 72 | D6 | 34 | LYS | Peptide |
| 72 | D6 | 97 | PRO | Peptide |
| 73 | D7 | 58 | SER | Peptide |
| 75 | D9 | 5 | ASN | Peptide |
| 75 | D9 | 6 | VAL | Peptide |
| 6 | L4 | 196 | ASN | Peptide |
| 7 | L5 | 124 | GLU | Peptide |
| 7 | L5 | 251 | PRO | Peptide |
| 7 | L5 | 258 | LYS | Peptide |
| 7 | L5 | 7 | ALA | Peptide |
| 7 | L5 | 8 | LYS | Peptide |
| 10 | L8 | 24 | ASN | Peptide |
| 10 | L8 | 30 | THR | Peptide |
| 10 | L8 | 76 | ALA | Peptide |
| 13 | M1 | 63 | GLU | Peptide |
| 14 | M3 | 86 | THR | Peptide |
| 16 | M5 | 74 | PRO | Peptide |
| 20 | M9 | 131 | ALA | Peptide |
| 21 | N0 | 166 | LYS | Peptide |
| 21 | N0 | 22 | PRO | Peptide |
| 21 | N0 | 69 | PRO | Peptide |
| 23 | N2 | 26 | GLY | Peptide |
| 23 | N2 | 90 | ARG | Peptide |
| 30 | N9 | 20 | GLY | Peptide |
| 31 | O0 | 36 | GLN | Peptide |
| 33 | O2 | 122 | PRO | Peptide |
| 43 | Q2 | 99 | GLN | Peptide |
| 47 | S1 | 157 | GLN | Peptide |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 47 | S1 | 23 | PRO | Peptide |
| 48 | S2 | 106 | ASP | Peptide |
| 51 | S5 | 44 | ASN | Peptide |
| 53 | S7 | 107 | ARG | Peptide |
| 53 | S7 | 131 | PHE | Peptide |
| 54 | S8 | 147 | ALA | Peptide |
| 78 | SM | 50 | ASN | Peptide |
| 77 | SR | 163 | ASP | Peptide |
| 77 | SR | 193 | ILE | Peptide |
| 57 | c1 | 120 | GLY | Peptide |
| 58 | c2 | 109 | GLU | Peptide |
| 58 | c2 | 130 | THR | Peptide |
| 61 | c5 | 51 | SER | Peptide |
| 62 | c6 | 40 | GLU | Peptide |
| 63 | c7 | 83 | GLN | Peptide |
| 70 | d4 | 29 | HIS | Peptide |
| 70 | d4 | 35 | VAL | Peptide |
| 70 | d4 | 50 | ALA | Peptide |
| 75 | d9 | 6 | VAL | Peptide |
| 4 | l2 | 215 | ASN | Peptide |
| 10 | l8 | 222 | PHE | Peptide |
| 10 | l8 | 24 | ASN | Peptide |
| 10 | l8 | 25 | PRO | Peptide |
| 13 | m1 | 151 | SER | Peptide |
| 15 | m4 | 48 | GLY | Peptide |
| 21 | n0 | 170 | THR | Peptide |
| 21 | n0 | 3 | HIS | Peptide |
| 26 | n5 | 47 | ALA | Peptide |
| 28 | n7 | 132 | SER | Peptide |
| 29 | n8 | 110 | GLY | Peptide |
| 30 | n9 | 19 | ASN | Peptide |
| 33 | o2 | 15 | LYS | Peptide |
| 35 | o4 | 47 | CYS | Peptide |
| 38 | o7 | 76 | ASN | Peptide |
| 48 | s2 | 106 | ASP | Peptide |
| 48 | s2 | 236 | PRO | Peptide |
| 49 | s3 | 219 | ALA | Peptide |
| 51 | s5 | 44 | ASN | Peptide |
| 53 | s7 | 10 | SER | Peptide |
| 53 | s7 | 11 | GLN | Peptide |
| 53 | s7 | 130 | VAL | Peptide |
| 53 | s7 | 29 | ASN | Peptide |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 53 | s7 | 64 | VAL | Peptide |
| 55 | s9 | 132 | ARG | Peptide |
| 55 | s9 | 133 | HIS | Peptide |
| 55 | s9 | 134 | ILE | Peptide |
| 55 | s9 | 89 | ASP | Peptide |
| 78 | sM | 64 | LYS | Peptide |
| 77 | sR | 146 | GLY | Peptide |

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | L2 | 246/248 (99%) | 236 (96%) | 10 (4%) | 0 | 100 | 100 |
| 4 | l2 | 246/248 (99%) | 229 (93%) | 16 (6%) | 1 (0%) | 34 | 66 |
| 5 | L3 | 384/386 (100%) | 355 (92%) | 27 (7%) | 2 (0%) | 29 | 61 |
| 5 | l3 | 384/386 (100%) | 359 (94%) | 25 (6%) | 0 | 100 | 100 |
| 6 | L4 | 359/361 (99%) | 334 (93%) | 24 (7%) | 1 (0%) | 41 | 71 |
| 6 | l4 | 359/361 (99%) | 318 (89%) | 39 (11%) | 2 (1%) | 25 | 57 |
| 7 | L5 | 291/296 (98%) | 260 (89%) | 29 (10%) | 2 (1%) | 22 | 54 |
| 7 | l5 | 292/296 (99%) | 261 (89%) | 30 (10%) | 1 (0%) | 41 | 71 |
| 8 | L6 | 152/176 (86%) | 142 (93%) | 8 (5%) | 2 (1%) | 12 | 40 |
| 8 | l6 | 153/176 (87%) | 136 (89%) | 16 (10%) | 1 (1%) | 22 | 54 |
| 9 | L7 | 224/226 (99%) | 206 (92%) | 17 (8%) | 1 (0%) | 34 | 66 |
| 9 | l7 | 221/226 (98%) | 202 (91%) | 18 (8%) | 1 (0%) | 29 | 61 |
| 10 | L8 | 229/231 (99%) | 199 (87%) | 27 (12%) | 3 (1%) | 12 | 40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 10 | l8 | 229/231 (99%) | 190 (83%) | 35 (15%) | 4 (2%) | 9 35 |
| 11 | L9 | 187/191 (98%) | 167 (89%) | 19 (10%) | 1 (0%) | 29 61 |
| 11 | l9 | 189/191 (99%) | 176 (93%) | 11 (6%) | 2 (1%) | 14 45 |
| 12 | M0 | 215/221 (97%) | 196 (91%) | 18 (8%) | 1 (0%) | 29 61 |
| 12 | m0 | 217/221 (98%) | 200 (92%) | 17 (8%) | 0 | 100 100 |
| 13 | M1 | 167/169 (99%) | 146 (87%) | 18 (11%) | 3 (2%) | 8 35 |
| 13 | m1 | 167/169 (99%) | 140 (84%) | 25 (15%) | 2 (1%) | 13 42 |
| 14 | M3 | 191/194 (98%) | 171 (90%) | 19 (10%) | 1 (0%) | 29 61 |
| 14 | m3 | 192/194 (99%) | 157 (82%) | 34 (18%) | 1 (0%) | 29 61 |
| 15 | M4 | 134/137 (98%) | 121 (90%) | 12 (9%) | 1 (1%) | 22 54 |
| 15 | m4 | 135/137 (98%) | 126 (93%) | 9 (7%) | 0 | 100 100 |
| 16 | M5 | 201/203 (99%) | 190 (94%) | 11 (6%) | 0 | 100 100 |
| 16 | m5 | 201/203 (99%) | 184 (92%) | 16 (8%) | 1 (0%) | 29 61 |
| 17 | M6 | 195/197 (99%) | 187 (96%) | 8 (4%) | 0 | 100 100 |
| 17 | m6 | 195/197 (99%) | 183 (94%) | 11 (6%) | 1 (0%) | 29 61 |
| 18 | M7 | 171/184 (93%) | 164 (96%) | 7 (4%) | 0 | 100 100 |
| 18 | m7 | 153/184 (83%) | 142 (93%) | 11 (7%) | 0 | 100 100 |
| 19 | M8 | 183/185 (99%) | 169 (92%) | 13 (7%) | 1 (0%) | 29 61 |
| 19 | m8 | 183/185 (99%) | 166 (91%) | 15 (8%) | 2 (1%) | 14 45 |
| 20 | M9 | 183/188 (97%) | 162 (88%) | 21 (12%) | 0 | 100 100 |
| 20 | m9 | 186/188 (99%) | 173 (93%) | 13 (7%) | 0 | 100 100 |
| 21 | N0 | 170/172 (99%) | 151 (89%) | 18 (11%) | 1 (1%) | 25 57 |
| 21 | n0 | 170/172 (99%) | 161 (95%) | 9 (5%) | 0 | 100 100 |
| 22 | N1 | 157/159 (99%) | 139 (88%) | 16 (10%) | 2 (1%) | 12 40 |
| 22 | n1 | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 57 |
| 23 | N2 | 97/99 (98%) | 88 (91%) | 7 (7%) | 2 (2%) | 7 31 |
| 23 | n2 | 96/99 (97%) | 86 (90%) | 10 (10%) | 0 | 100 100 |
| 24 | N3 | 130/136 (96%) | 124 (95%) | 6 (5%) | 0 | 100 100 |
| 24 | n3 | 134/136 (98%) | 132 (98%) | 2 (2%) | 0 | 100 100 |
| 25 | N4 | 61/155 (39%) | 56 (92%) | 5 (8%) | 0 | 100 100 |
| 25 | n4 | 133/155 (86%) | 121 (91%) | 10 (8%) | 2 (2%) | 10 38 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 26 | N5 | 116/120 (97%) | 104 (90%) | 11 (10%) | 1 (1%) | 17 48 |
| 26 | n5 | 118/120 (98%) | 105 (89%) | 11 (9%) | 2 (2%) | 9 35 |
| 27 | N6 | 123/125 (98%) | 119 (97%) | 4 (3%) | 0 | 100 100 |
| 27 | n6 | 121/125 (97%) | 114 (94%) | 7 (6%) | 0 | 100 100 |
| 28 | N7 | 133/135 (98%) | 118 (89%) | 15 (11%) | 0 | 100 100 |
| 28 | n7 | 133/135 (98%) | 117 (88%) | 15 (11%) | 1 (1%) | 19 51 |
| 29 | N8 | 146/148 (99%) | 133 (91%) | 12 (8%) | 1 (1%) | 22 54 |
| 29 | n8 | 146/148 (99%) | 128 (88%) | 18 (12%) | 0 | 100 100 |
| 30 | N9 | 54/58 (93%) | 46 (85%) | 8 (15%) | 0 | 100 100 |
| 30 | n9 | 56/58 (97%) | 47 (84%) | 8 (14%) | 1 (2%) | 8 35 |
| 31 | O0 | 95/100 (95%) | 91 (96%) | 3 (3%) | 1 (1%) | 14 45 |
| 31 | o0 | 98/100 (98%) | 86 (88%) | 11 (11%) | 1 (1%) | 15 46 |
| 32 | O1 | 102/112 (91%) | 98 (96%) | 3 (3%) | 1 (1%) | 15 46 |
| 32 | o1 | 107/112 (96%) | 96 (90%) | 11 (10%) | 0 | 100 100 |
| 33 | O2 | 123/127 (97%) | 114 (93%) | 8 (6%) | 1 (1%) | 19 51 |
| 33 | o2 | 125/127 (98%) | 117 (94%) | 8 (6%) | 0 | 100 100 |
| 34 | O3 | 104/106 (98%) | 98 (94%) | 6 (6%) | 0 | 100 100 |
| 34 | o3 | 104/106 (98%) | 98 (94%) | 6 (6%) | 0 | 100 100 |
| 35 | O4 | 110/112 (98%) | 101 (92%) | 9 (8%) | 0 | 100 100 |
| 35 | o4 | 110/112 (98%) | 99 (90%) | 10 (9%) | 1 (1%) | 17 48 |
| 36 | O5 | 117/119 (98%) | 107 (92%) | 9 (8%) | 1 (1%) | 17 48 |
| 36 | o5 | 117/119 (98%) | 103 (88%) | 14 (12%) | 0 | 100 100 |
| 37 | O6 | 95/99 (96%) | 83 (87%) | 11 (12%) | 1 (1%) | 14 45 |
| 37 | o6 | 97/99 (98%) | 83 (86%) | 14 (14%) | 0 | 100 100 |
| 38 | O7 | 82/87 (94%) | 78 (95%) | 4 (5%) | 0 | 100 100 |
| 38 | o7 | 85/87 (98%) | 78 (92%) | 7 (8%) | 0 | 100 100 |
| 39 | O8 | 75/77 (97%) | 66 (88%) | 9 (12%) | 0 | 100 100 |
| 39 | o8 | 75/77 (97%) | 63 (84%) | 12 (16%) | 0 | 100 100 |
| 40 | O9 | 48/50 (96%) | 44 (92%) | 4 (8%) | 0 | 100 100 |
| 40 | o9 | 48/50 (96%) | 43 (90%) | 5 (10%) | 0 | 100 100 |
| 41 | Q0 | 50/52 (96%) | 45 (90%) | 5 (10%) | 0 | 100 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 41 | q0 | 50/52 (96%) | 47 (94%) | 2 (4%) | 1 (2%) | 7 32 |
| 42 | Q1 | 23/25 (92%) | 21 (91%) | 2 (9%) | 0 | 100 100 |
| 42 | q1 | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 100 |
| 43 | Q2 | 103/105 (98%) | 88 (85%) | 15 (15%) | 0 | 100 100 |
| 43 | q2 | 103/105 (98%) | 96 (93%) | 7 (7%) | 0 | 100 100 |
| 44 | Q3 | 89/91 (98%) | 80 (90%) | 9 (10%) | 0 | 100 100 |
| 44 | q3 | 89/91 (98%) | 80 (90%) | 9 (10%) | 0 | 100 100 |
| 46 | S0 | 204/206 (99%) | 179 (88%) | 22 (11%) | 3 (2%) | 10 38 |
| 46 | s0 | 204/206 (99%) | 177 (87%) | 26 (13%) | 1 (0%) | 29 61 |
| 47 | S1 | 209/216 (97%) | 161 (77%) | 40 (19%) | 8 (4%) | 3 19 |
| 47 | s1 | 214/216 (99%) | 186 (87%) | 26 (12%) | 2 (1%) | 17 48 |
| 48 | S2 | 215/217 (99%) | 194 (90%) | 19 (9%) | 2 (1%) | 17 48 |
| 48 | s2 | 215/217 (99%) | 187 (87%) | 28 (13%) | 0 | 100 100 |
| 49 | S3 | 207/223 (93%) | 188 (91%) | 19 (9%) | 0 | 100 100 |
| 49 | s3 | 221/223 (99%) | 187 (85%) | 33 (15%) | 1 (0%) | 29 61 |
| 50 | S4 | 252/260 (97%) | 219 (87%) | 31 (12%) | 2 (1%) | 19 51 |
| 50 | s4 | 258/260 (99%) | 224 (87%) | 34 (13%) | 0 | 100 100 |
| 51 | S5 | 204/206 (99%) | 173 (85%) | 29 (14%) | 2 (1%) | 15 46 |
| 51 | s5 | 204/206 (99%) | 177 (87%) | 25 (12%) | 2 (1%) | 15 46 |
| 52 | S6 | 194/236 (82%) | 174 (90%) | 20 (10%) | 0 | 100 100 |
| 53 | S7 | 175/186 (94%) | 138 (79%) | 35 (20%) | 2 (1%) | 14 45 |
| 53 | s7 | 184/186 (99%) | 155 (84%) | 28 (15%) | 1 (0%) | 29 61 |
| 54 | S8 | 181/200 (90%) | 157 (87%) | 22 (12%) | 2 (1%) | 14 45 |
| 54 | s8 | 184/200 (92%) | 162 (88%) | 21 (11%) | 1 (0%) | 29 61 |
| 55 | S9 | 172/185 (93%) | 140 (81%) | 31 (18%) | 1 (1%) | 25 57 |
| 55 | s9 | 183/185 (99%) | 165 (90%) | 18 (10%) | 0 | 100 100 |
| 56 | C0 | 88/105 (84%) | 73 (83%) | 14 (16%) | 1 (1%) | 14 45 |
| 56 | c0 | 92/105 (88%) | 65 (71%) | 19 (21%) | 8 (9%) | 1 5 |
| 57 | C1 | 137/146 (94%) | 126 (92%) | 10 (7%) | 1 (1%) | 22 54 |
| 57 | c1 | 144/146 (99%) | 130 (90%) | 12 (8%) | 2 (1%) | 11 38 |
| 58 | C2 | 98/143 (68%) | 70 (71%) | 25 (26%) | 3 (3%) | 4 23 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 58 | c2 | 122/143 (85%) | 91 (75%) | 28 (23%) | 3 (2%) | 5 27 |
| 59 | C3 | 148/150 (99%) | 129 (87%) | 18 (12%) | 1 (1%) | 22 54 |
| 59 | c3 | 148/150 (99%) | 130 (88%) | 15 (10%) | 3 (2%) | 7 32 |
| 60 | C4 | 125/128 (98%) | 98 (78%) | 25 (20%) | 2 (2%) | 9 36 |
| 60 | c4 | 126/128 (98%) | 108 (86%) | 17 (14%) | 1 (1%) | 19 51 |
| 61 | C5 | 114/141 (81%) | 101 (89%) | 13 (11%) | 0 | 100 100 |
| 61 | c5 | 133/141 (94%) | 100 (75%) | 29 (22%) | 4 (3%) | 4 24 |
| 62 | C6 | 134/142 (94%) | 114 (85%) | 19 (14%) | 1 (1%) | 22 54 |
| 62 | c6 | 140/142 (99%) | 132 (94%) | 8 (6%) | 0 | 100 100 |
| 63 | C7 | 111/136 (82%) | 94 (85%) | 14 (13%) | 3 (3%) | 5 26 |
| 63 | c7 | 113/136 (83%) | 95 (84%) | 12 (11%) | 6 (5%) | 2 12 |
| 64 | C8 | 141/145 (97%) | 111 (79%) | 28 (20%) | 2 (1%) | 11 38 |
| 64 | c8 | 143/145 (99%) | 126 (88%) | 15 (10%) | 2 (1%) | 11 38 |
| 65 | C9 | 135/143 (94%) | 120 (89%) | 14 (10%) | 1 (1%) | 22 54 |
| 65 | c9 | 141/143 (99%) | 125 (89%) | 15 (11%) | 1 (1%) | 22 54 |
| 66 | D0 | 100/109 (92%) | 90 (90%) | 10 (10%) | 0 | 100 100 |
| 66 | d0 | 107/109 (98%) | 95 (89%) | 11 (10%) | 1 (1%) | 17 48 |
| 67 | D1 | 85/87 (98%) | 67 (79%) | 15 (18%) | 3 (4%) | 3 21 |
| 67 | d1 | 85/87 (98%) | 74 (87%) | 10 (12%) | 1 (1%) | 13 42 |
| 68 | D2 | 127/129 (98%) | 111 (87%) | 14 (11%) | 2 (2%) | 9 36 |
| 68 | d2 | 127/129 (98%) | 113 (89%) | 13 (10%) | 1 (1%) | 19 51 |
| 69 | D3 | 142/144 (99%) | 120 (84%) | 21 (15%) | 1 (1%) | 22 54 |
| 69 | d3 | 142/144 (99%) | 125 (88%) | 17 (12%) | 0 | 100 100 |
| 70 | D4 | 132/134 (98%) | 117 (89%) | 13 (10%) | 2 (2%) | 10 38 |
| 70 | d4 | 132/134 (98%) | 118 (89%) | 14 (11%) | 0 | 100 100 |
| 71 | D5 | 68/70 (97%) | 54 (79%) | 11 (16%) | 3 (4%) | 2 16 |
| 71 | d5 | 67/70 (96%) | 56 (84%) | 11 (16%) | 0 | 100 100 |
| 72 | D6 | 95/97 (98%) | 69 (73%) | 22 (23%) | 4 (4%) | 3 17 |
| 72 | d6 | 95/97 (98%) | 75 (79%) | 18 (19%) | 2 (2%) | 7 31 |
| 73 | D7 | 79/81 (98%) | 71 (90%) | 8 (10%) | 0 | 100 100 |
| 73 | d7 | 79/81 (98%) | 72 (91%) | 7 (9%) | 0 | 100 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 74 | D8 | 61/63 (97%) | 51 (84%) | 10 (16%) | 0 | 100 100 |
| 74 | d8 | 61/63 (97%) | 48 (79%) | 12 (20%) | 1 (2%) | 9 36 |
| 75 | D9 | 51/53 (96%) | 43 (84%) | 7 (14%) | 1 (2%) | 7 32 |
| 75 | d9 | 51/53 (96%) | 43 (84%) | 8 (16%) | 0 | 100 100 |
| 76 | E0 | 58/62 (94%) | 50 (86%) | 7 (12%) | 1 (2%) | 9 35 |
| 76 | e0 | 60/62 (97%) | 51 (85%) | 7 (12%) | 2 (3%) | 4 22 |
| 77 | SR | 315/318 (99%) | 274 (87%) | 41 (13%) | 0 | 100 100 |
| 77 | sR | 316/318 (99%) | 278 (88%) | 37 (12%) | 1 (0%) | 41 71 |
| 78 | SM | 143/272 (53%) | 117 (82%) | 25 (18%) | 1 (1%) | 22 54 |
| 78 | sM | 89/272 (33%) | 73 (82%) | 15 (17%) | 1 (1%) | 14 45 |
| 79 | s6 | 216/218 (99%) | 183 (85%) | 30 (14%) | 3 (1%) | 11 38 |
| All | All | 21808/22972 (95%) | 19331 (89%) | 2311 (11%) | 166 (1%) | 19 51 |

All (166) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | L6 | 98 | VAL |
| 10 | L8 | 36 | ILE |
| 10 | L8 | 116 | VAL |
| 11 | L9 | 50 | ASN |
| 33 | O2 | 123 | LYS |
| 51 | S5 | 64 | VAL |
| 56 | C0 | 88 | PRO |
| 57 | C1 | 7 | VAL |
| 63 | C7 | 85 | VAL |
| 68 | D2 | 83 | ILE |
| 71 | D5 | 88 | ILE |
| 8 | l6 | 98 | VAL |
| 10 | l8 | 203 | VAL |
| 19 | m8 | 124 | LEU |
| 26 | n5 | 47 | ALA |
| 30 | n9 | 21 | ILE |
| 31 | o0 | 100 | ILE |
| 56 | c0 | 83 | PRO |
| 56 | c0 | 88 | PRO |
| 56 | c0 | 97 | PRO |
| 57 | c1 | 7 | VAL |
| 59 | c3 | 66 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 63 | c7 | 97 | ASN |
| 63 | c7 | 99 | VAL |
| 65 | c9 | 34 | VAL |
| 76 | e0 | 45 | VAL |
| 5 | L3 | 140 | ASP |
| 6 | L4 | 195 | ARG |
| 13 | M1 | 114 | ILE |
| 23 | N2 | 11 | ILE |
| 23 | N2 | 88 | GLN |
| 58 | C2 | 89 | ILE |
| 60 | C4 | 42 | VAL |
| 63 | C7 | 84 | TYR |
| 71 | D5 | 41 | ILE |
| 72 | D6 | 75 | VAL |
| 25 | n4 | 63 | ILE |
| 25 | n4 | 76 | VAL |
| 35 | o4 | 48 | GLY |
| 46 | s0 | 189 | VAL |
| 51 | s5 | 36 | ALA |
| 53 | s7 | 109 | VAL |
| 56 | c0 | 78 | GLU |
| 56 | c0 | 82 | LEU |
| 56 | c0 | 92 | ILE |
| 63 | c7 | 117 | LEU |
| 63 | c7 | 118 | PRO |
| 66 | d0 | 18 | GLN |
| 68 | d2 | 6 | VAL |
| 74 | d8 | 7 | VAL |
| 12 | M0 | 24 | ARG |
| 13 | M1 | 56 | THR |
| 13 | M1 | 173 | ASP |
| 31 | O0 | 37 | GLY |
| 36 | O5 | 98 | SER |
| 47 | S1 | 49 | ASN |
| 47 | S1 | 62 | LYS |
| 63 | C7 | 88 | VAL |
| 67 | D1 | 29 | HIS |
| 68 | D2 | 31 | SER |
| 71 | D5 | 71 | ILE |
| 72 | D6 | 58 | VAL |
| 14 | m3 | 47 | ALA |
| 49 | s3 | 217 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 56 | c0 | 96 | ASN |
| 61 | c5 | 12 | PHE |
| 61 | c5 | 50 | THR |
| 67 | d1 | 29 | HIS |
| 14 | M3 | 47 | ALA |
| 15 | M4 | 8 | LYS |
| 19 | M8 | 99 | THR |
| 22 | N1 | 22 | HIS |
| 22 | N1 | 124 | VAL |
| 29 | N8 | 48 | TYR |
| 46 | S0 | 68 | PRO |
| 47 | S1 | 130 | SER |
| 51 | S5 | 51 | VAL |
| 54 | S8 | 152 | ILE |
| 70 | D4 | 5 | VAL |
| 9 | l7 | 191 | VAL |
| 13 | m1 | 11 | ASP |
| 16 | m5 | 149 | ASN |
| 19 | m8 | 99 | THR |
| 58 | c2 | 91 | VAL |
| 58 | c2 | 106 | ILE |
| 58 | c2 | 131 | ASP |
| 63 | c7 | 104 | ASN |
| 64 | c8 | 92 | ILE |
| 72 | d6 | 61 | GLU |
| 7 | L5 | 9 | SER |
| 8 | L6 | 97 | ASN |
| 26 | N5 | 50 | ALA |
| 47 | S1 | 56 | SER |
| 47 | S1 | 94 | LYS |
| 48 | S2 | 144 | TRP |
| 54 | S8 | 148 | ALA |
| 58 | C2 | 69 | ALA |
| 72 | D6 | 64 | LEU |
| 10 | l8 | 117 | ALA |
| 13 | m1 | 114 | ILE |
| 22 | n1 | 83 | ARG |
| 59 | c3 | 22 | ALA |
| 59 | c3 | 87 | ASP |
| 60 | c4 | 133 | ARG |
| 61 | c5 | 130 | ARG |
| 47 | S1 | 68 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | S2 | 126 | ARG |
| 50 | S4 | 179 | LYS |
| 65 | C9 | 53 | TRP |
| 72 | D6 | 65 | PRO |
| 4 | l2 | 49 | VAL |
| 6 | l4 | 144 | LYS |
| 7 | l5 | 125 | VAL |
| 10 | l8 | 240 | ASN |
| 26 | n5 | 62 | VAL |
| 28 | n7 | 103 | GLN |
| 51 | s5 | 35 | GLN |
| 76 | e0 | 50 | VAL |
| 77 | sR | 308 | ASN |
| 78 | sM | 51 | ARG |
| 10 | L8 | 157 | VAL |
| 46 | S0 | 158 | VAL |
| 50 | S4 | 195 | ILE |
| 58 | C2 | 91 | VAL |
| 75 | D9 | 11 | PRO |
| 6 | l4 | 145 | ILE |
| 11 | l9 | 144 | ILE |
| 21 | N0 | 167 | ARG |
| 32 | O1 | 7 | VAL |
| 37 | O6 | 3 | VAL |
| 47 | S1 | 66 | VAL |
| 67 | D1 | 6 | GLY |
| 67 | D1 | 32 | VAL |
| 47 | s1 | 225 | VAL |
| 79 | s6 | 69 | LEU |
| 56 | c0 | 35 | ILE |
| 61 | c5 | 5 | VAL |
| 9 | L7 | 178 | ILE |
| 47 | S1 | 210 | ILE |
| 53 | S7 | 98 | ILE |
| 59 | C3 | 22 | ALA |
| 64 | C8 | 14 | ILE |
| 76 | E0 | 47 | VAL |
| 10 | l8 | 237 | ILE |
| 41 | q0 | 78 | ILE |
| 47 | s1 | 22 | ASP |
| 79 | s6 | 153 | VAL |
| 54 | s8 | 78 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 57 | c1 | 129 | ARG |
| 64 | c8 | 14 | ILE |
| 5 | L3 | 317 | ILE |
| 46 | S0 | 103 | THR |
| 60 | C4 | 39 | ILE |
| 62 | C6 | 39 | VAL |
| 64 | C8 | 5 | VAL |
| 69 | D3 | 130 | VAL |
| 70 | D4 | 35 | VAL |
| 78 | SM | 12 | VAL |
| 11 | l9 | 167 | VAL |
| 79 | s6 | 162 | VAL |
| 72 | d6 | 58 | VAL |
| 7 | L5 | 125 | VAL |
| 53 | S7 | 181 | ILE |
| 55 | S9 | 134 | ILE |
| 17 | m6 | 4 | GLU |
| 63 | c7 | 98 | GLY |

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 4 | L2 | 190/190 (100%) | 169 (89%) | 21 (11%) | 6 23 |
| 4 | l2 | 190/190 (100%) | 174 (92%) | 16 (8%) | 11 35 |
| 5 | L3 | 322/322 (100%) | 280 (87%) | 42 (13%) | 4 17 |
| 5 | l3 | 322/322 (100%) | 287 (89%) | 35 (11%) | 6 24 |
| 6 | L4 | 288/288 (100%) | 258 (90%) | 30 (10%) | 7 25 |
| 6 | l4 | 288/288 (100%) | 253 (88%) | 35 (12%) | 5 20 |
| 7 | L5 | 242/244 (99%) | 220 (91%) | 22 (9%) | 9 31 |
| 7 | l5 | 243/244 (100%) | 223 (92%) | 20 (8%) | 11 36 |
| 8 | L6 | 134/153 (88%) | 118 (88%) | 16 (12%) | 5 21 |
| 8 | l6 | 135/153 (88%) | 123 (91%) | 12 (9%) | 9 32 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 9 | L7 | 190/190 (100%) | 169 (89%) | 21 (11%) | 6 23 |
| 9 | l7 | 187/190 (98%) | 164 (88%) | 23 (12%) | 4 20 |
| 10 | L8 | 186/190 (98%) | 169 (91%) | 17 (9%) | 9 31 |
| 10 | l8 | 177/190 (93%) | 155 (88%) | 22 (12%) | 4 19 |
| 11 | L9 | 169/171 (99%) | 143 (85%) | 26 (15%) | 2 12 |
| 11 | l9 | 171/171 (100%) | 144 (84%) | 27 (16%) | 2 11 |
| 12 | M0 | 185/187 (99%) | 163 (88%) | 22 (12%) | 5 21 |
| 12 | m0 | 186/187 (100%) | 162 (87%) | 24 (13%) | 4 18 |
| 13 | M1 | 147/147 (100%) | 127 (86%) | 20 (14%) | 3 16 |
| 13 | m1 | 147/147 (100%) | 125 (85%) | 22 (15%) | 3 13 |
| 14 | M3 | 154/154 (100%) | 139 (90%) | 15 (10%) | 8 29 |
| 14 | m3 | 154/154 (100%) | 140 (91%) | 14 (9%) | 9 31 |
| 15 | M4 | 107/108 (99%) | 99 (92%) | 8 (8%) | 13 39 |
| 15 | m4 | 108/108 (100%) | 95 (88%) | 13 (12%) | 5 20 |
| 16 | M5 | 175/175 (100%) | 164 (94%) | 11 (6%) | 18 47 |
| 16 | m5 | 175/175 (100%) | 162 (93%) | 13 (7%) | 13 40 |
| 17 | M6 | 160/160 (100%) | 147 (92%) | 13 (8%) | 11 36 |
| 17 | m6 | 160/160 (100%) | 150 (94%) | 10 (6%) | 18 47 |
| 18 | M7 | 139/146 (95%) | 120 (86%) | 19 (14%) | 3 16 |
| 18 | m7 | 125/146 (86%) | 110 (88%) | 15 (12%) | 5 20 |
| 19 | M8 | 150/150 (100%) | 134 (89%) | 16 (11%) | 6 25 |
| 19 | m8 | 150/150 (100%) | 135 (90%) | 15 (10%) | 7 27 |
| 20 | M9 | 151/153 (99%) | 135 (89%) | 16 (11%) | 6 25 |
| 20 | m9 | 153/153 (100%) | 136 (89%) | 17 (11%) | 6 23 |
| 21 | N0 | 156/156 (100%) | 134 (86%) | 22 (14%) | 3 16 |
| 21 | n0 | 156/156 (100%) | 136 (87%) | 20 (13%) | 4 18 |
| 22 | N1 | 136/136 (100%) | 116 (85%) | 20 (15%) | 3 14 |
| 22 | n1 | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 33 |
| 23 | N2 | 86/86 (100%) | 73 (85%) | 13 (15%) | 3 13 |
| 23 | n2 | 85/86 (99%) | 77 (91%) | 8 (9%) | 8 30 |
| 24 | N3 | 102/104 (98%) | 91 (89%) | 11 (11%) | 6 24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 24 | n3 | 104/104 (100%) | 94 (90%) | 10 (10%) | 8 29 |
| 25 | N4 | 55/129 (43%) | 54 (98%) | 1 (2%) | 59 78 |
| 25 | n4 | 100/129 (78%) | 93 (93%) | 7 (7%) | 15 43 |
| 26 | N5 | 103/104 (99%) | 88 (85%) | 15 (15%) | 3 14 |
| 26 | n5 | 104/104 (100%) | 92 (88%) | 12 (12%) | 5 22 |
| 27 | N6 | 108/108 (100%) | 100 (93%) | 8 (7%) | 13 40 |
| 27 | n6 | 106/108 (98%) | 98 (92%) | 8 (8%) | 13 39 |
| 28 | N7 | 115/115 (100%) | 103 (90%) | 12 (10%) | 7 25 |
| 28 | n7 | 115/115 (100%) | 108 (94%) | 7 (6%) | 18 48 |
| 29 | N8 | 118/118 (100%) | 102 (86%) | 16 (14%) | 3 16 |
| 29 | n8 | 118/118 (100%) | 108 (92%) | 10 (8%) | 10 35 |
| 30 | N9 | 44/46 (96%) | 40 (91%) | 4 (9%) | 9 31 |
| 30 | n9 | 46/46 (100%) | 41 (89%) | 5 (11%) | 6 24 |
| 31 | O0 | 81/84 (96%) | 72 (89%) | 9 (11%) | 6 23 |
| 31 | o0 | 84/84 (100%) | 75 (89%) | 9 (11%) | 6 25 |
| 32 | O1 | 89/96 (93%) | 81 (91%) | 8 (9%) | 9 32 |
| 32 | o1 | 94/96 (98%) | 84 (89%) | 10 (11%) | 6 25 |
| 33 | O2 | 108/109 (99%) | 94 (87%) | 14 (13%) | 4 17 |
| 33 | o2 | 109/109 (100%) | 101 (93%) | 8 (7%) | 14 41 |
| 34 | O3 | 90/90 (100%) | 83 (92%) | 7 (8%) | 12 38 |
| 34 | o3 | 90/90 (100%) | 85 (94%) | 5 (6%) | 21 52 |
| 35 | O4 | 95/95 (100%) | 88 (93%) | 7 (7%) | 13 40 |
| 35 | o4 | 95/95 (100%) | 88 (93%) | 7 (7%) | 13 40 |
| 36 | O5 | 104/104 (100%) | 96 (92%) | 8 (8%) | 13 38 |
| 36 | o5 | 103/104 (99%) | 98 (95%) | 5 (5%) | 25 56 |
| 37 | O6 | 79/81 (98%) | 74 (94%) | 5 (6%) | 18 47 |
| 37 | o6 | 81/81 (100%) | 73 (90%) | 8 (10%) | 8 28 |
| 38 | O7 | 69/70 (99%) | 60 (87%) | 9 (13%) | 4 17 |
| 38 | o7 | 70/70 (100%) | 63 (90%) | 7 (10%) | 7 27 |
| 39 | O8 | 68/68 (100%) | 63 (93%) | 5 (7%) | 13 40 |
| 39 | o8 | 67/68 (98%) | 56 (84%) | 11 (16%) | 2 10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 40 | O9 | 45/45 (100%) | 39 (87%) | 6 (13%) | 4 17 |
| 40 | o9 | 45/45 (100%) | 43 (96%) | 2 (4%) | 28 59 |
| 41 | Q0 | 47/47 (100%) | 45 (96%) | 2 (4%) | 29 59 |
| 41 | q0 | 47/47 (100%) | 41 (87%) | 6 (13%) | 4 18 |
| 42 | Q1 | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 8 |
| 42 | q1 | 23/23 (100%) | 17 (74%) | 6 (26%) | 0 2 |
| 43 | Q2 | 90/90 (100%) | 79 (88%) | 11 (12%) | 5 20 |
| 43 | q2 | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 23 |
| 44 | Q3 | 71/71 (100%) | 61 (86%) | 10 (14%) | 3 16 |
| 44 | q3 | 71/71 (100%) | 64 (90%) | 7 (10%) | 8 28 |
| 46 | S0 | 166/173 (96%) | 149 (90%) | 17 (10%) | 7 27 |
| 46 | s0 | 166/173 (96%) | 150 (90%) | 16 (10%) | 8 29 |
| 47 | S1 | 189/192 (98%) | 156 (82%) | 33 (18%) | 2 8 |
| 47 | s1 | 192/192 (100%) | 172 (90%) | 20 (10%) | 7 25 |
| 48 | S2 | 176/176 (100%) | 158 (90%) | 18 (10%) | 7 27 |
| 48 | s2 | 176/176 (100%) | 166 (94%) | 10 (6%) | 20 51 |
| 49 | S3 | 169/182 (93%) | 151 (89%) | 18 (11%) | 6 25 |
| 49 | s3 | 182/182 (100%) | 165 (91%) | 17 (9%) | 9 30 |
| 50 | S4 | 219/221 (99%) | 203 (93%) | 16 (7%) | 14 41 |
| 50 | s4 | 221/221 (100%) | 200 (90%) | 21 (10%) | 8 29 |
| 51 | S5 | 173/173 (100%) | 155 (90%) | 18 (10%) | 7 25 |
| 51 | s5 | 173/173 (100%) | 161 (93%) | 12 (7%) | 15 44 |
| 52 | S6 | 167/201 (83%) | 154 (92%) | 13 (8%) | 12 38 |
| 53 | S7 | 160/166 (96%) | 145 (91%) | 15 (9%) | 8 30 |
| 53 | s7 | 166/166 (100%) | 150 (90%) | 16 (10%) | 8 29 |
| 54 | S8 | 148/161 (92%) | 135 (91%) | 13 (9%) | 10 33 |
| 54 | s8 | 150/161 (93%) | 142 (95%) | 8 (5%) | 22 53 |
| 55 | S9 | 152/158 (96%) | 141 (93%) | 11 (7%) | 14 41 |
| 55 | s9 | 158/158 (100%) | 146 (92%) | 12 (8%) | 13 39 |
| 56 | C0 | 77/98 (79%) | 71 (92%) | 6 (8%) | 12 38 |
| 56 | c0 | 73/98 (74%) | 68 (93%) | 5 (7%) | 16 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 57 | C1 | 126/129 (98%) | 110 (87%) | 16 (13%) | 4 19 |
| 57 | c1 | 129/129 (100%) | 117 (91%) | 12 (9%) | 9 30 |
| 58 | C2 | 82/119 (69%) | 69 (84%) | 13 (16%) | 2 11 |
| 58 | c2 | 88/119 (74%) | 72 (82%) | 16 (18%) | 1 7 |
| 59 | C3 | 127/127 (100%) | 118 (93%) | 9 (7%) | 14 42 |
| 59 | c3 | 127/127 (100%) | 116 (91%) | 11 (9%) | 10 34 |
| 60 | C4 | 81/97 (84%) | 68 (84%) | 13 (16%) | 2 11 |
| 60 | c4 | 97/97 (100%) | 84 (87%) | 13 (13%) | 4 16 |
| 61 | C5 | 96/117 (82%) | 91 (95%) | 5 (5%) | 23 54 |
| 61 | c5 | 103/117 (88%) | 86 (84%) | 17 (16%) | 2 10 |
| 62 | C6 | 113/118 (96%) | 100 (88%) | 13 (12%) | 5 22 |
| 62 | c6 | 118/118 (100%) | 108 (92%) | 10 (8%) | 10 35 |
| 63 | C7 | 94/124 (76%) | 81 (86%) | 13 (14%) | 3 16 |
| 63 | c7 | 92/124 (74%) | 86 (94%) | 6 (6%) | 17 46 |
| 64 | C8 | 126/128 (98%) | 111 (88%) | 15 (12%) | 5 21 |
| 64 | c8 | 128/128 (100%) | 114 (89%) | 14 (11%) | 6 24 |
| 65 | C9 | 110/115 (96%) | 98 (89%) | 12 (11%) | 6 24 |
| 65 | c9 | 115/115 (100%) | 104 (90%) | 11 (10%) | 8 29 |
| 66 | D0 | 96/102 (94%) | 85 (88%) | 11 (12%) | 5 22 |
| 66 | d0 | 102/102 (100%) | 88 (86%) | 14 (14%) | 3 16 |
| 67 | D1 | 74/74 (100%) | 68 (92%) | 6 (8%) | 11 36 |
| 67 | d1 | 74/74 (100%) | 63 (85%) | 11 (15%) | 3 13 |
| 68 | D2 | 110/110 (100%) | 98 (89%) | 12 (11%) | 6 24 |
| 68 | d2 | 110/110 (100%) | 97 (88%) | 13 (12%) | 5 21 |
| 69 | D3 | 119/119 (100%) | 111 (93%) | 8 (7%) | 16 45 |
| 69 | d3 | 119/119 (100%) | 112 (94%) | 7 (6%) | 19 49 |
| 70 | D4 | 112/112 (100%) | 99 (88%) | 13 (12%) | 5 22 |
| 70 | d4 | 112/112 (100%) | 104 (93%) | 8 (7%) | 14 42 |
| 71 | D5 | 61/61 (100%) | 51 (84%) | 10 (16%) | 2 10 |
| 71 | d5 | 61/61 (100%) | 51 (84%) | 10 (16%) | 2 10 |
| 72 | D6 | 83/83 (100%) | 69 (83%) | 14 (17%) | 2 9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 72 | d6 | 83/83 (100%) | 73 (88%) | 10 (12%) | 5 20 |
| 73 | D7 | 70/70 (100%) | 63 (90%) | 7 (10%) | 7 27 |
| 73 | d7 | 70/70 (100%) | 64 (91%) | 6 (9%) | 10 35 |
| 74 | D8 | 56/56 (100%) | 51 (91%) | 5 (9%) | 9 32 |
| 74 | d8 | 56/56 (100%) | 50 (89%) | 6 (11%) | 6 25 |
| 75 | D9 | 47/47 (100%) | 44 (94%) | 3 (6%) | 17 46 |
| 75 | d9 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 13 |
| 76 | E0 | 51/53 (96%) | 42 (82%) | 9 (18%) | 2 8 |
| 76 | e0 | 53/53 (100%) | 46 (87%) | 7 (13%) | 4 17 |
| 77 | SR | 259/261 (99%) | 246 (95%) | 13 (5%) | 24 55 |
| 77 | sR | 259/261 (99%) | 238 (92%) | 21 (8%) | 11 36 |
| 78 | SM | 97/227 (43%) | 85 (88%) | 12 (12%) | 4 19 |
| 78 | sM | 54/227 (24%) | 50 (93%) | 4 (7%) | 13 40 |
| 79 | s6 | 187/187 (100%) | 168 (90%) | 19 (10%) | 7 27 |
| All | All | 18408/19292 (95%) | 16513 (90%) | 1895 (10%) | 7 26 |

All (1895) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | L2 | 20 | THR |
| 4 | L2 | 23 | ARG |
| 4 | L2 | 32 | LEU |
| 4 | L2 | 45 | VAL |
| 4 | L2 | 62 | VAL |
| 4 | L2 | 74 | GLU |
| 4 | L2 | 93 | LYS |
| 4 | L2 | 97 | ASN |
| 4 | L2 | 113 | VAL |
| 4 | L2 | 114 | SER |
| 4 | L2 | 116 | VAL |
| 4 | L2 | 142 | ASP |
| 4 | L2 | 159 | SER |
| 4 | L2 | 165 | VAL |
| 4 | L2 | 179 | LEU |
| 4 | L2 | 181 | LYS |
| 4 | L2 | 195 | SER |
| 4 | L2 | 204 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | L2 | 207 | VAL |
| 4 | L2 | 227 | ARG |
| 4 | L2 | 246 | LEU |
| 5 | L3 | 7 | GLU |
| 5 | L3 | 17 | LEU |
| 5 | L3 | 19 | ARG |
| 5 | L3 | 37 | ARG |
| 5 | L3 | 41 | VAL |
| 5 | L3 | 70 | ARG |
| 5 | L3 | 73 | VAL |
| 5 | L3 | 77 | THR |
| 5 | L3 | 81 | THR |
| 5 | L3 | 84 | VAL |
| 5 | L3 | 85 | VAL |
| 5 | L3 | 89 | VAL |
| 5 | L3 | 93 | VAL |
| 5 | L3 | 99 | LEU |
| 5 | L3 | 103 | THR |
| 5 | L3 | 139 | GLN |
| 5 | L3 | 140 | ASP |
| 5 | L3 | 154 | TYR |
| 5 | L3 | 160 | VAL |
| 5 | L3 | 169 | THR |
| 5 | L3 | 189 | SER |
| 5 | L3 | 196 | ARG |
| 5 | L3 | 202 | THR |
| 5 | L3 | 205 | VAL |
| 5 | L3 | 211 | GLN |
| 5 | L3 | 214 | MET |
| 5 | L3 | 236 | LYS |
| 5 | L3 | 238 | LEU |
| 5 | L3 | 246 | LEU |
| 5 | L3 | 252 | ILE |
| 5 | L3 | 260 | VAL |
| 5 | L3 | 284 | ARG |
| 5 | L3 | 290 | ASP |
| 5 | L3 | 291 | GLU |
| 5 | L3 | 293 | ASN |
| 5 | L3 | 324 | VAL |
| 5 | L3 | 332 | ARG |
| 5 | L3 | 343 | TYR |
| 5 | L3 | 348 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | L3 | 372 | THR |
| 5 | L3 | 375 | GLU |
| 5 | L3 | 385 | LYS |
| 6 | L4 | 54 | GLU |
| 6 | L4 | 73 | ARG |
| 6 | L4 | 74 | ILE |
| 6 | L4 | 93 | MET |
| 6 | L4 | 99 | MET |
| 6 | L4 | 112 | LYS |
| 6 | L4 | 120 | TYR |
| 6 | L4 | 133 | SER |
| 6 | L4 | 138 | ARG |
| 6 | L4 | 144 | LYS |
| 6 | L4 | 150 | LEU |
| 6 | L4 | 160 | GLN |
| 6 | L4 | 179 | LEU |
| 6 | L4 | 188 | ARG |
| 6 | L4 | 194 | TYR |
| 6 | L4 | 195 | ARG |
| 6 | L4 | 197 | ARG |
| 6 | L4 | 206 | LEU |
| 6 | L4 | 211 | GLU |
| 6 | L4 | 216 | VAL |
| 6 | L4 | 220 | ARG |
| 6 | L4 | 230 | VAL |
| 6 | L4 | 246 | ARG |
| 6 | L4 | 258 | LEU |
| 6 | L4 | 271 | LYS |
| 6 | L4 | 313 | LEU |
| 6 | L4 | 323 | VAL |
| 6 | L4 | 327 | LEU |
| 6 | L4 | 332 | LYS |
| 6 | L4 | 349 | THR |
| 7 | L5 | 13 | SER |
| 7 | L5 | 15 | ARG |
| 7 | L5 | 22 | ARG |
| 7 | L5 | 23 | ARG |
| 7 | L5 | 35 | ARG |
| 7 | L5 | 41 | LYS |
| 7 | L5 | 56 | THR |
| 7 | L5 | 81 | HIS |
| 7 | L5 | 92 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | L5 | 99 | TYR |
| 7 | L5 | 152 | ARG |
| 7 | L5 | 155 | THR |
| 7 | L5 | 158 | ARG |
| 7 | L5 | 185 | PHE |
| 7 | L5 | 187 | THR |
| 7 | L5 | 188 | GLU |
| 7 | L5 | 218 | ARG |
| 7 | L5 | 222 | LEU |
| 7 | L5 | 258 | LYS |
| 7 | L5 | 259 | LYS |
| 7 | L5 | 265 | TYR |
| 7 | L5 | 277 | LEU |
| 8 | L6 | 15 | VAL |
| 8 | L6 | 18 | LEU |
| 8 | L6 | 21 | THR |
| 8 | L6 | 30 | LEU |
| 8 | L6 | 52 | VAL |
| 8 | L6 | 64 | LEU |
| 8 | L6 | 84 | VAL |
| 8 | L6 | 89 | THR |
| 8 | L6 | 93 | VAL |
| 8 | L6 | 98 | VAL |
| 8 | L6 | 99 | GLU |
| 8 | L6 | 109 | GLU |
| 8 | L6 | 152 | THR |
| 8 | L6 | 154 | LEU |
| 8 | L6 | 156 | LYS |
| 8 | L6 | 175 | LYS |
| 9 | L7 | 21 | LYS |
| 9 | L7 | 30 | ARG |
| 9 | L7 | 52 | GLN |
| 9 | L7 | 59 | GLU |
| 9 | L7 | 60 | ARG |
| 9 | L7 | 80 | GLN |
| 9 | L7 | 84 | VAL |
| 9 | L7 | 87 | VAL |
| 9 | L7 | 93 | ASN |
| 9 | L7 | 98 | LYS |
| 9 | L7 | 140 | SER |
| 9 | L7 | 150 | LYS |
| 9 | L7 | 151 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | L7 | 157 | ASN |
| 9 | L7 | 158 | LYS |
| 9 | L7 | 173 | LEU |
| 9 | L7 | 176 | TYR |
| 9 | L7 | 179 | LEU |
| 9 | L7 | 200 | ASN |
| 9 | L7 | 234 | GLU |
| 9 | L7 | 239 | LEU |
| 10 | L8 | 27 | THR |
| 10 | L8 | 36 | ILE |
| 10 | L8 | 38 | GLN |
| 10 | L8 | 74 | THR |
| 10 | L8 | 79 | GLN |
| 10 | L8 | 124 | ASP |
| 10 | L8 | 136 | LEU |
| 10 | L8 | 157 | VAL |
| 10 | L8 | 169 | LEU |
| 10 | L8 | 172 | LYS |
| 10 | L8 | 180 | VAL |
| 10 | L8 | 181 | LYS |
| 10 | L8 | 185 | ARG |
| 10 | L8 | 227 | ASP |
| 10 | L8 | 230 | LYS |
| 10 | L8 | 245 | LYS |
| 10 | L8 | 249 | ARG |
| 11 | L9 | 16 | VAL |
| 11 | L9 | 18 | VAL |
| 11 | L9 | 42 | ASP |
| 11 | L9 | 44 | THR |
| 11 | L9 | 50 | ASN |
| 11 | L9 | 52 | LEU |
| 11 | L9 | 62 | ARG |
| 11 | L9 | 68 | LEU |
| 11 | L9 | 69 | ARG |
| 11 | L9 | 70 | THR |
| 11 | L9 | 80 | THR |
| 11 | L9 | 92 | TYR |
| 11 | L9 | 93 | VAL |
| 11 | L9 | 104 | VAL |
| 11 | L9 | 118 | LEU |
| 11 | L9 | 140 | VAL |
| 11 | L9 | 146 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | L9 | 151 | VAL |
| 11 | L9 | 153 | ASP |
| 11 | L9 | 157 | ASN |
| 11 | L9 | 161 | LEU |
| 11 | L9 | 168 | ARG |
| 11 | L9 | 173 | ARG |
| 11 | L9 | 177 | ASP |
| 11 | L9 | 180 | TYR |
| 11 | L9 | 189 | GLU |
| 12 | M0 | 3 | ARG |
| 12 | M0 | 21 | ARG |
| 12 | M0 | 22 | TYR |
| 12 | M0 | 24 | ARG |
| 12 | M0 | 30 | LYS |
| 12 | M0 | 32 | ARG |
| 12 | M0 | 36 | LEU |
| 12 | M0 | 52 | LEU |
| 12 | M0 | 60 | LEU |
| 12 | M0 | 87 | LEU |
| 12 | M0 | 102 | MET |
| 12 | M0 | 109 | ASP |
| 12 | M0 | 110 | ARG |
| 12 | M0 | 112 | GLN |
| 12 | M0 | 142 | ASP |
| 12 | M0 | 149 | VAL |
| 12 | M0 | 177 | ASP |
| 12 | M0 | 197 | VAL |
| 12 | M0 | 206 | LEU |
| 12 | M0 | 210 | ILE |
| 12 | M0 | 212 | GLU |
| 12 | M0 | 213 | PHE |
| 13 | M1 | 11 | ASP |
| 13 | M1 | 22 | SER |
| 13 | M1 | 28 | ASP |
| 13 | M1 | 44 | THR |
| 13 | M1 | 64 | LYS |
| 13 | M1 | 71 | VAL |
| 13 | M1 | 80 | LEU |
| 13 | M1 | 94 | ARG |
| 13 | M1 | 95 | ASN |
| 13 | M1 | 114 | ILE |
| 13 | M1 | 125 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M1 | 130 | VAL |
| 13 | M1 | 132 | ASN |
| 13 | M1 | 140 | ARG |
| 13 | M1 | 148 | VAL |
| 13 | M1 | 155 | THR |
| 13 | M1 | 171 | VAL |
| 13 | M1 | 172 | LEU |
| 13 | M1 | 173 | ASP |
| 13 | M1 | 174 | LYS |
| 14 | M3 | 13 | HIS |
| 14 | M3 | 15 | ARG |
| 14 | M3 | 17 | HIS |
| 14 | M3 | 37 | ASN |
| 14 | M3 | 54 | LEU |
| 14 | M3 | 55 | ARG |
| 14 | M3 | 58 | VAL |
| 14 | M3 | 85 | LEU |
| 14 | M3 | 104 | ARG |
| 14 | M3 | 114 | GLN |
| 14 | M3 | 131 | LYS |
| 14 | M3 | 164 | GLU |
| 14 | M3 | 168 | ARG |
| 14 | M3 | 176 | GLU |
| 14 | M3 | 194 | GLU |
| 15 | M4 | 6 | ILE |
| 15 | M4 | 8 | LYS |
| 15 | M4 | 50 | LYS |
| 15 | M4 | 53 | VAL |
| 15 | M4 | 69 | THR |
| 15 | M4 | 72 | LEU |
| 15 | M4 | 102 | LYS |
| 15 | M4 | 107 | GLU |
| 16 | M5 | 10 | LEU |
| 16 | M5 | 19 | LEU |
| 16 | M5 | 80 | THR |
| 16 | M5 | 83 | LYS |
| 16 | M5 | 109 | ARG |
| 16 | M5 | 117 | ASN |
| 16 | M5 | 133 | ILE |
| 16 | M5 | 138 | GLN |
| 16 | M5 | 151 | ILE |
| 16 | M5 | 182 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | M5 | 183 | THR |
| 17 | M6 | 4 | GLU |
| 17 | M6 | 10 | ASP |
| 17 | M6 | 12 | LYS |
| 17 | M6 | 66 | LYS |
| 17 | M6 | 68 | ARG |
| 17 | M6 | 78 | ARG |
| 17 | M6 | 84 | LEU |
| 17 | M6 | 85 | ARG |
| 17 | M6 | 89 | SER |
| 17 | M6 | 94 | ARG |
| 17 | M6 | 119 | VAL |
| 17 | M6 | 128 | ARG |
| 17 | M6 | 143 | THR |
| 18 | M7 | 7 | THR |
| 18 | M7 | 14 | SER |
| 18 | M7 | 24 | VAL |
| 18 | M7 | 32 | THR |
| 18 | M7 | 36 | ILE |
| 18 | M7 | 52 | LEU |
| 18 | M7 | 55 | GLN |
| 18 | M7 | 56 | ARG |
| 18 | M7 | 69 | ARG |
| 18 | M7 | 96 | GLN |
| 18 | M7 | 112 | LEU |
| 18 | M7 | 120 | ASN |
| 18 | M7 | 121 | GLN |
| 18 | M7 | 127 | ARG |
| 18 | M7 | 128 | ARG |
| 18 | M7 | 142 | SER |
| 18 | M7 | 144 | SER |
| 18 | M7 | 165 | VAL |
| 18 | M7 | 168 | LEU |
| 19 | M8 | 7 | SER |
| 19 | M8 | 13 | SER |
| 19 | M8 | 26 | LEU |
| 19 | M8 | 31 | LYS |
| 19 | M8 | 32 | LEU |
| 19 | M8 | 39 | ARG |
| 19 | M8 | 46 | LYS |
| 19 | M8 | 49 | LEU |
| 19 | M8 | 82 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | M8 | 86 | THR |
| 19 | M8 | 135 | GLN |
| 19 | M8 | 138 | LEU |
| 19 | M8 | 168 | THR |
| 19 | M8 | 170 | ARG |
| 19 | M8 | 178 | ARG |
| 19 | M8 | 180 | ARG |
| 20 | M9 | 8 | LYS |
| 20 | M9 | 22 | VAL |
| 20 | M9 | 39 | ASN |
| 20 | M9 | 46 | LYS |
| 20 | M9 | 47 | ASN |
| 20 | M9 | 60 | LYS |
| 20 | M9 | 91 | SER |
| 20 | M9 | 103 | ARG |
| 20 | M9 | 108 | LYS |
| 20 | M9 | 134 | HIS |
| 20 | M9 | 138 | LEU |
| 20 | M9 | 144 | GLN |
| 20 | M9 | 152 | GLU |
| 20 | M9 | 156 | ASN |
| 20 | M9 | 163 | ARG |
| 20 | M9 | 180 | LYS |
| 21 | N0 | 1 | MET |
| 21 | N0 | 3 | HIS |
| 21 | N0 | 14 | LEU |
| 21 | N0 | 18 | SER |
| 21 | N0 | 23 | LYS |
| 21 | N0 | 45 | LEU |
| 21 | N0 | 47 | LYS |
| 21 | N0 | 51 | VAL |
| 21 | N0 | 80 | ARG |
| 21 | N0 | 85 | SER |
| 21 | N0 | 87 | THR |
| 21 | N0 | 100 | VAL |
| 21 | N0 | 117 | ARG |
| 21 | N0 | 120 | SER |
| 21 | N0 | 125 | LYS |
| 21 | N0 | 132 | THR |
| 21 | N0 | 136 | LYS |
| 21 | N0 | 137 | ARG |
| 21 | N0 | 155 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | N0 | 156 | VAL |
| 21 | N0 | 167 | ARG |
| 21 | N0 | 172 | TYR |
| 22 | N1 | 12 | ARG |
| 22 | N1 | 14 | MET |
| 22 | N1 | 27 | LEU |
| 22 | N1 | 52 | MET |
| 22 | N1 | 78 | LYS |
| 22 | N1 | 79 | MET |
| 22 | N1 | 83 | ARG |
| 22 | N1 | 88 | ARG |
| 22 | N1 | 100 | LYS |
| 22 | N1 | 102 | ARG |
| 22 | N1 | 103 | GLN |
| 22 | N1 | 104 | GLU |
| 22 | N1 | 122 | GLN |
| 22 | N1 | 126 | VAL |
| 22 | N1 | 128 | LEU |
| 22 | N1 | 139 | ARG |
| 22 | N1 | 143 | THR |
| 22 | N1 | 144 | GLU |
| 22 | N1 | 146 | ASN |
| 22 | N1 | 155 | PRO |
| 23 | N2 | 16 | THR |
| 23 | N2 | 29 | ASP |
| 23 | N2 | 39 | ASP |
| 23 | N2 | 43 | VAL |
| 23 | N2 | 44 | GLU |
| 23 | N2 | 52 | ASN |
| 23 | N2 | 70 | LYS |
| 23 | N2 | 72 | SER |
| 23 | N2 | 80 | THR |
| 23 | N2 | 87 | ASN |
| 23 | N2 | 95 | PHE |
| 23 | N2 | 100 | THR |
| 23 | N2 | 107 | PHE |
| 24 | N3 | 12 | ARG |
| 24 | N3 | 32 | ARG |
| 24 | N3 | 33 | ASN |
| 24 | N3 | 47 | ASN |
| 24 | N3 | 64 | LYS |
| 24 | N3 | 69 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | N3 | 102 | ILE |
| 24 | N3 | 108 | GLU |
| 24 | N3 | 112 | SER |
| 24 | N3 | 115 | THR |
| 24 | N3 | 125 | LEU |
| 25 | N4 | 32 | GLN |
| 26 | N5 | 40 | LEU |
| 26 | N5 | 49 | LYS |
| 26 | N5 | 51 | VAL |
| 26 | N5 | 55 | ASN |
| 26 | N5 | 69 | SER |
| 26 | N5 | 70 | GLU |
| 26 | N5 | 71 | THR |
| 26 | N5 | 87 | SER |
| 26 | N5 | 96 | LYS |
| 26 | N5 | 105 | VAL |
| 26 | N5 | 109 | LYS |
| 26 | N5 | 115 | ARG |
| 26 | N5 | 125 | ARG |
| 26 | N5 | 134 | ASP |
| 26 | N5 | 135 | ILE |
| 27 | N6 | 13 | ARG |
| 27 | N6 | 37 | LYS |
| 27 | N6 | 51 | ARG |
| 27 | N6 | 55 | GLU |
| 27 | N6 | 56 | VAL |
| 27 | N6 | 74 | TYR |
| 27 | N6 | 76 | LEU |
| 27 | N6 | 126 | LEU |
| 28 | N7 | 14 | VAL |
| 28 | N7 | 15 | ARG |
| 28 | N7 | 30 | ASP |
| 28 | N7 | 53 | VAL |
| 28 | N7 | 55 | LYS |
| 28 | N7 | 56 | LYS |
| 28 | N7 | 64 | LYS |
| 28 | N7 | 65 | ARG |
| 28 | N7 | 75 | VAL |
| 28 | N7 | 81 | LEU |
| 28 | N7 | 102 | GLU |
| 28 | N7 | 126 | LYS |
| 29 | N8 | 4 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 29 | N8 | 8 | THR |
| 29 | N8 | 10 | LYS |
| 29 | N8 | 16 | SER |
| 29 | N8 | 25 | HIS |
| 29 | N8 | 26 | ARG |
| 29 | N8 | 46 | ASP |
| 29 | N8 | 56 | VAL |
| 29 | N8 | 60 | TYR |
| 29 | N8 | 65 | GLN |
| 29 | N8 | 72 | VAL |
| 29 | N8 | 73 | LEU |
| 29 | N8 | 76 | ASP |
| 29 | N8 | 78 | LEU |
| 29 | N8 | 85 | ASP |
| 29 | N8 | 133 | LEU |
| 30 | N9 | 18 | ARG |
| 30 | N9 | 19 | ASN |
| 30 | N9 | 28 | LYS |
| 30 | N9 | 33 | LYS |
| 31 | O0 | 16 | LEU |
| 31 | O0 | 36 | GLN |
| 31 | O0 | 41 | LEU |
| 31 | O0 | 57 | GLU |
| 31 | O0 | 61 | MET |
| 31 | O0 | 83 | LYS |
| 31 | O0 | 97 | ASP |
| 31 | O0 | 99 | ASP |
| 31 | O0 | 104 | LEU |
| 32 | O1 | 26 | LYS |
| 32 | O1 | 73 | LEU |
| 32 | O1 | 79 | ARG |
| 32 | O1 | 86 | LYS |
| 32 | O1 | 96 | VAL |
| 32 | O1 | 102 | LYS |
| 32 | O1 | 106 | THR |
| 32 | O1 | 110 | GLU |
| 33 | O2 | 14 | THR |
| 33 | O2 | 15 | LYS |
| 33 | O2 | 24 | ARG |
| 33 | O2 | 34 | LYS |
| 33 | O2 | 35 | GLN |
| 33 | O2 | 54 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | O2 | 73 | THR |
| 33 | O2 | 75 | LEU |
| 33 | O2 | 87 | MET |
| 33 | O2 | 88 | HIS |
| 33 | O2 | 90 | LYS |
| 33 | O2 | 109 | LEU |
| 33 | O2 | 113 | LYS |
| 33 | O2 | 120 | THR |
| 34 | O3 | 4 | SER |
| 34 | O3 | 15 | SER |
| 34 | O3 | 21 | ARG |
| 34 | O3 | 54 | ARG |
| 34 | O3 | 73 | ARG |
| 34 | O3 | 74 | THR |
| 34 | O3 | 98 | VAL |
| 35 | O4 | 51 | LEU |
| 35 | O4 | 71 | THR |
| 35 | O4 | 79 | SER |
| 35 | O4 | 81 | CYS |
| 35 | O4 | 83 | ASN |
| 35 | O4 | 86 | LYS |
| 35 | O4 | 103 | LYS |
| 36 | O5 | 4 | VAL |
| 36 | O5 | 28 | LEU |
| 36 | O5 | 31 | LEU |
| 36 | O5 | 74 | LYS |
| 36 | O5 | 79 | ASP |
| 36 | O5 | 89 | ARG |
| 36 | O5 | 90 | ARG |
| 36 | O5 | 119 | LYS |
| 37 | O6 | 21 | THR |
| 37 | O6 | 43 | LEU |
| 37 | O6 | 57 | LEU |
| 37 | O6 | 76 | ARG |
| 37 | O6 | 81 | THR |
| 38 | O7 | 12 | HIS |
| 38 | O7 | 17 | THR |
| 38 | O7 | 21 | ARG |
| 38 | O7 | 25 | ARG |
| 38 | O7 | 33 | THR |
| 38 | O7 | 44 | THR |
| 38 | O7 | 59 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | O7 | 67 | LEU |
| 38 | O7 | 68 | LYS |
| 39 | O8 | 12 | LEU |
| 39 | O8 | 24 | THR |
| 39 | O8 | 41 | THR |
| 39 | O8 | 69 | LEU |
| 39 | O8 | 77 | ARG |
| 40 | O9 | 13 | MET |
| 40 | O9 | 19 | GLN |
| 40 | O9 | 21 | ARG |
| 40 | O9 | 36 | ARG |
| 40 | O9 | 45 | ARG |
| 40 | O9 | 51 | ILE |
| 41 | Q0 | 109 | ASN |
| 41 | Q0 | 128 | LYS |
| 42 | Q1 | 2 | ARG |
| 42 | Q1 | 9 | ARG |
| 42 | Q1 | 11 | ARG |
| 42 | Q1 | 13 | LEU |
| 43 | Q2 | 7 | THR |
| 43 | Q2 | 16 | THR |
| 43 | Q2 | 29 | LYS |
| 43 | Q2 | 35 | LEU |
| 43 | Q2 | 45 | ARG |
| 43 | Q2 | 71 | ARG |
| 43 | Q2 | 74 | CYS |
| 43 | Q2 | 83 | LEU |
| 43 | Q2 | 84 | THR |
| 43 | Q2 | 105 | GLN |
| 43 | Q2 | 106 | PHE |
| 44 | Q3 | 5 | THR |
| 44 | Q3 | 11 | THR |
| 44 | Q3 | 24 | ARG |
| 44 | Q3 | 38 | ASP |
| 44 | Q3 | 45 | LYS |
| 44 | Q3 | 49 | ARG |
| 44 | Q3 | 60 | CYS |
| 44 | Q3 | 71 | VAL |
| 44 | Q3 | 78 | THR |
| 44 | Q3 | 84 | ARG |
| 46 | S0 | 2 | SER |
| 46 | S0 | 6 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 46 | S0 | 7 | PHE |
| 46 | S0 | 9 | LEU |
| 46 | S0 | 24 | LEU |
| 46 | S0 | 33 | GLN |
| 46 | S0 | 62 | ARG |
| 46 | S0 | 87 | LEU |
| 46 | S0 | 119 | ARG |
| 46 | S0 | 139 | VAL |
| 46 | S0 | 157 | ASP |
| 46 | S0 | 162 | CYS |
| 46 | S0 | 185 | ARG |
| 46 | S0 | 188 | LEU |
| 46 | S0 | 198 | MET |
| 46 | S0 | 200 | ASP |
| 46 | S0 | 203 | PHE |
| 47 | S1 | 26 | ARG |
| 47 | S1 | 30 | PHE |
| 47 | S1 | 38 | PHE |
| 47 | S1 | 43 | VAL |
| 47 | S1 | 61 | LEU |
| 47 | S1 | 66 | VAL |
| 47 | S1 | 70 | LEU |
| 47 | S1 | 73 | LEU |
| 47 | S1 | 78 | ASP |
| 47 | S1 | 79 | HIS |
| 47 | S1 | 81 | PHE |
| 47 | S1 | 89 | ASP |
| 47 | S1 | 95 | ASN |
| 47 | S1 | 96 | LEU |
| 47 | S1 | 97 | LEU |
| 47 | S1 | 98 | THR |
| 47 | S1 | 105 | PHE |
| 47 | S1 | 111 | ARG |
| 47 | S1 | 126 | THR |
| 47 | S1 | 130 | SER |
| 47 | S1 | 133 | TYR |
| 47 | S1 | 148 | ASN |
| 47 | S1 | 150 | VAL |
| 47 | S1 | 167 | VAL |
| 47 | S1 | 181 | LEU |
| 47 | S1 | 202 | LYS |
| 47 | S1 | 203 | ASP |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | S1 | 205 | PHE |
| 47 | S1 | 211 | HIS |
| 47 | S1 | 217 | LEU |
| 47 | S1 | 220 | GLN |
| 47 | S1 | 222 | LYS |
| 47 | S1 | 223 | PHE |
| 48 | S2 | 44 | LEU |
| 48 | S2 | 55 | GLU |
| 48 | S2 | 73 | LEU |
| 48 | S2 | 111 | VAL |
| 48 | S2 | 116 | LYS |
| 48 | S2 | 140 | ARG |
| 48 | S2 | 141 | ARG |
| 48 | S2 | 152 | HIS |
| 48 | S2 | 204 | THR |
| 48 | S2 | 205 | ARG |
| 48 | S2 | 206 | THR |
| 48 | S2 | 221 | THR |
| 48 | S2 | 222 | TYR |
| 48 | S2 | 225 | LEU |
| 48 | S2 | 233 | GLN |
| 48 | S2 | 235 | LEU |
| 48 | S2 | 241 | ASP |
| 48 | S2 | 244 | SER |
| 49 | S3 | 9 | ARG |
| 49 | S3 | 17 | PHE |
| 49 | S3 | 45 | LYS |
| 49 | S3 | 64 | ARG |
| 49 | S3 | 65 | ARG |
| 49 | S3 | 76 | ARG |
| 49 | S3 | 79 | TYR |
| 49 | S3 | 83 | THR |
| 49 | S3 | 87 | TYR |
| 49 | S3 | 91 | VAL |
| 49 | S3 | 108 | LYS |
| 49 | S3 | 172 | THR |
| 49 | S3 | 175 | VAL |
| 49 | S3 | 176 | LEU |
| 49 | S3 | 177 | MET |
| 49 | S3 | 178 | ARG |
| 49 | S3 | 181 | VAL |
| 49 | S3 | 190 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | S4 | 26 | CYS |
| 50 | S4 | 30 | ARG |
| 50 | S4 | 38 | LEU |
| 50 | S4 | 56 | LEU |
| 50 | S4 | 73 | ASP |
| 50 | S4 | 77 | ARG |
| 50 | S4 | 78 | THR |
| 50 | S4 | 105 | VAL |
| 50 | S4 | 117 | GLU |
| 50 | S4 | 130 | GLN |
| 50 | S4 | 139 | VAL |
| 50 | S4 | 182 | TYR |
| 50 | S4 | 206 | ASP |
| 50 | S4 | 226 | PHE |
| 50 | S4 | 227 | VAL |
| 50 | S4 | 231 | GLN |
| 51 | S5 | 20 | PHE |
| 51 | S5 | 24 | VAL |
| 51 | S5 | 41 | LYS |
| 51 | S5 | 48 | PHE |
| 51 | S5 | 51 | VAL |
| 51 | S5 | 64 | VAL |
| 51 | S5 | 65 | ARG |
| 51 | S5 | 69 | PHE |
| 51 | S5 | 76 | ARG |
| 51 | S5 | 79 | ASN |
| 51 | S5 | 93 | LEU |
| 51 | S5 | 103 | ASN |
| 51 | S5 | 108 | LEU |
| 51 | S5 | 112 | ARG |
| 51 | S5 | 116 | HIS |
| 51 | S5 | 122 | ASN |
| 51 | S5 | 194 | LEU |
| 51 | S5 | 212 | LYS |
| 52 | S6 | 4 | ASN |
| 52 | S6 | 7 | TYR |
| 52 | S6 | 23 | ARG |
| 52 | S6 | 25 | ARG |
| 52 | S6 | 58 | LYS |
| 52 | S6 | 68 | LEU |
| 52 | S6 | 89 | ASP |
| 52 | S6 | 115 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | S6 | 133 | LEU |
| 52 | S6 | 160 | ARG |
| 52 | S6 | 177 | ARG |
| 52 | S6 | 190 | GLN |
| 52 | S6 | 211 | LEU |
| 53 | S7 | 46 | ILE |
| 53 | S7 | 51 | VAL |
| 53 | S7 | 60 | ILE |
| 53 | S7 | 62 | VAL |
| 53 | S7 | 64 | VAL |
| 53 | S7 | 77 | LEU |
| 53 | S7 | 82 | GLU |
| 53 | S7 | 85 | PHE |
| 53 | S7 | 109 | VAL |
| 53 | S7 | 114 | ARG |
| 53 | S7 | 117 | THR |
| 53 | S7 | 130 | VAL |
| 53 | S7 | 131 | PHE |
| 53 | S7 | 159 | VAL |
| 53 | S7 | 163 | ASP |
| 54 | S8 | 29 | LEU |
| 54 | S8 | 36 | THR |
| 54 | S8 | 58 | LEU |
| 54 | S8 | 70 | GLU |
| 54 | S8 | 92 | ARG |
| 54 | S8 | 93 | THR |
| 54 | S8 | 110 | ARG |
| 54 | S8 | 116 | HIS |
| 54 | S8 | 121 | LEU |
| 54 | S8 | 137 | LYS |
| 54 | S8 | 142 | LYS |
| 54 | S8 | 168 | CYS |
| 54 | S8 | 179 | CYS |
| 55 | S9 | 3 | ARG |
| 55 | S9 | 28 | LEU |
| 55 | S9 | 71 | PHE |
| 55 | S9 | 103 | ASP |
| 55 | S9 | 109 | LEU |
| 55 | S9 | 132 | ARG |
| 55 | S9 | 134 | ILE |
| 55 | S9 | 141 | VAL |
| 55 | S9 | 152 | SER |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | S9 | 171 | ARG |
| 55 | S9 | 175 | ARG |
| 56 | C0 | 1 | MET |
| 56 | C0 | 13 | GLN |
| 56 | C0 | 22 | VAL |
| 56 | C0 | 49 | LEU |
| 56 | C0 | 51 | SER |
| 56 | C0 | 56 | LYS |
| 57 | C1 | 7 | VAL |
| 57 | C1 | 8 | GLN |
| 57 | C1 | 10 | GLU |
| 57 | C1 | 15 | LYS |
| 57 | C1 | 16 | GLN |
| 57 | C1 | 20 | PHE |
| 57 | C1 | 40 | LEU |
| 57 | C1 | 63 | LEU |
| 57 | C1 | 67 | ARG |
| 57 | C1 | 69 | LYS |
| 57 | C1 | 80 | MET |
| 57 | C1 | 83 | THR |
| 57 | C1 | 116 | ARG |
| 57 | C1 | 125 | VAL |
| 57 | C1 | 127 | GLN |
| 57 | C1 | 129 | ARG |
| 58 | C2 | 28 | LEU |
| 58 | C2 | 29 | LYS |
| 58 | C2 | 43 | ARG |
| 58 | C2 | 52 | LEU |
| 58 | C2 | 61 | VAL |
| 58 | C2 | 62 | LEU |
| 58 | C2 | 63 | VAL |
| 58 | C2 | 66 | VAL |
| 58 | C2 | 88 | LEU |
| 58 | C2 | 100 | TRP |
| 58 | C2 | 121 | VAL |
| 58 | C2 | 124 | LYS |
| 58 | C2 | 130 | THR |
| 59 | C3 | 3 | ARG |
| 59 | C3 | 64 | ARG |
| 59 | C3 | 84 | ILE |
| 59 | C3 | 107 | LYS |
| 59 | C3 | 115 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 59 | C3 | 125 | LEU |
| 59 | C3 | 134 | VAL |
| 59 | C3 | 140 | LYS |
| 59 | C3 | 145 | THR |
| 60 | C4 | 16 | VAL |
| 60 | C4 | 20 | TYR |
| 60 | C4 | 29 | HIS |
| 60 | C4 | 31 | THR |
| 60 | C4 | 41 | ARG |
| 60 | C4 | 42 | VAL |
| 60 | C4 | 43 | THR |
| 60 | C4 | 81 | VAL |
| 60 | C4 | 92 | LYS |
| 60 | C4 | 99 | GLN |
| 60 | C4 | 111 | ARG |
| 60 | C4 | 123 | SER |
| 60 | C4 | 135 | ARG |
| 61 | C5 | 36 | LEU |
| 61 | C5 | 44 | ARG |
| 61 | C5 | 50 | THR |
| 61 | C5 | 57 | MET |
| 61 | C5 | 124 | THR |
| 62 | C6 | 28 | LEU |
| 62 | C6 | 43 | ILE |
| 62 | C6 | 47 | LYS |
| 62 | C6 | 52 | LEU |
| 62 | C6 | 53 | LEU |
| 62 | C6 | 58 | ASP |
| 62 | C6 | 60 | PHE |
| 62 | C6 | 66 | ARG |
| 62 | C6 | 69 | VAL |
| 62 | C6 | 97 | VAL |
| 62 | C6 | 103 | ASN |
| 62 | C6 | 118 | ILE |
| 62 | C6 | 123 | ARG |
| 63 | C7 | 3 | ARG |
| 63 | C7 | 23 | LYS |
| 63 | C7 | 25 | THR |
| 63 | C7 | 36 | ASP |
| 63 | C7 | 46 | LEU |
| 63 | C7 | 71 | PHE |
| 63 | C7 | 84 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 63 | C7 | 85 | VAL |
| 63 | C7 | 87 | GLU |
| 63 | C7 | 88 | VAL |
| 63 | C7 | 105 | GLN |
| 63 | C7 | 108 | ASP |
| 63 | C7 | 119 | LEU |
| 64 | C8 | 4 | VAL |
| 64 | C8 | 11 | PHE |
| 64 | C8 | 25 | ASN |
| 64 | C8 | 28 | ILE |
| 64 | C8 | 55 | HIS |
| 64 | C8 | 79 | TYR |
| 64 | C8 | 80 | LYS |
| 64 | C8 | 81 | ILE |
| 64 | C8 | 85 | PHE |
| 64 | C8 | 100 | THR |
| 64 | C8 | 132 | ARG |
| 64 | C8 | 133 | VAL |
| 64 | C8 | 136 | GLN |
| 64 | C8 | 143 | ARG |
| 64 | C8 | 145 | ARG |
| 65 | C9 | 18 | TYR |
| 65 | C9 | 29 | GLU |
| 65 | C9 | 33 | TYR |
| 65 | C9 | 35 | ASP |
| 65 | C9 | 67 | MET |
| 65 | C9 | 69 | LYS |
| 65 | C9 | 70 | GLN |
| 65 | C9 | 75 | LYS |
| 65 | C9 | 114 | VAL |
| 65 | C9 | 126 | GLU |
| 65 | C9 | 130 | ARG |
| 65 | C9 | 134 | ARG |
| 66 | D0 | 18 | GLN |
| 66 | D0 | 22 | ILE |
| 66 | D0 | 30 | LYS |
| 66 | D0 | 48 | HIS |
| 66 | D0 | 57 | ARG |
| 66 | D0 | 58 | LEU |
| 66 | D0 | 70 | THR |
| 66 | D0 | 72 | ASN |
| 66 | D0 | 74 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 66 | D0 | 87 | HIS |
| 66 | D0 | 109 | GLU |
| 67 | D1 | 1 | MET |
| 67 | D1 | 60 | ARG |
| 67 | D1 | 67 | ASP |
| 67 | D1 | 80 | LYS |
| 67 | D1 | 81 | ASN |
| 67 | D1 | 86 | SER |
| 68 | D2 | 4 | SER |
| 68 | D2 | 25 | VAL |
| 68 | D2 | 31 | SER |
| 68 | D2 | 56 | HIS |
| 68 | D2 | 65 | LEU |
| 68 | D2 | 76 | SER |
| 68 | D2 | 81 | VAL |
| 68 | D2 | 93 | LEU |
| 68 | D2 | 117 | ARG |
| 68 | D2 | 126 | LEU |
| 68 | D2 | 128 | PHE |
| 68 | D2 | 129 | VAL |
| 69 | D3 | 18 | HIS |
| 69 | D3 | 19 | ARG |
| 69 | D3 | 73 | ARG |
| 69 | D3 | 75 | GLN |
| 69 | D3 | 92 | CYS |
| 69 | D3 | 107 | PHE |
| 69 | D3 | 132 | LEU |
| 69 | D3 | 135 | LEU |
| 70 | D4 | 10 | ARG |
| 70 | D4 | 28 | LEU |
| 70 | D4 | 35 | VAL |
| 70 | D4 | 57 | VAL |
| 70 | D4 | 61 | ARG |
| 70 | D4 | 62 | THR |
| 70 | D4 | 72 | PHE |
| 70 | D4 | 93 | ARG |
| 70 | D4 | 111 | LYS |
| 70 | D4 | 115 | ASP |
| 70 | D4 | 124 | ARG |
| 70 | D4 | 131 | ARG |
| 70 | D4 | 132 | ARG |
| 71 | D5 | 40 | VAL |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 71 | D5 | 42 | LEU |
| 71 | D5 | 49 | ARG |
| 71 | D5 | 58 | ARG |
| 71 | D5 | 60 | VAL |
| 71 | D5 | 63 | SER |
| 71 | D5 | 64 | VAL |
| 71 | D5 | 69 | LEU |
| 71 | D5 | 85 | LYS |
| 71 | D5 | 97 | LYS |
| 72 | D6 | 7 | SER |
| 72 | D6 | 10 | ARG |
| 72 | D6 | 12 | LYS |
| 72 | D6 | 15 | ARG |
| 72 | D6 | 37 | LYS |
| 72 | D6 | 39 | MET |
| 72 | D6 | 58 | VAL |
| 72 | D6 | 66 | LYS |
| 72 | D6 | 69 | ASN |
| 72 | D6 | 82 | ARG |
| 72 | D6 | 84 | VAL |
| 72 | D6 | 85 | ARG |
| 72 | D6 | 88 | SER |
| 72 | D6 | 90 | GLU |
| 73 | D7 | 3 | LEU |
| 73 | D7 | 33 | LEU |
| 73 | D7 | 49 | HIS |
| 73 | D7 | 56 | CYS |
| 73 | D7 | 59 | CYS |
| 73 | D7 | 77 | THR |
| 73 | D7 | 79 | PHE |
| 74 | D8 | 5 | THR |
| 74 | D8 | 7 | VAL |
| 74 | D8 | 15 | VAL |
| 74 | D8 | 58 | GLU |
| 74 | D8 | 67 | ARG |
| 75 | D9 | 7 | TRP |
| 75 | D9 | 27 | HIS |
| 75 | D9 | 32 | ARG |
| 76 | E0 | 21 | VAL |
| 76 | E0 | 26 | LYS |
| 76 | E0 | 48 | THR |
| 76 | E0 | 49 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | E0 | 50 | VAL |
| 76 | E0 | 51 | ASN |
| 76 | E0 | 53 | LYS |
| 76 | E0 | 54 | ARG |
| 76 | E0 | 56 | MET |
| 77 | SR | 50 | ASP |
| 77 | SR | 52 | GLN |
| 77 | SR | 53 | LYS |
| 77 | SR | 64 | HIS |
| 77 | SR | 102 | ARG |
| 77 | SR | 121 | MET |
| 77 | SR | 141 | LEU |
| 77 | SR | 149 | ASP |
| 77 | SR | 156 | VAL |
| 77 | SR | 234 | LEU |
| 77 | SR | 248 | ASN |
| 77 | SR | 278 | PHE |
| 77 | SR | 290 | VAL |
| 78 | SM | 23 | LYS |
| 78 | SM | 24 | GLU |
| 78 | SM | 37 | VAL |
| 78 | SM | 49 | LYS |
| 78 | SM | 68 | ARG |
| 78 | SM | 69 | ARG |
| 78 | SM | 72 | ARG |
| 78 | SM | 73 | SER |
| 78 | SM | 84 | LYS |
| 78 | SM | 89 | ARG |
| 78 | SM | 102 | THR |
| 78 | SM | 134 | ASP |
| 4 | l2 | 44 | ILE |
| 4 | l2 | 45 | VAL |
| 4 | l2 | 61 | VAL |
| 4 | l2 | 109 | GLU |
| 4 | l2 | 113 | VAL |
| 4 | l2 | 142 | ASP |
| 4 | l2 | 147 | ARG |
| 4 | l2 | 179 | LEU |
| 4 | l2 | 180 | LEU |
| 4 | l2 | 193 | ARG |
| 4 | l2 | 207 | VAL |
| 4 | l2 | 215 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | l2 | 217 | GLN |
| 4 | l2 | 227 | ARG |
| 4 | l2 | 242 | ARG |
| 4 | l2 | 246 | LEU |
| 5 | l3 | 2 | SER |
| 5 | l3 | 3 | HIS |
| 5 | l3 | 4 | ARG |
| 5 | l3 | 10 | ARG |
| 5 | l3 | 24 | SER |
| 5 | l3 | 37 | ARG |
| 5 | l3 | 41 | VAL |
| 5 | l3 | 44 | THR |
| 5 | l3 | 84 | VAL |
| 5 | l3 | 85 | VAL |
| 5 | l3 | 99 | LEU |
| 5 | l3 | 103 | THR |
| 5 | l3 | 112 | ASP |
| 5 | l3 | 114 | VAL |
| 5 | l3 | 120 | LYS |
| 5 | l3 | 139 | GLN |
| 5 | l3 | 140 | ASP |
| 5 | l3 | 148 | LEU |
| 5 | l3 | 156 | SER |
| 5 | l3 | 169 | THR |
| 5 | l3 | 183 | LEU |
| 5 | l3 | 210 | GLU |
| 5 | l3 | 229 | VAL |
| 5 | l3 | 232 | ARG |
| 5 | l3 | 238 | LEU |
| 5 | l3 | 246 | LEU |
| 5 | l3 | 259 | HIS |
| 5 | l3 | 260 | VAL |
| 5 | l3 | 274 | SER |
| 5 | l3 | 284 | ARG |
| 5 | l3 | 328 | ILE |
| 5 | l3 | 332 | ARG |
| 5 | l3 | 338 | LEU |
| 5 | l3 | 348 | ARG |
| 5 | l3 | 369 | ARG |
| 6 | l4 | 3 | ARG |
| 6 | l4 | 10 | SER |
| 6 | l4 | 37 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | l4 | 47 | ARG |
| 6 | l4 | 54 | GLU |
| 6 | l4 | 63 | GLU |
| 6 | l4 | 92 | ASN |
| 6 | l4 | 94 | CYS |
| 6 | l4 | 120 | TYR |
| 6 | l4 | 138 | ARG |
| 6 | l4 | 143 | GLU |
| 6 | l4 | 144 | LYS |
| 6 | l4 | 156 | LEU |
| 6 | l4 | 188 | ARG |
| 6 | l4 | 194 | TYR |
| 6 | l4 | 197 | ARG |
| 6 | l4 | 198 | ARG |
| 6 | l4 | 206 | LEU |
| 6 | l4 | 217 | LYS |
| 6 | l4 | 220 | ARG |
| 6 | l4 | 243 | HIS |
| 6 | l4 | 246 | ARG |
| 6 | l4 | 256 | THR |
| 6 | l4 | 258 | LEU |
| 6 | l4 | 259 | ASP |
| 6 | l4 | 261 | VAL |
| 6 | l4 | 279 | HIS |
| 6 | l4 | 283 | THR |
| 6 | l4 | 284 | SER |
| 6 | l4 | 294 | GLU |
| 6 | l4 | 313 | LEU |
| 6 | l4 | 319 | LYS |
| 6 | l4 | 323 | VAL |
| 6 | l4 | 327 | LEU |
| 6 | l4 | 362 | ASP |
| 7 | l5 | 34 | LYS |
| 7 | l5 | 45 | ASN |
| 7 | l5 | 50 | ARG |
| 7 | l5 | 75 | LEU |
| 7 | l5 | 81 | HIS |
| 7 | l5 | 123 | GLU |
| 7 | l5 | 124 | GLU |
| 7 | l5 | 128 | GLU |
| 7 | l5 | 131 | LEU |
| 7 | l5 | 140 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | l5 | 152 | ARG |
| 7 | l5 | 155 | THR |
| 7 | l5 | 185 | PHE |
| 7 | l5 | 222 | LEU |
| 7 | l5 | 237 | GLU |
| 7 | l5 | 259 | LYS |
| 7 | l5 | 260 | PHE |
| 7 | l5 | 268 | GLU |
| 7 | l5 | 273 | ARG |
| 7 | l5 | 279 | LYS |
| 8 | l6 | 21 | THR |
| 8 | l6 | 26 | ARG |
| 8 | l6 | 30 | LEU |
| 8 | l6 | 64 | LEU |
| 8 | l6 | 65 | ILE |
| 8 | l6 | 87 | THR |
| 8 | l6 | 90 | LYS |
| 8 | l6 | 93 | VAL |
| 8 | l6 | 134 | ARG |
| 8 | l6 | 152 | THR |
| 8 | l6 | 154 | LEU |
| 8 | l6 | 155 | LEU |
| 9 | l7 | 45 | LEU |
| 9 | l7 | 46 | GLU |
| 9 | l7 | 60 | ARG |
| 9 | l7 | 83 | LEU |
| 9 | l7 | 84 | VAL |
| 9 | l7 | 87 | VAL |
| 9 | l7 | 88 | ARG |
| 9 | l7 | 111 | ILE |
| 9 | l7 | 112 | ASN |
| 9 | l7 | 128 | LYS |
| 9 | l7 | 151 | ARG |
| 9 | l7 | 166 | ASN |
| 9 | l7 | 173 | LEU |
| 9 | l7 | 179 | LEU |
| 9 | l7 | 180 | SER |
| 9 | l7 | 182 | ASP |
| 9 | l7 | 184 | LEU |
| 9 | l7 | 190 | THR |
| 9 | l7 | 191 | VAL |
| 9 | l7 | 228 | SER |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | l7 | 229 | PHE |
| 9 | l7 | 234 | GLU |
| 9 | l7 | 239 | LEU |
| 10 | l8 | 61 | GLN |
| 10 | l8 | 71 | VAL |
| 10 | l8 | 93 | LEU |
| 10 | l8 | 98 | ARG |
| 10 | l8 | 108 | ARG |
| 10 | l8 | 111 | LYS |
| 10 | l8 | 134 | TYR |
| 10 | l8 | 136 | LEU |
| 10 | l8 | 149 | LYS |
| 10 | l8 | 150 | LEU |
| 10 | l8 | 155 | ASN |
| 10 | l8 | 173 | MET |
| 10 | l8 | 180 | VAL |
| 10 | l8 | 183 | LYS |
| 10 | l8 | 200 | LEU |
| 10 | l8 | 202 | GLU |
| 10 | l8 | 204 | ARG |
| 10 | l8 | 213 | LYS |
| 10 | l8 | 222 | PHE |
| 10 | l8 | 226 | TYR |
| 10 | l8 | 228 | GLU |
| 10 | l8 | 238 | LEU |
| 11 | l9 | 3 | TYR |
| 11 | l9 | 5 | GLN |
| 11 | l9 | 6 | THR |
| 11 | l9 | 16 | VAL |
| 11 | l9 | 22 | SER |
| 11 | l9 | 33 | THR |
| 11 | l9 | 52 | LEU |
| 11 | l9 | 55 | VAL |
| 11 | l9 | 68 | LEU |
| 11 | l9 | 82 | VAL |
| 11 | l9 | 92 | TYR |
| 11 | l9 | 93 | VAL |
| 11 | l9 | 104 | VAL |
| 11 | l9 | 105 | GLU |
| 11 | l9 | 110 | LYS |
| 11 | l9 | 130 | ASP |
| 11 | l9 | 138 | THR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | l9 | 140 | VAL |
| 11 | l9 | 143 | GLU |
| 11 | l9 | 146 | LEU |
| 11 | l9 | 149 | ASN |
| 11 | l9 | 151 | VAL |
| 11 | l9 | 161 | LEU |
| 11 | l9 | 165 | CYS |
| 11 | l9 | 172 | ILE |
| 11 | l9 | 177 | ASP |
| 11 | l9 | 191 | LEU |
| 12 | m0 | 24 | ARG |
| 12 | m0 | 26 | VAL |
| 12 | m0 | 29 | SER |
| 12 | m0 | 36 | LEU |
| 12 | m0 | 42 | THR |
| 12 | m0 | 44 | ASP |
| 12 | m0 | 52 | LEU |
| 12 | m0 | 82 | ARG |
| 12 | m0 | 101 | LYS |
| 12 | m0 | 105 | CYS |
| 12 | m0 | 110 | ARG |
| 12 | m0 | 111 | LEU |
| 12 | m0 | 112 | GLN |
| 12 | m0 | 130 | ASP |
| 12 | m0 | 139 | ARG |
| 12 | m0 | 140 | THR |
| 12 | m0 | 142 | ASP |
| 12 | m0 | 150 | GLU |
| 12 | m0 | 163 | GLN |
| 12 | m0 | 186 | GLU |
| 12 | m0 | 197 | VAL |
| 12 | m0 | 208 | ASN |
| 12 | m0 | 217 | PHE |
| 12 | m0 | 220 | GLN |
| 13 | m1 | 10 | ARG |
| 13 | m1 | 11 | ASP |
| 13 | m1 | 12 | LEU |
| 13 | m1 | 25 | GLU |
| 13 | m1 | 28 | ASP |
| 13 | m1 | 30 | LEU |
| 13 | m1 | 68 | HIS |
| 13 | m1 | 92 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | m1 | 101 | ASN |
| 13 | m1 | 107 | ASP |
| 13 | m1 | 108 | GLU |
| 13 | m1 | 110 | ILE |
| 13 | m1 | 111 | ASP |
| 13 | m1 | 112 | LEU |
| 13 | m1 | 115 | LYS |
| 13 | m1 | 116 | TYR |
| 13 | m1 | 127 | PHE |
| 13 | m1 | 133 | ARG |
| 13 | m1 | 152 | HIS |
| 13 | m1 | 153 | LYS |
| 13 | m1 | 155 | THR |
| 13 | m1 | 174 | LYS |
| 14 | m3 | 22 | VAL |
| 14 | m3 | 45 | LYS |
| 14 | m3 | 46 | ILE |
| 14 | m3 | 54 | LEU |
| 14 | m3 | 58 | VAL |
| 14 | m3 | 59 | ARG |
| 14 | m3 | 67 | ARG |
| 14 | m3 | 69 | VAL |
| 14 | m3 | 92 | THR |
| 14 | m3 | 100 | ARG |
| 14 | m3 | 107 | GLU |
| 14 | m3 | 114 | GLN |
| 14 | m3 | 162 | ASN |
| 14 | m3 | 186 | ARG |
| 15 | m4 | 20 | VAL |
| 15 | m4 | 21 | VAL |
| 15 | m4 | 42 | LYS |
| 15 | m4 | 63 | VAL |
| 15 | m4 | 69 | THR |
| 15 | m4 | 72 | LEU |
| 15 | m4 | 80 | THR |
| 15 | m4 | 90 | VAL |
| 15 | m4 | 91 | CYS |
| 15 | m4 | 98 | SER |
| 15 | m4 | 102 | LYS |
| 15 | m4 | 108 | ARG |
| 15 | m4 | 129 | TYR |
| 16 | m5 | 10 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | m5 | 13 | LYS |
| 16 | m5 | 17 | ASP |
| 16 | m5 | 24 | ARG |
| 16 | m5 | 37 | HIS |
| 16 | m5 | 49 | ARG |
| 16 | m5 | 68 | ARG |
| 16 | m5 | 75 | VAL |
| 16 | m5 | 109 | ARG |
| 16 | m5 | 116 | LEU |
| 16 | m5 | 122 | ASN |
| 16 | m5 | 190 | THR |
| 16 | m5 | 201 | ARG |
| 17 | m6 | 66 | LYS |
| 17 | m6 | 67 | THR |
| 17 | m6 | 68 | ARG |
| 17 | m6 | 106 | GLU |
| 17 | m6 | 108 | ILE |
| 17 | m6 | 115 | LYS |
| 17 | m6 | 119 | VAL |
| 17 | m6 | 178 | VAL |
| 17 | m6 | 182 | ASN |
| 17 | m6 | 187 | GLU |
| 18 | m7 | 23 | ARG |
| 18 | m7 | 24 | VAL |
| 18 | m7 | 31 | GLU |
| 18 | m7 | 32 | THR |
| 18 | m7 | 46 | LYS |
| 18 | m7 | 53 | ASP |
| 18 | m7 | 56 | ARG |
| 18 | m7 | 64 | ASN |
| 18 | m7 | 75 | GLU |
| 18 | m7 | 96 | GLN |
| 18 | m7 | 107 | LEU |
| 18 | m7 | 116 | HIS |
| 18 | m7 | 125 | GLN |
| 18 | m7 | 126 | ARG |
| 18 | m7 | 144 | SER |
| 19 | m8 | 3 | ILE |
| 19 | m8 | 20 | LYS |
| 19 | m8 | 26 | LEU |
| 19 | m8 | 49 | LEU |
| 19 | m8 | 55 | SER |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | m8 | 86 | THR |
| 19 | m8 | 135 | GLN |
| 19 | m8 | 138 | LEU |
| 19 | m8 | 141 | ARG |
| 19 | m8 | 148 | GLU |
| 19 | m8 | 150 | VAL |
| 19 | m8 | 155 | MET |
| 19 | m8 | 170 | ARG |
| 19 | m8 | 174 | ARG |
| 19 | m8 | 178 | ARG |
| 20 | m9 | 7 | GLN |
| 20 | m9 | 9 | ARG |
| 20 | m9 | 10 | LEU |
| 20 | m9 | 29 | THR |
| 20 | m9 | 43 | LYS |
| 20 | m9 | 70 | LYS |
| 20 | m9 | 74 | ARG |
| 20 | m9 | 99 | LEU |
| 20 | m9 | 105 | LEU |
| 20 | m9 | 128 | LYS |
| 20 | m9 | 134 | HIS |
| 20 | m9 | 144 | GLN |
| 20 | m9 | 150 | GLN |
| 20 | m9 | 164 | LEU |
| 20 | m9 | 180 | LYS |
| 20 | m9 | 184 | LEU |
| 20 | m9 | 188 | ASP |
| 21 | n0 | 1 | MET |
| 21 | n0 | 3 | HIS |
| 21 | n0 | 13 | ARG |
| 21 | n0 | 40 | ARG |
| 21 | n0 | 51 | VAL |
| 21 | n0 | 80 | ARG |
| 21 | n0 | 87 | THR |
| 21 | n0 | 88 | HIS |
| 21 | n0 | 113 | ARG |
| 21 | n0 | 115 | ARG |
| 21 | n0 | 120 | SER |
| 21 | n0 | 131 | LYS |
| 21 | n0 | 132 | THR |
| 21 | n0 | 137 | ARG |
| 21 | n0 | 155 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | n0 | 160 | THR |
| 21 | n0 | 162 | THR |
| 21 | n0 | 164 | SER |
| 21 | n0 | 167 | ARG |
| 21 | n0 | 172 | TYR |
| 22 | n1 | 12 | ARG |
| 22 | n1 | 18 | ASP |
| 22 | n1 | 26 | HIS |
| 22 | n1 | 32 | LYS |
| 22 | n1 | 83 | ARG |
| 22 | n1 | 88 | ARG |
| 22 | n1 | 89 | LEU |
| 22 | n1 | 98 | HIS |
| 22 | n1 | 104 | GLU |
| 22 | n1 | 124 | VAL |
| 22 | n1 | 129 | LYS |
| 22 | n1 | 139 | ARG |
| 23 | n2 | 21 | SER |
| 23 | n2 | 39 | ASP |
| 23 | n2 | 50 | LEU |
| 23 | n2 | 78 | TYR |
| 23 | n2 | 86 | LYS |
| 23 | n2 | 90 | ARG |
| 23 | n2 | 91 | ASP |
| 23 | n2 | 100 | THR |
| 24 | n3 | 7 | GLN |
| 24 | n3 | 13 | ILE |
| 24 | n3 | 32 | ARG |
| 24 | n3 | 45 | ARG |
| 24 | n3 | 54 | LEU |
| 24 | n3 | 83 | LYS |
| 24 | n3 | 88 | ARG |
| 24 | n3 | 115 | THR |
| 24 | n3 | 128 | ARG |
| 24 | n3 | 135 | VAL |
| 25 | n4 | 1 | MET |
| 25 | n4 | 19 | THR |
| 25 | n4 | 39 | LEU |
| 25 | n4 | 57 | LYS |
| 25 | n4 | 96 | LEU |
| 25 | n4 | 105 | ARG |
| 25 | n4 | 123 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | n5 | 42 | ARG |
| 26 | n5 | 48 | SER |
| 26 | n5 | 49 | LYS |
| 26 | n5 | 51 | VAL |
| 26 | n5 | 57 | LEU |
| 26 | n5 | 87 | SER |
| 26 | n5 | 104 | GLU |
| 26 | n5 | 108 | LEU |
| 26 | n5 | 115 | ARG |
| 26 | n5 | 133 | LEU |
| 26 | n5 | 135 | ILE |
| 26 | n5 | 139 | ILE |
| 27 | n6 | 7 | ASP |
| 27 | n6 | 8 | VAL |
| 27 | n6 | 37 | LYS |
| 27 | n6 | 56 | VAL |
| 27 | n6 | 74 | TYR |
| 27 | n6 | 89 | LYS |
| 27 | n6 | 94 | SER |
| 27 | n6 | 115 | ARG |
| 28 | n7 | 4 | PHE |
| 28 | n7 | 26 | VAL |
| 28 | n7 | 65 | ARG |
| 28 | n7 | 75 | VAL |
| 28 | n7 | 81 | LEU |
| 28 | n7 | 102 | GLU |
| 28 | n7 | 127 | ASN |
| 29 | n8 | 6 | THR |
| 29 | n8 | 8 | THR |
| 29 | n8 | 24 | LYS |
| 29 | n8 | 42 | ARG |
| 29 | n8 | 46 | ASP |
| 29 | n8 | 60 | TYR |
| 29 | n8 | 78 | LEU |
| 29 | n8 | 80 | THR |
| 29 | n8 | 84 | GLU |
| 29 | n8 | 85 | ASP |
| 30 | n9 | 18 | ARG |
| 30 | n9 | 21 | ILE |
| 30 | n9 | 23 | LYS |
| 30 | n9 | 25 | LYS |
| 30 | n9 | 27 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | o0 | 10 | ILE |
| 31 | o0 | 18 | ILE |
| 31 | o0 | 41 | LEU |
| 31 | o0 | 55 | GLU |
| 31 | o0 | 61 | MET |
| 31 | o0 | 64 | LYS |
| 31 | o0 | 83 | LYS |
| 31 | o0 | 86 | ARG |
| 31 | o0 | 100 | ILE |
| 32 | o1 | 16 | LEU |
| 32 | o1 | 24 | SER |
| 32 | o1 | 28 | ARG |
| 32 | o1 | 31 | ARG |
| 32 | o1 | 44 | MET |
| 32 | o1 | 62 | ARG |
| 32 | o1 | 64 | VAL |
| 32 | o1 | 91 | SER |
| 32 | o1 | 106 | THR |
| 32 | o1 | 111 | GLU |
| 33 | o2 | 19 | ARG |
| 33 | o2 | 33 | ARG |
| 33 | o2 | 73 | THR |
| 33 | o2 | 75 | LEU |
| 33 | o2 | 82 | LEU |
| 33 | o2 | 87 | MET |
| 33 | o2 | 125 | ARG |
| 33 | o2 | 126 | LEU |
| 34 | o3 | 21 | ARG |
| 34 | o3 | 49 | ILE |
| 34 | o3 | 59 | VAL |
| 34 | o3 | 60 | ARG |
| 34 | o3 | 81 | VAL |
| 35 | o4 | 15 | THR |
| 35 | o4 | 33 | GLN |
| 35 | o4 | 44 | CYS |
| 35 | o4 | 60 | ARG |
| 35 | o4 | 71 | THR |
| 35 | o4 | 80 | ARG |
| 35 | o4 | 88 | ARG |
| 36 | o5 | 4 | VAL |
| 36 | o5 | 23 | ASP |
| 36 | o5 | 31 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 36 | o5 | 43 | LYS |
| 36 | o5 | 101 | THR |
| 37 | o6 | 3 | VAL |
| 37 | o6 | 13 | LYS |
| 37 | o6 | 17 | VAL |
| 37 | o6 | 43 | LEU |
| 37 | o6 | 68 | ARG |
| 37 | o6 | 70 | ARG |
| 37 | o6 | 98 | ARG |
| 37 | o6 | 100 | HIS |
| 38 | o7 | 12 | HIS |
| 38 | o7 | 37 | CYS |
| 38 | o7 | 44 | THR |
| 38 | o7 | 45 | ARG |
| 38 | o7 | 55 | ARG |
| 38 | o7 | 67 | LEU |
| 38 | o7 | 76 | ASN |
| 39 | o8 | 16 | ARG |
| 39 | o8 | 19 | ASP |
| 39 | o8 | 24 | THR |
| 39 | o8 | 28 | ASN |
| 39 | o8 | 32 | ASN |
| 39 | o8 | 41 | THR |
| 39 | o8 | 46 | ARG |
| 39 | o8 | 53 | THR |
| 39 | o8 | 54 | LEU |
| 39 | o8 | 64 | LYS |
| 39 | o8 | 69 | LEU |
| 40 | o9 | 21 | ARG |
| 40 | o9 | 23 | LEU |
| 41 | q0 | 85 | LEU |
| 41 | q0 | 92 | ASP |
| 41 | q0 | 93 | LYS |
| 41 | q0 | 99 | CYS |
| 41 | q0 | 106 | ARG |
| 41 | q0 | 127 | LEU |
| 42 | q1 | 2 | ARG |
| 42 | q1 | 6 | ARG |
| 42 | q1 | 13 | LEU |
| 42 | q1 | 19 | LYS |
| 42 | q1 | 21 | ARG |
| 42 | q1 | 24 | SER |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 43 | q2 | 2 | VAL |
| 43 | q2 | 4 | VAL |
| 43 | q2 | 8 | ARG |
| 43 | q2 | 38 | GLN |
| 43 | q2 | 71 | ARG |
| 43 | q2 | 77 | CYS |
| 43 | q2 | 80 | ARG |
| 43 | q2 | 84 | THR |
| 43 | q2 | 85 | LEU |
| 43 | q2 | 93 | LEU |
| 44 | q3 | 4 | ARG |
| 44 | q3 | 6 | LYS |
| 44 | q3 | 16 | VAL |
| 44 | q3 | 20 | SER |
| 44 | q3 | 59 | CYS |
| 44 | q3 | 62 | LYS |
| 44 | q3 | 90 | VAL |
| 46 | s0 | 22 | THR |
| 46 | s0 | 23 | HIS |
| 46 | s0 | 24 | LEU |
| 46 | s0 | 29 | VAL |
| 46 | s0 | 30 | GLN |
| 46 | s0 | 31 | VAL |
| 46 | s0 | 55 | GLU |
| 46 | s0 | 59 | LEU |
| 46 | s0 | 139 | VAL |
| 46 | s0 | 151 | SER |
| 46 | s0 | 179 | ARG |
| 46 | s0 | 183 | ARG |
| 46 | s0 | 185 | ARG |
| 46 | s0 | 188 | LEU |
| 46 | s0 | 195 | TRP |
| 46 | s0 | 200 | ASP |
| 47 | s1 | 21 | VAL |
| 47 | s1 | 25 | THR |
| 47 | s1 | 47 | LEU |
| 47 | s1 | 49 | ASN |
| 47 | s1 | 66 | VAL |
| 47 | s1 | 70 | LEU |
| 47 | s1 | 77 | GLU |
| 47 | s1 | 85 | LYS |
| 47 | s1 | 105 | PHE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | s1 | 108 | ASP |
| 47 | s1 | 115 | ARG |
| 47 | s1 | 128 | LYS |
| 47 | s1 | 150 | VAL |
| 47 | s1 | 180 | THR |
| 47 | s1 | 181 | LEU |
| 47 | s1 | 194 | ASN |
| 47 | s1 | 205 | PHE |
| 47 | s1 | 209 | ASN |
| 47 | s1 | 223 | PHE |
| 47 | s1 | 224 | ASP |
| 48 | s2 | 53 | ILE |
| 48 | s2 | 73 | LEU |
| 48 | s2 | 90 | THR |
| 48 | s2 | 97 | ARG |
| 48 | s2 | 111 | VAL |
| 48 | s2 | 136 | VAL |
| 48 | s2 | 141 | ARG |
| 48 | s2 | 161 | LYS |
| 48 | s2 | 164 | SER |
| 48 | s2 | 222 | TYR |
| 49 | s3 | 4 | LEU |
| 49 | s3 | 9 | ARG |
| 49 | s3 | 10 | LYS |
| 49 | s3 | 57 | ASP |
| 49 | s3 | 61 | GLU |
| 49 | s3 | 76 | ARG |
| 49 | s3 | 90 | ARG |
| 49 | s3 | 91 | VAL |
| 49 | s3 | 128 | GLU |
| 49 | s3 | 134 | CYS |
| 49 | s3 | 142 | LEU |
| 49 | s3 | 156 | PHE |
| 49 | s3 | 157 | LEU |
| 49 | s3 | 164 | VAL |
| 49 | s3 | 181 | VAL |
| 49 | s3 | 212 | LYS |
| 49 | s3 | 218 | LEU |
| 50 | s4 | 7 | LYS |
| 50 | s4 | 17 | HIS |
| 50 | s4 | 39 | ARG |
| 50 | s4 | 51 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | s4 | 68 | ARG |
| 50 | s4 | 73 | ASP |
| 50 | s4 | 100 | ARG |
| 50 | s4 | 105 | VAL |
| 50 | s4 | 126 | VAL |
| 50 | s4 | 139 | VAL |
| 50 | s4 | 140 | VAL |
| 50 | s4 | 180 | LEU |
| 50 | s4 | 182 | TYR |
| 50 | s4 | 189 | LEU |
| 50 | s4 | 192 | ILE |
| 50 | s4 | 214 | LEU |
| 50 | s4 | 215 | ASP |
| 50 | s4 | 222 | LEU |
| 50 | s4 | 226 | PHE |
| 50 | s4 | 246 | LEU |
| 50 | s4 | 248 | ILE |
| 51 | s5 | 24 | VAL |
| 51 | s5 | 29 | ILE |
| 51 | s5 | 43 | PHE |
| 51 | s5 | 76 | ARG |
| 51 | s5 | 94 | THR |
| 51 | s5 | 112 | ARG |
| 51 | s5 | 114 | ILE |
| 51 | s5 | 131 | GLN |
| 51 | s5 | 149 | VAL |
| 51 | s5 | 156 | ARG |
| 51 | s5 | 157 | ARG |
| 51 | s5 | 194 | LEU |
| 79 | s6 | 7 | TYR |
| 79 | s6 | 71 | THR |
| 79 | s6 | 108 | VAL |
| 79 | s6 | 111 | LEU |
| 79 | s6 | 115 | LYS |
| 79 | s6 | 122 | GLU |
| 79 | s6 | 124 | LEU |
| 79 | s6 | 125 | THR |
| 79 | s6 | 136 | LYS |
| 79 | s6 | 151 | ASP |
| 79 | s6 | 153 | VAL |
| 79 | s6 | 156 | PHE |
| 79 | s6 | 164 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 79 | s6 | 169 | TYR |
| 79 | s6 | 177 | ARG |
| 79 | s6 | 193 | LEU |
| 79 | s6 | 197 | ASN |
| 79 | s6 | 212 | LEU |
| 79 | s6 | 216 | LEU |
| 53 | s7 | 2 | SER |
| 53 | s7 | 34 | LEU |
| 53 | s7 | 38 | LEU |
| 53 | s7 | 50 | ASP |
| 53 | s7 | 55 | LYS |
| 53 | s7 | 64 | VAL |
| 53 | s7 | 97 | ARG |
| 53 | s7 | 110 | GLN |
| 53 | s7 | 112 | ARG |
| 53 | s7 | 114 | ARG |
| 53 | s7 | 116 | ARG |
| 53 | s7 | 127 | GLU |
| 53 | s7 | 139 | ARG |
| 53 | s7 | 157 | LYS |
| 53 | s7 | 159 | VAL |
| 53 | s7 | 163 | ASP |
| 54 | s8 | 29 | LEU |
| 54 | s8 | 36 | THR |
| 54 | s8 | 46 | VAL |
| 54 | s8 | 72 | ILE |
| 54 | s8 | 88 | ASN |
| 54 | s8 | 158 | SER |
| 54 | s8 | 199 | LYS |
| 54 | s8 | 200 | LYS |
| 55 | s9 | 13 | SER |
| 55 | s9 | 14 | THR |
| 55 | s9 | 17 | ARG |
| 55 | s9 | 28 | LEU |
| 55 | s9 | 39 | LYS |
| 55 | s9 | 59 | LEU |
| 55 | s9 | 78 | ARG |
| 55 | s9 | 105 | LEU |
| 55 | s9 | 130 | THR |
| 55 | s9 | 141 | VAL |
| 55 | s9 | 149 | ARG |
| 55 | s9 | 154 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 56 | c0 | 3 | MET |
| 56 | c0 | 15 | LEU |
| 56 | c0 | 28 | ASN |
| 56 | c0 | 41 | TYR |
| 56 | c0 | 55 | VAL |
| 57 | c1 | 5 | LEU |
| 57 | c1 | 16 | GLN |
| 57 | c1 | 28 | SER |
| 57 | c1 | 33 | ARG |
| 57 | c1 | 60 | PHE |
| 57 | c1 | 67 | ARG |
| 57 | c1 | 82 | ARG |
| 57 | c1 | 102 | LYS |
| 57 | c1 | 116 | ARG |
| 57 | c1 | 121 | ASP |
| 57 | c1 | 129 | ARG |
| 57 | c1 | 138 | ASN |
| 58 | c2 | 25 | GLU |
| 58 | c2 | 54 | ARG |
| 58 | c2 | 58 | LEU |
| 58 | c2 | 61 | VAL |
| 58 | c2 | 62 | LEU |
| 58 | c2 | 63 | VAL |
| 58 | c2 | 74 | LEU |
| 58 | c2 | 85 | LYS |
| 58 | c2 | 88 | LEU |
| 58 | c2 | 89 | ILE |
| 58 | c2 | 97 | LEU |
| 58 | c2 | 103 | LEU |
| 58 | c2 | 126 | TRP |
| 58 | c2 | 129 | GLU |
| 58 | c2 | 138 | GLU |
| 58 | c2 | 140 | PHE |
| 59 | c3 | 12 | SER |
| 59 | c3 | 20 | ARG |
| 59 | c3 | 64 | ARG |
| 59 | c3 | 65 | VAL |
| 59 | c3 | 70 | LYS |
| 59 | c3 | 72 | MET |
| 59 | c3 | 94 | LYS |
| 59 | c3 | 115 | LEU |
| 59 | c3 | 125 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 59 | c3 | 139 | TRP |
| 59 | c3 | 141 | TYR |
| 60 | c4 | 10 | ASN |
| 60 | c4 | 14 | PHE |
| 60 | c4 | 16 | VAL |
| 60 | c4 | 20 | TYR |
| 60 | c4 | 58 | TYR |
| 60 | c4 | 66 | ASP |
| 60 | c4 | 102 | LEU |
| 60 | c4 | 110 | LEU |
| 60 | c4 | 116 | GLU |
| 60 | c4 | 118 | VAL |
| 60 | c4 | 124 | ASP |
| 60 | c4 | 136 | ARG |
| 60 | c4 | 137 | LEU |
| 61 | c5 | 10 | ARG |
| 61 | c5 | 22 | LEU |
| 61 | c5 | 36 | LEU |
| 61 | c5 | 40 | ARG |
| 61 | c5 | 49 | MET |
| 61 | c5 | 50 | THR |
| 61 | c5 | 52 | LYS |
| 61 | c5 | 56 | PHE |
| 61 | c5 | 69 | GLU |
| 61 | c5 | 77 | ARG |
| 61 | c5 | 93 | VAL |
| 61 | c5 | 102 | PHE |
| 61 | c5 | 107 | ILE |
| 61 | c5 | 124 | THR |
| 61 | c5 | 126 | VAL |
| 61 | c5 | 128 | HIS |
| 61 | c5 | 130 | ARG |
| 62 | c6 | 23 | LYS |
| 62 | c6 | 26 | LYS |
| 62 | c6 | 40 | GLU |
| 62 | c6 | 62 | ASN |
| 62 | c6 | 64 | ASP |
| 62 | c6 | 66 | ARG |
| 62 | c6 | 68 | ARG |
| 62 | c6 | 97 | VAL |
| 62 | c6 | 109 | PHE |
| 62 | c6 | 114 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 63 | c7 | 24 | LEU |
| 63 | c7 | 29 | GLN |
| 63 | c7 | 78 | ARG |
| 63 | c7 | 79 | GLU |
| 63 | c7 | 84 | TYR |
| 63 | c7 | 108 | ASP |
| 64 | c8 | 7 | GLU |
| 64 | c8 | 26 | ILE |
| 64 | c8 | 61 | LEU |
| 64 | c8 | 66 | LEU |
| 64 | c8 | 85 | PHE |
| 64 | c8 | 88 | ARG |
| 64 | c8 | 91 | ASP |
| 64 | c8 | 94 | ASP |
| 64 | c8 | 97 | ASP |
| 64 | c8 | 104 | ASN |
| 64 | c8 | 112 | ASP |
| 64 | c8 | 115 | ARG |
| 64 | c8 | 116 | LEU |
| 64 | c8 | 136 | GLN |
| 65 | c9 | 18 | TYR |
| 65 | c9 | 33 | TYR |
| 65 | c9 | 34 | VAL |
| 65 | c9 | 41 | SER |
| 65 | c9 | 70 | GLN |
| 65 | c9 | 95 | ASP |
| 65 | c9 | 111 | ILE |
| 65 | c9 | 122 | ARG |
| 65 | c9 | 123 | ARG |
| 65 | c9 | 133 | ASP |
| 65 | c9 | 141 | GLU |
| 66 | d0 | 14 | GLN |
| 66 | d0 | 15 | GLN |
| 66 | d0 | 16 | GLN |
| 66 | d0 | 18 | GLN |
| 66 | d0 | 19 | ILE |
| 66 | d0 | 21 | LYS |
| 66 | d0 | 23 | ARG |
| 66 | d0 | 34 | LEU |
| 66 | d0 | 46 | GLU |
| 66 | d0 | 57 | ARG |
| 66 | d0 | 61 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 66 | d0 | 74 | GLU |
| 66 | d0 | 102 | ARG |
| 66 | d0 | 116 | VAL |
| 67 | d1 | 3 | ASN |
| 67 | d1 | 5 | LYS |
| 67 | d1 | 11 | LEU |
| 67 | d1 | 41 | GLU |
| 67 | d1 | 44 | ARG |
| 67 | d1 | 59 | VAL |
| 67 | d1 | 62 | ARG |
| 67 | d1 | 70 | ASN |
| 67 | d1 | 71 | ARG |
| 67 | d1 | 76 | ASP |
| 67 | d1 | 78 | LEU |
| 68 | d2 | 4 | SER |
| 68 | d2 | 6 | VAL |
| 68 | d2 | 25 | VAL |
| 68 | d2 | 28 | ARG |
| 68 | d2 | 37 | PHE |
| 68 | d2 | 42 | GLN |
| 68 | d2 | 55 | ASP |
| 68 | d2 | 68 | ARG |
| 68 | d2 | 93 | LEU |
| 68 | d2 | 98 | GLN |
| 68 | d2 | 103 | ILE |
| 68 | d2 | 126 | LEU |
| 68 | d2 | 129 | VAL |
| 69 | d3 | 9 | LEU |
| 69 | d3 | 19 | ARG |
| 69 | d3 | 99 | ASN |
| 69 | d3 | 107 | PHE |
| 69 | d3 | 131 | SER |
| 69 | d3 | 132 | LEU |
| 69 | d3 | 144 | ARG |
| 70 | d4 | 10 | ARG |
| 70 | d4 | 28 | LEU |
| 70 | d4 | 35 | VAL |
| 70 | d4 | 37 | LYS |
| 70 | d4 | 49 | LYS |
| 70 | d4 | 72 | PHE |
| 70 | d4 | 91 | LEU |
| 70 | d4 | 93 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 71 | d5 | 37 | GLN |
| 71 | d5 | 46 | LYS |
| 71 | d5 | 49 | ARG |
| 71 | d5 | 52 | LYS |
| 71 | d5 | 53 | GLU |
| 71 | d5 | 60 | VAL |
| 71 | d5 | 67 | ASP |
| 71 | d5 | 85 | LYS |
| 71 | d5 | 89 | ILE |
| 71 | d5 | 98 | GLN |
| 72 | d6 | 7 | SER |
| 72 | d6 | 26 | CYS |
| 72 | d6 | 27 | SER |
| 72 | d6 | 28 | LYS |
| 72 | d6 | 46 | GLU |
| 72 | d6 | 53 | LEU |
| 72 | d6 | 58 | VAL |
| 72 | d6 | 61 | GLU |
| 72 | d6 | 82 | ARG |
| 72 | d6 | 84 | VAL |
| 73 | d7 | 23 | THR |
| 73 | d7 | 42 | ASN |
| 73 | d7 | 56 | CYS |
| 73 | d7 | 59 | CYS |
| 73 | d7 | 77 | THR |
| 73 | d7 | 81 | ARG |
| 74 | d8 | 7 | VAL |
| 74 | d8 | 8 | THR |
| 74 | d8 | 15 | VAL |
| 74 | d8 | 32 | PHE |
| 74 | d8 | 61 | ARG |
| 74 | d8 | 64 | ARG |
| 75 | d9 | 5 | ASN |
| 75 | d9 | 8 | PHE |
| 75 | d9 | 14 | TYR |
| 75 | d9 | 30 | LEU |
| 75 | d9 | 32 | ARG |
| 75 | d9 | 44 | ARG |
| 75 | d9 | 54 | LYS |
| 76 | e0 | 44 | PHE |
| 76 | e0 | 46 | ASN |
| 76 | e0 | 49 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | e0 | 51 | ASN |
| 76 | e0 | 53 | LYS |
| 76 | e0 | 54 | ARG |
| 76 | e0 | 56 | MET |
| 77 | sR | 4 | ASN |
| 77 | sR | 5 | GLU |
| 77 | sR | 9 | LEU |
| 77 | sR | 16 | HIS |
| 77 | sR | 29 | GLN |
| 77 | sR | 38 | ARG |
| 77 | sR | 60 | SER |
| 77 | sR | 106 | HIS |
| 77 | sR | 127 | ARG |
| 77 | sR | 139 | GLN |
| 77 | sR | 140 | CYS |
| 77 | sR | 145 | LEU |
| 77 | sR | 163 | ASP |
| 77 | sR | 167 | VAL |
| 77 | sR | 185 | GLN |
| 77 | sR | 207 | ASP |
| 77 | sR | 248 | ASN |
| 77 | sR | 250 | TYR |
| 77 | sR | 251 | TRP |
| 77 | sR | 290 | VAL |
| 77 | sR | 316 | MET |
| 78 | sM | 30 | THR |
| 78 | sM | 53 | ARG |
| 78 | sM | 63 | ASP |
| 78 | sM | 83 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | L2 | 209 | HIS |
| 4 | L2 | 216 | HIS |
| 7 | L5 | 40 | HIS |
| 10 | L8 | 79 | GLN |
| 12 | M0 | 112 | GLN |
| 13 | M1 | 109 | HIS |
| 14 | M3 | 99 | HIS |
| 16 | M5 | 194 | GLN |
| 18 | M7 | 10 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | N0 | 62 | ASN |
| 22 | N1 | 77 | ASN |
| 24 | N3 | 33 | ASN |
| 46 | S0 | 23 | HIS |
| 46 | S0 | 30 | GLN |
| 47 | S1 | 149 | GLN |
| 50 | S4 | 130 | GLN |
| 51 | S5 | 44 | ASN |
| 52 | S6 | 13 | GLN |
| 52 | S6 | 176 | GLN |
| 55 | S9 | 48 | GLN |
| 56 | C0 | 39 | ASN |
| 60 | C4 | 29 | HIS |
| 67 | D1 | 3 | ASN |
| 68 | D2 | 56 | HIS |
| 69 | D3 | 48 | HIS |
| 70 | D4 | 29 | HIS |
| 72 | D6 | 25 | ASN |
| 4 | l2 | 50 | HIS |
| 6 | l4 | 316 | ASN |
| 12 | m0 | 112 | GLN |
| 21 | n0 | 8 | GLN |
| 24 | n3 | 33 | ASN |
| 24 | n3 | 47 | ASN |
| 25 | n4 | 32 | GLN |
| 28 | n7 | 57 | HIS |
| 28 | n7 | 78 | ASN |
| 51 | s5 | 63 | GLN |
| 51 | s5 | 122 | ASN |
| 79 | s6 | 201 | GLN |
| 53 | s7 | 86 | GLN |
| 53 | s7 | 180 | GLN |
| 56 | c0 | 12 | HIS |
| 56 | c0 | 32 | HIS |
| 56 | c0 | 47 | GLN |
| 57 | c1 | 104 | HIS |
| 64 | c8 | 99 | HIS |
| 66 | d0 | 16 | GLN |
| 66 | d0 | 72 | ASN |
| 74 | d8 | 27 | GLN |
| 77 | sR | 182 | ASN |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1 | 3069/3396 (90%) | 618 (20%) | 56 (1%) |
| 1 | 5 | 3080/3396 (90%) | 657 (21%) | 53 (1%) |
| 2 | 3 | 120/121 (99%) | 22 (18%) | 1 (0%) |
| 2 | 7 | 120/121 (99%) | 20 (16%) | 0 |
| 3 | 4 | 156/158 (98%) | 35 (22%) | 4 (2%) |
| 3 | 8 | 157/158 (99%) | 35 (22%) | 7 (4%) |
| 45 | 2 | 1708/1800 (94%) | 485 (28%) | 33 (1%) |
| 45 | 6 | 1678/1800 (93%) | 453 (26%) | 39 (2%) |
| All | All | 10088/10950 (92%) | 2325 (23%) | 193 (1%) |

All (2325) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 6 | A |
| 1 | 1 | 25 | U |
| 1 | 1 | 26 | A |
| 1 | 1 | 30 | G |
| 1 | 1 | 40 | A |
| 1 | 1 | 42 | C |
| 1 | 1 | 49 | A |
| 1 | 1 | 57 | A |
| 1 | 1 | 59 | G |
| 1 | 1 | 60 | A |
| 1 | 1 | 65 | A |
| 1 | 1 | 66 | A |
| 1 | 1 | 76 | G |
| 1 | 1 | 87 | U |
| 1 | 1 | 88 | A |
| 1 | 1 | 92 | G |
| 1 | 1 | 93 | C |
| 1 | 1 | 99 | A |
| 1 | 1 | 109 | A |
| 1 | 1 | 110 | G |
| 1 | 1 | 111 | C |
| 1 | 1 | 116 | A |
| 1 | 1 | 121 | A |
| 1 | 1 | 122 | A |
| 1 | 1 | 132 | C |
| 1 | 1 | 133 | U |
| 1 | 1 | 135 | C |
| 1 | 1 | 136 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 139 | G |
| 1 | 1 | 146 | U |
| 1 | 1 | 154 | U |
| 1 | 1 | 156 | G |
| 1 | 1 | 157 | A |
| 1 | 1 | 162 | G |
| 1 | 1 | 163 | C |
| 1 | 1 | 166 | C |
| 1 | 1 | 187 | A |
| 1 | 1 | 190 | U |
| 1 | 1 | 191 | U |
| 1 | 1 | 192 | C |
| 1 | 1 | 200 | C |
| 1 | 1 | 210 | U |
| 1 | 1 | 211 | A |
| 1 | 1 | 213 | A |
| 1 | 1 | 218 | G |
| 1 | 1 | 219 | A |
| 1 | 1 | 230 | U |
| 1 | 1 | 231 | G |
| 1 | 1 | 235 | A |
| 1 | 1 | 240 | U |
| 1 | 1 | 241 | G |
| 1 | 1 | 242 | C |
| 1 | 1 | 243 | G |
| 1 | 1 | 244 | G |
| 1 | 1 | 245 | U |
| 1 | 1 | 246 | U |
| 1 | 1 | 250 | U |
| 1 | 1 | 251 | G |
| 1 | 1 | 252 | U |
| 1 | 1 | 253 | A |
| 1 | 1 | 269 | G |
| 1 | 1 | 282 | G |
| 1 | 1 | 286 | U |
| 1 | 1 | 295 | A |
| 1 | 1 | 298 | U |
| 1 | 1 | 305 | U |
| 1 | 1 | 315 | C |
| 1 | 1 | 323 | A |
| 1 | 1 | 329 | U |
| 1 | 1 | 338 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 339 | C |
| 1 | 1 | 350 | C |
| 1 | 1 | 351 | A |
| 1 | 1 | 376 | G |
| 1 | 1 | 391 | A |
| 1 | 1 | 397 | A |
| 1 | 1 | 398 | A |
| 1 | 1 | 399 | A |
| 1 | 1 | 401 | U |
| 1 | 1 | 402 | A |
| 1 | 1 | 403 | C |
| 1 | 1 | 420 | G |
| 1 | 1 | 421 | G |
| 1 | 1 | 422 | A |
| 1 | 1 | 436 | A |
| 1 | 1 | 437 | G |
| 1 | 1 | 495 | G |
| 1 | 1 | 496 | C |
| 1 | 1 | 520 | U |
| 1 | 1 | 521 | A |
| 1 | 1 | 532 | A |
| 1 | 1 | 535 | G |
| 1 | 1 | 545 | U |
| 1 | 1 | 548 | G |
| 1 | 1 | 549 | U |
| 1 | 1 | 552 | G |
| 1 | 1 | 556 | U |
| 1 | 1 | 557 | A |
| 1 | 1 | 558 | U |
| 1 | 1 | 559 | A |
| 1 | 1 | 568 | G |
| 1 | 1 | 569 | A |
| 1 | 1 | 578 | A |
| 1 | 1 | 579 | G |
| 1 | 1 | 589 | A |
| 1 | 1 | 594 | U |
| 1 | 1 | 600 | G |
| 1 | 1 | 604 | G |
| 1 | 1 | 607 | A |
| 1 | 1 | 609 | G |
| 1 | 1 | 611 | A |
| 1 | 1 | 619 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 620 | U |
| 1 | 1 | 621 | A |
| 1 | 1 | 622 | A |
| 1 | 1 | 625 | G |
| 1 | 1 | 636 | C |
| 1 | 1 | 637 | C |
| 1 | 1 | 638 | C |
| 1 | 1 | 649 | A |
| 1 | 1 | 660 | A |
| 1 | 1 | 677 | A |
| 1 | 1 | 681 | U |
| 1 | 1 | 689 | U |
| 1 | 1 | 697 | A |
| 1 | 1 | 705 | A |
| 1 | 1 | 712 | G |
| 1 | 1 | 715 | A |
| 1 | 1 | 716 | A |
| 1 | 1 | 718 | G |
| 1 | 1 | 720 | A |
| 1 | 1 | 721 | G |
| 1 | 1 | 741 | U |
| 1 | 1 | 764 | U |
| 1 | 1 | 765 | C |
| 1 | 1 | 767 | U |
| 1 | 1 | 768 | C |
| 1 | 1 | 773 | G |
| 1 | 1 | 774 | G |
| 1 | 1 | 775 | A |
| 1 | 1 | 776 | U |
| 1 | 1 | 777 | U |
| 1 | 1 | 781 | G |
| 1 | 1 | 785 | G |
| 1 | 1 | 806 | A |
| 1 | 1 | 817 | A |
| 1 | 1 | 818 | C |
| 1 | 1 | 830 | A |
| 1 | 1 | 849 | C |
| 1 | 1 | 861 | C |
| 1 | 1 | 863 | C |
| 1 | 1 | 869 | G |
| 1 | 1 | 871 | U |
| 1 | 1 | 874 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 879 | U |
| 1 | 1 | 890 | C |
| 1 | 1 | 896 | A |
| 1 | 1 | 907 | G |
| 1 | 1 | 908 | G |
| 1 | 1 | 914 | A |
| 1 | 1 | 916 | G |
| 1 | 1 | 917 | A |
| 1 | 1 | 920 | A |
| 1 | 1 | 921 | A |
| 1 | 1 | 924 | G |
| 1 | 1 | 926 | A |
| 1 | 1 | 934 | G |
| 1 | 1 | 937 | G |
| 1 | 1 | 944 | C |
| 1 | 1 | 959 | C |
| 1 | 1 | 960 | U |
| 1 | 1 | 964 | G |
| 1 | 1 | 979 | U |
| 1 | 1 | 980 | A |
| 1 | 1 | 982 | C |
| 1 | 1 | 995 | U |
| 1 | 1 | 1000 | C |
| 1 | 1 | 1001 | G |
| 1 | 1 | 1002 | A |
| 1 | 1 | 1010 | G |
| 1 | 1 | 1015 | U |
| 1 | 1 | 1017 | C |
| 1 | 1 | 1018 | G |
| 1 | 1 | 1020 | G |
| 1 | 1 | 1021 | G |
| 1 | 1 | 1032 | C |
| 1 | 1 | 1036 | A |
| 1 | 1 | 1038 | C |
| 1 | 1 | 1041 | U |
| 1 | 1 | 1046 | A |
| 1 | 1 | 1047 | A |
| 1 | 1 | 1049 | C |
| 1 | 1 | 1064 | A |
| 1 | 1 | 1065 | A |
| 1 | 1 | 1066 | G |
| 1 | 1 | 1068 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1071 | U |
| 1 | 1 | 1072 | G |
| 1 | 1 | 1081 | U |
| 1 | 1 | 1082 | U |
| 1 | 1 | 1088 | U |
| 1 | 1 | 1093 | A |
| 1 | 1 | 1094 | U |
| 1 | 1 | 1095 | U |
| 1 | 1 | 1096 | U |
| 1 | 1 | 1097 | G |
| 1 | 1 | 1098 | A |
| 1 | 1 | 1103 | A |
| 1 | 1 | 1104 | G |
| 1 | 1 | 1105 | A |
| 1 | 1 | 1117 | G |
| 1 | 1 | 1128 | U |
| 1 | 1 | 1131 | G |
| 1 | 1 | 1140 | G |
| 1 | 1 | 1144 | U |
| 1 | 1 | 1153 | A |
| 1 | 1 | 1159 | A |
| 1 | 1 | 1161 | G |
| 1 | 1 | 1177 | G |
| 1 | 1 | 1179 | A |
| 1 | 1 | 1180 | A |
| 1 | 1 | 1181 | U |
| 1 | 1 | 1182 | A |
| 1 | 1 | 1191 | U |
| 1 | 1 | 1192 | C |
| 1 | 1 | 1193 | A |
| 1 | 1 | 1196 | C |
| 1 | 1 | 1201 | C |
| 1 | 1 | 1209 | G |
| 1 | 1 | 1212 | A |
| 1 | 1 | 1216 | C |
| 1 | 1 | 1222 | G |
| 1 | 1 | 1229 | G |
| 1 | 1 | 1230 | G |
| 1 | 1 | 1285 | G |
| 1 | 1 | 1286 | A |
| 1 | 1 | 1287 | A |
| 1 | 1 | 1292 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1300 | G |
| 1 | 1 | 1307 | G |
| 1 | 1 | 1313 | G |
| 1 | 1 | 1318 | A |
| 1 | 1 | 1330 | A |
| 1 | 1 | 1345 | G |
| 1 | 1 | 1348 | U |
| 1 | 1 | 1356 | U |
| 1 | 1 | 1357 | G |
| 1 | 1 | 1385 | C |
| 1 | 1 | 1386 | A |
| 1 | 1 | 1399 | A |
| 1 | 1 | 1400 | G |
| 1 | 1 | 1416 | C |
| 1 | 1 | 1417 | G |
| 1 | 1 | 1418 | A |
| 1 | 1 | 1419 | A |
| 1 | 1 | 1431 | G |
| 1 | 1 | 1434 | G |
| 1 | 1 | 1437 | C |
| 1 | 1 | 1438 | U |
| 1 | 1 | 1446 | A |
| 1 | 1 | 1450 | G |
| 1 | 1 | 1460 | A |
| 1 | 1 | 1481 | A |
| 1 | 1 | 1482 | A |
| 1 | 1 | 1483 | G |
| 1 | 1 | 1485 | G |
| 1 | 1 | 1488 | G |
| 1 | 1 | 1502 | C |
| 1 | 1 | 1508 | C |
| 1 | 1 | 1523 | U |
| 1 | 1 | 1527 | C |
| 1 | 1 | 1528 | G |
| 1 | 1 | 1529 | A |
| 1 | 1 | 1533 | U |
| 1 | 1 | 1536 | G |
| 1 | 1 | 1539 | A |
| 1 | 1 | 1541 | G |
| 1 | 1 | 1553 | U |
| 1 | 1 | 1554 | U |
| 1 | 1 | 1555 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1556 | C |
| 1 | 1 | 1557 | A |
| 1 | 1 | 1561 | G |
| 1 | 1 | 1563 | C |
| 1 | 1 | 1564 | U |
| 1 | 1 | 1565 | G |
| 1 | 1 | 1566 | A |
| 1 | 1 | 1567 | U |
| 1 | 1 | 1568 | U |
| 1 | 1 | 1569 | U |
| 1 | 1 | 1570 | U |
| 1 | 1 | 1571 | A |
| 1 | 1 | 1572 | U |
| 1 | 1 | 1573 | G |
| 1 | 1 | 1574 | C |
| 1 | 1 | 1575 | A |
| 1 | 1 | 1576 | G |
| 1 | 1 | 1578 | C |
| 1 | 1 | 1579 | C |
| 1 | 1 | 1580 | A |
| 1 | 1 | 1581 | C |
| 1 | 1 | 1582 | C |
| 1 | 1 | 1583 | A |
| 1 | 1 | 1587 | A |
| 1 | 1 | 1589 | A |
| 1 | 1 | 1605 | A |
| 1 | 1 | 1607 | U |
| 1 | 1 | 1620 | U |
| 1 | 1 | 1629 | U |
| 1 | 1 | 1632 | A |
| 1 | 1 | 1639 | C |
| 1 | 1 | 1641 | U |
| 1 | 1 | 1642 | A |
| 1 | 1 | 1643 | A |
| 1 | 1 | 1644 | C |
| 1 | 1 | 1645 | U |
| 1 | 1 | 1657 | C |
| 1 | 1 | 1658 | G |
| 1 | 1 | 1673 | G |
| 1 | 1 | 1675 | G |
| 1 | 1 | 1683 | A |
| 1 | 1 | 1688 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1716 | U |
| 1 | 1 | 1717 | U |
| 1 | 1 | 1724 | U |
| 1 | 1 | 1725 | C |
| 1 | 1 | 1740 | U |
| 1 | 1 | 1743 | G |
| 1 | 1 | 1750 | A |
| 1 | 1 | 1751 | G |
| 1 | 1 | 1760 | A |
| 1 | 1 | 1763 | U |
| 1 | 1 | 1764 | U |
| 1 | 1 | 1770 | G |
| 1 | 1 | 1780 | G |
| 1 | 1 | 1787 | A |
| 1 | 1 | 1790 | G |
| 1 | 1 | 1797 | A |
| 1 | 1 | 1808 | G |
| 1 | 1 | 1813 | A |
| 1 | 1 | 1816 | A |
| 1 | 1 | 1821 | U |
| 1 | 1 | 1841 | A |
| 1 | 1 | 1842 | A |
| 1 | 1 | 1846 | C |
| 1 | 1 | 1847 | A |
| 1 | 1 | 1850 | A |
| 1 | 1 | 1866 | C |
| 1 | 1 | 1867 | A |
| 1 | 1 | 1877 | U |
| 1 | 1 | 1879 | A |
| 1 | 1 | 1886 | A |
| 1 | 1 | 1906 | G |
| 1 | 1 | 1952 | G |
| 1 | 1 | 2093 | A |
| 1 | 1 | 2094 | C |
| 1 | 1 | 2100 | A |
| 1 | 1 | 2101 | C |
| 1 | 1 | 2102 | U |
| 1 | 1 | 2113 | A |
| 1 | 1 | 2114 | C |
| 1 | 1 | 2121 | G |
| 1 | 1 | 2122 | G |
| 1 | 1 | 2130 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2131 | A |
| 1 | 1 | 2140 | U |
| 1 | 1 | 2144 | A |
| 1 | 1 | 2158 | A |
| 1 | 1 | 2169 | G |
| 1 | 1 | 2170 | U |
| 1 | 1 | 2188 | A |
| 1 | 1 | 2205 | U |
| 1 | 1 | 2206 | G |
| 1 | 1 | 2207 | A |
| 1 | 1 | 2209 | U |
| 1 | 1 | 2210 | G |
| 1 | 1 | 2223 | A |
| 1 | 1 | 2246 | G |
| 1 | 1 | 2248 | C |
| 1 | 1 | 2249 | G |
| 1 | 1 | 2250 | G |
| 1 | 1 | 2251 | G |
| 1 | 1 | 2252 | A |
| 1 | 1 | 2256 | A |
| 1 | 1 | 2257 | C |
| 1 | 1 | 2272 | G |
| 1 | 1 | 2273 | G |
| 1 | 1 | 2276 | G |
| 1 | 1 | 2280 | A |
| 1 | 1 | 2281 | A |
| 1 | 1 | 2282 | U |
| 1 | 1 | 2288 | G |
| 1 | 1 | 2295 | A |
| 1 | 1 | 2306 | C |
| 1 | 1 | 2307 | G |
| 1 | 1 | 2308 | C |
| 1 | 1 | 2309 | A |
| 1 | 1 | 2310 | U |
| 1 | 1 | 2313 | A |
| 1 | 1 | 2314 | U |
| 1 | 1 | 2315 | G |
| 1 | 1 | 2319 | U |
| 1 | 1 | 2334 | U |
| 1 | 1 | 2336 | U |
| 1 | 1 | 2361 | A |
| 1 | 1 | 2372 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2373 | A |
| 1 | 1 | 2374 | C |
| 1 | 1 | 2375 | G |
| 1 | 1 | 2383 | C |
| 1 | 1 | 2385 | G |
| 1 | 1 | 2388 | U |
| 1 | 1 | 2393 | G |
| 1 | 1 | 2394 | G |
| 1 | 1 | 2397 | A |
| 1 | 1 | 2402 | A |
| 1 | 1 | 2403 | G |
| 1 | 1 | 2404 | A |
| 1 | 1 | 2406 | C |
| 1 | 1 | 2411 | U |
| 1 | 1 | 2413 | A |
| 1 | 1 | 2414 | G |
| 1 | 1 | 2418 | G |
| 1 | 1 | 2419 | A |
| 1 | 1 | 2435 | G |
| 1 | 1 | 2441 | A |
| 1 | 1 | 2442 | G |
| 1 | 1 | 2507 | C |
| 1 | 1 | 2510 | U |
| 1 | 1 | 2511 | A |
| 1 | 1 | 2514 | U |
| 1 | 1 | 2515 | A |
| 1 | 1 | 2522 | G |
| 1 | 1 | 2533 | G |
| 1 | 1 | 2536 | A |
| 1 | 1 | 2537 | U |
| 1 | 1 | 2538 | U |
| 1 | 1 | 2539 | C |
| 1 | 1 | 2540 | A |
| 1 | 1 | 2541 | U |
| 1 | 1 | 2542 | U |
| 1 | 1 | 2543 | U |
| 1 | 1 | 2544 | U |
| 1 | 1 | 2545 | C |
| 1 | 1 | 2546 | C |
| 1 | 1 | 2549 | G |
| 1 | 1 | 2552 | C |
| 1 | 1 | 2554 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2555 | G |
| 1 | 1 | 2569 | A |
| 1 | 1 | 2570 | U |
| 1 | 1 | 2571 | U |
| 1 | 1 | 2572 | C |
| 1 | 1 | 2573 | G |
| 1 | 1 | 2585 | G |
| 1 | 1 | 2593 | A |
| 1 | 1 | 2594 | C |
| 1 | 1 | 2606 | G |
| 1 | 1 | 2607 | G |
| 1 | 1 | 2614 | G |
| 1 | 1 | 2626 | A |
| 1 | 1 | 2629 | U |
| 1 | 1 | 2637 | A |
| 1 | 1 | 2638 | C |
| 1 | 1 | 2652 | U |
| 1 | 1 | 2656 | A |
| 1 | 1 | 2657 | A |
| 1 | 1 | 2674 | A |
| 1 | 1 | 2676 | A |
| 1 | 1 | 2677 | G |
| 1 | 1 | 2678 | A |
| 1 | 1 | 2681 | U |
| 1 | 1 | 2688 | U |
| 1 | 1 | 2689 | A |
| 1 | 1 | 2691 | A |
| 1 | 1 | 2694 | A |
| 1 | 1 | 2696 | A |
| 1 | 1 | 2705 | A |
| 1 | 1 | 2714 | G |
| 1 | 1 | 2723 | U |
| 1 | 1 | 2728 | G |
| 1 | 1 | 2737 | C |
| 1 | 1 | 2752 | U |
| 1 | 1 | 2753 | G |
| 1 | 1 | 2762 | A |
| 1 | 1 | 2772 | C |
| 1 | 1 | 2777 | G |
| 1 | 1 | 2778 | G |
| 1 | 1 | 2779 | A |
| 1 | 1 | 2796 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2800 | G |
| 1 | 1 | 2801 | A |
| 1 | 1 | 2810 | C |
| 1 | 1 | 2814 | G |
| 1 | 1 | 2817 | A |
| 1 | 1 | 2818 | U |
| 1 | 1 | 2837 | A |
| 1 | 1 | 2842 | U |
| 1 | 1 | 2845 | A |
| 1 | 1 | 2847 | A |
| 1 | 1 | 2853 | A |
| 1 | 1 | 2861 | U |
| 1 | 1 | 2871 | G |
| 1 | 1 | 2872 | A |
| 1 | 1 | 2873 | U |
| 1 | 1 | 2876 | C |
| 1 | 1 | 2887 | A |
| 1 | 1 | 2889 | C |
| 1 | 1 | 2899 | C |
| 1 | 1 | 2904 | U |
| 1 | 1 | 2910 | A |
| 1 | 1 | 2923 | U |
| 1 | 1 | 2935 | U |
| 1 | 1 | 2936 | A |
| 1 | 1 | 2938 | G |
| 1 | 1 | 2942 | C |
| 1 | 1 | 2947 | G |
| 1 | 1 | 2949 | U |
| 1 | 1 | 2954 | U |
| 1 | 1 | 2971 | A |
| 1 | 1 | 2972 | G |
| 1 | 1 | 2977 | G |
| 1 | 1 | 2983 | C |
| 1 | 1 | 2990 | G |
| 1 | 1 | 2992 | U |
| 1 | 1 | 2996 | U |
| 1 | 1 | 2997 | G |
| 1 | 1 | 3012 | A |
| 1 | 1 | 3030 | G |
| 1 | 1 | 3033 | A |
| 1 | 1 | 3056 | U |
| 1 | 1 | 3058 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 3059 | G |
| 1 | 1 | 3078 | U |
| 1 | 1 | 3079 | U |
| 1 | 1 | 3086 | A |
| 1 | 1 | 3092 | C |
| 1 | 1 | 3113 | A |
| 1 | 1 | 3122 | A |
| 1 | 1 | 3130 | A |
| 1 | 1 | 3131 | U |
| 1 | 1 | 3142 | A |
| 1 | 1 | 3143 | C |
| 1 | 1 | 3150 | A |
| 1 | 1 | 3151 | U |
| 1 | 1 | 3152 | U |
| 1 | 1 | 3163 | A |
| 1 | 1 | 3164 | C |
| 1 | 1 | 3165 | A |
| 1 | 1 | 3167 | A |
| 1 | 1 | 3168 | A |
| 1 | 1 | 3169 | U |
| 1 | 1 | 3170 | A |
| 1 | 1 | 3171 | U |
| 1 | 1 | 3173 | G |
| 1 | 1 | 3174 | A |
| 1 | 1 | 3176 | G |
| 1 | 1 | 3179 | U |
| 1 | 1 | 3180 | A |
| 1 | 1 | 3181 | C |
| 1 | 1 | 3187 | A |
| 1 | 1 | 3194 | C |
| 1 | 1 | 3196 | U |
| 1 | 1 | 3202 | G |
| 1 | 1 | 3207 | U |
| 1 | 1 | 3210 | A |
| 1 | 1 | 3217 | C |
| 1 | 1 | 3218 | A |
| 1 | 1 | 3219 | G |
| 1 | 1 | 3228 | C |
| 1 | 1 | 3229 | G |
| 1 | 1 | 3244 | A |
| 1 | 1 | 3245 | A |
| 1 | 1 | 3247 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 3253 | G |
| 1 | 1 | 3254 | G |
| 1 | 1 | 3259 | U |
| 1 | 1 | 3263 | G |
| 1 | 1 | 3270 | U |
| 1 | 1 | 3271 | G |
| 1 | 1 | 3273 | A |
| 1 | 1 | 3275 | U |
| 1 | 1 | 3276 | G |
| 1 | 1 | 3279 | A |
| 1 | 1 | 3281 | U |
| 1 | 1 | 3286 | G |
| 1 | 1 | 3287 | U |
| 1 | 1 | 3288 | G |
| 1 | 1 | 3289 | G |
| 1 | 1 | 3295 | A |
| 1 | 1 | 3304 | U |
| 1 | 1 | 3309 | G |
| 1 | 1 | 3316 | A |
| 1 | 1 | 3317 | U |
| 1 | 1 | 3318 | G |
| 1 | 1 | 3319 | U |
| 1 | 1 | 3320 | A |
| 1 | 1 | 3335 | A |
| 1 | 1 | 3341 | U |
| 1 | 1 | 3342 | A |
| 1 | 1 | 3345 | G |
| 1 | 1 | 3347 | A |
| 1 | 1 | 3350 | C |
| 1 | 1 | 3351 | U |
| 1 | 1 | 3352 | U |
| 1 | 1 | 3353 | G |
| 1 | 1 | 3354 | U |
| 1 | 1 | 3355 | U |
| 1 | 1 | 3367 | C |
| 1 | 1 | 3369 | G |
| 1 | 1 | 3375 | A |
| 1 | 1 | 3378 | C |
| 1 | 1 | 3383 | G |
| 1 | 1 | 3386 | G |
| 1 | 1 | 3389 | U |
| 1 | 1 | 3390 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 3394 | U |
| 1 | 1 | 3396 | U |
| 2 | 3 | 7 | G |
| 2 | 3 | 10 | C |
| 2 | 3 | 22 | A |
| 2 | 3 | 23 | A |
| 2 | 3 | 33 | U |
| 2 | 3 | 38 | U |
| 2 | 3 | 41 | G |
| 2 | 3 | 42 | A |
| 2 | 3 | 51 | A |
| 2 | 3 | 53 | U |
| 2 | 3 | 54 | U |
| 2 | 3 | 65 | G |
| 2 | 3 | 74 | C |
| 2 | 3 | 76 | A |
| 2 | 3 | 90 | U |
| 2 | 3 | 91 | G |
| 2 | 3 | 99 | G |
| 2 | 3 | 102 | A |
| 2 | 3 | 104 | A |
| 2 | 3 | 110 | G |
| 2 | 3 | 112 | G |
| 2 | 3 | 121 | U |
| 3 | 4 | 21 | C |
| 3 | 4 | 23 | U |
| 3 | 4 | 34 | U |
| 3 | 4 | 35 | C |
| 3 | 4 | 50 | C |
| 3 | 4 | 51 | G |
| 3 | 4 | 53 | A |
| 3 | 4 | 59 | A |
| 3 | 4 | 62 | C |
| 3 | 4 | 63 | G |
| 3 | 4 | 80 | A |
| 3 | 4 | 81 | U |
| 3 | 4 | 82 | U |
| 3 | 4 | 83 | C |
| 3 | 4 | 84 | C |
| 3 | 4 | 86 | U |
| 3 | 4 | 87 | G |
| 3 | 4 | 89 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 4 | 90 | U |
| 3 | 4 | 91 | C |
| 3 | 4 | 95 | G |
| 3 | 4 | 104 | A |
| 3 | 4 | 105 | A |
| 3 | 4 | 106 | C |
| 3 | 4 | 111 | A |
| 3 | 4 | 113 | U |
| 3 | 4 | 125 | U |
| 3 | 4 | 126 | A |
| 3 | 4 | 127 | U |
| 3 | 4 | 128 | U |
| 3 | 4 | 138 | A |
| 3 | 4 | 148 | G |
| 3 | 4 | 149 | A |
| 3 | 4 | 151 | C |
| 3 | 4 | 155 | A |
| 45 | 2 | 2 | A |
| 45 | 2 | 16 | G |
| 45 | 2 | 17 | C |
| 45 | 2 | 25 | C |
| 45 | 2 | 26 | A |
| 45 | 2 | 27 | U |
| 45 | 2 | 34 | G |
| 45 | 2 | 37 | U |
| 45 | 2 | 45 | U |
| 45 | 2 | 47 | A |
| 45 | 2 | 48 | G |
| 45 | 2 | 57 | G |
| 45 | 2 | 60 | U |
| 45 | 2 | 61 | A |
| 45 | 2 | 62 | A |
| 45 | 2 | 66 | U |
| 45 | 2 | 67 | A |
| 45 | 2 | 68 | A |
| 45 | 2 | 69 | G |
| 45 | 2 | 72 | A |
| 45 | 2 | 73 | U |
| 45 | 2 | 74 | U |
| 45 | 2 | 75 | U |
| 45 | 2 | 77 | U |
| 45 | 2 | 78 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 79 | C |
| 45 | 2 | 80 | A |
| 45 | 2 | 81 | G |
| 45 | 2 | 94 | U |
| 45 | 2 | 99 | C |
| 45 | 2 | 100 | A |
| 45 | 2 | 101 | U |
| 45 | 2 | 103 | A |
| 45 | 2 | 104 | A |
| 45 | 2 | 110 | U |
| 45 | 2 | 114 | C |
| 45 | 2 | 115 | G |
| 45 | 2 | 116 | U |
| 45 | 2 | 117 | U |
| 45 | 2 | 123 | G |
| 45 | 2 | 124 | A |
| 45 | 2 | 127 | G |
| 45 | 2 | 128 | U |
| 45 | 2 | 130 | C |
| 45 | 2 | 131 | C |
| 45 | 2 | 133 | U |
| 45 | 2 | 134 | U |
| 45 | 2 | 135 | A |
| 45 | 2 | 136 | C |
| 45 | 2 | 137 | U |
| 45 | 2 | 138 | A |
| 45 | 2 | 140 | A |
| 45 | 2 | 141 | U |
| 45 | 2 | 144 | U |
| 45 | 2 | 145 | A |
| 45 | 2 | 146 | U |
| 45 | 2 | 149 | C |
| 45 | 2 | 151 | G |
| 45 | 2 | 158 | U |
| 45 | 2 | 159 | U |
| 45 | 2 | 168 | A |
| 45 | 2 | 178 | U |
| 45 | 2 | 185 | U |
| 45 | 2 | 186 | C |
| 45 | 2 | 187 | G |
| 45 | 2 | 192 | U |
| 45 | 2 | 193 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 194 | U |
| 45 | 2 | 195 | G |
| 45 | 2 | 197 | A |
| 45 | 2 | 200 | A |
| 45 | 2 | 209 | U |
| 45 | 2 | 215 | A |
| 45 | 2 | 217 | A |
| 45 | 2 | 218 | A |
| 45 | 2 | 219 | A |
| 45 | 2 | 225 | A |
| 45 | 2 | 229 | U |
| 45 | 2 | 231 | U |
| 45 | 2 | 232 | U |
| 45 | 2 | 233 | C |
| 45 | 2 | 234 | G |
| 45 | 2 | 238 | U |
| 45 | 2 | 239 | C |
| 45 | 2 | 240 | U |
| 45 | 2 | 241 | U |
| 45 | 2 | 246 | G |
| 45 | 2 | 250 | C |
| 45 | 2 | 254 | A |
| 45 | 2 | 257 | A |
| 45 | 2 | 260 | U |
| 45 | 2 | 261 | U |
| 45 | 2 | 262 | U |
| 45 | 2 | 265 | A |
| 45 | 2 | 266 | A |
| 45 | 2 | 267 | U |
| 45 | 2 | 269 | G |
| 45 | 2 | 270 | C |
| 45 | 2 | 271 | A |
| 45 | 2 | 272 | U |
| 45 | 2 | 276 | C |
| 45 | 2 | 277 | U |
| 45 | 2 | 278 | U |
| 45 | 2 | 279 | G |
| 45 | 2 | 280 | U |
| 45 | 2 | 281 | G |
| 45 | 2 | 283 | U |
| 45 | 2 | 284 | G |
| 45 | 2 | 288 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 292 | U |
| 45 | 2 | 299 | A |
| 45 | 2 | 302 | U |
| 45 | 2 | 306 | U |
| 45 | 2 | 309 | C |
| 45 | 2 | 314 | C |
| 45 | 2 | 316 | A |
| 45 | 2 | 320 | U |
| 45 | 2 | 321 | C |
| 45 | 2 | 324 | U |
| 45 | 2 | 333 | A |
| 45 | 2 | 337 | G |
| 45 | 2 | 338 | C |
| 45 | 2 | 352 | A |
| 45 | 2 | 359 | A |
| 45 | 2 | 360 | A |
| 45 | 2 | 361 | C |
| 45 | 2 | 369 | A |
| 45 | 2 | 381 | C |
| 45 | 2 | 390 | G |
| 45 | 2 | 399 | A |
| 45 | 2 | 400 | A |
| 45 | 2 | 402 | C |
| 45 | 2 | 403 | G |
| 45 | 2 | 404 | G |
| 45 | 2 | 416 | A |
| 45 | 2 | 417 | A |
| 45 | 2 | 418 | G |
| 45 | 2 | 422 | G |
| 45 | 2 | 424 | C |
| 45 | 2 | 425 | A |
| 45 | 2 | 426 | G |
| 45 | 2 | 427 | C |
| 45 | 2 | 428 | A |
| 45 | 2 | 434 | G |
| 45 | 2 | 437 | A |
| 45 | 2 | 439 | U |
| 45 | 2 | 444 | C |
| 45 | 2 | 447 | U |
| 45 | 2 | 448 | C |
| 45 | 2 | 452 | A |
| 45 | 2 | 454 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 455 | C |
| 45 | 2 | 468 | A |
| 45 | 2 | 469 | C |
| 45 | 2 | 474 | A |
| 45 | 2 | 475 | A |
| 45 | 2 | 477 | A |
| 45 | 2 | 483 | A |
| 45 | 2 | 484 | C |
| 45 | 2 | 485 | A |
| 45 | 2 | 486 | G |
| 45 | 2 | 487 | G |
| 45 | 2 | 502 | U |
| 45 | 2 | 504 | U |
| 45 | 2 | 505 | A |
| 45 | 2 | 506 | A |
| 45 | 2 | 507 | U |
| 45 | 2 | 510 | G |
| 45 | 2 | 511 | A |
| 45 | 2 | 512 | A |
| 45 | 2 | 513 | U |
| 45 | 2 | 515 | A |
| 45 | 2 | 516 | G |
| 45 | 2 | 532 | U |
| 45 | 2 | 535 | A |
| 45 | 2 | 536 | C |
| 45 | 2 | 538 | A |
| 45 | 2 | 539 | G |
| 45 | 2 | 540 | G |
| 45 | 2 | 541 | A |
| 45 | 2 | 542 | A |
| 45 | 2 | 543 | C |
| 45 | 2 | 544 | A |
| 45 | 2 | 548 | G |
| 45 | 2 | 554 | C |
| 45 | 2 | 555 | A |
| 45 | 2 | 556 | A |
| 45 | 2 | 557 | G |
| 45 | 2 | 558 | U |
| 45 | 2 | 559 | C |
| 45 | 2 | 560 | U |
| 45 | 2 | 561 | G |
| 45 | 2 | 565 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 567 | A |
| 45 | 2 | 568 | G |
| 45 | 2 | 570 | A |
| 45 | 2 | 576 | G |
| 45 | 2 | 579 | A |
| 45 | 2 | 580 | A |
| 45 | 2 | 582 | U |
| 45 | 2 | 583 | C |
| 45 | 2 | 594 | A |
| 45 | 2 | 595 | G |
| 45 | 2 | 613 | G |
| 45 | 2 | 619 | A |
| 45 | 2 | 620 | A |
| 45 | 2 | 621 | A |
| 45 | 2 | 622 | A |
| 45 | 2 | 623 | A |
| 45 | 2 | 624 | G |
| 45 | 2 | 638 | U |
| 45 | 2 | 639 | U |
| 45 | 2 | 640 | U |
| 45 | 2 | 650 | U |
| 45 | 2 | 654 | C |
| 45 | 2 | 655 | G |
| 45 | 2 | 656 | G |
| 45 | 2 | 658 | C |
| 45 | 2 | 677 | G |
| 45 | 2 | 679 | U |
| 45 | 2 | 683 | C |
| 45 | 2 | 684 | A |
| 45 | 2 | 686 | C |
| 45 | 2 | 694 | U |
| 45 | 2 | 695 | U |
| 45 | 2 | 696 | C |
| 45 | 2 | 697 | C |
| 45 | 2 | 699 | U |
| 45 | 2 | 702 | G |
| 45 | 2 | 703 | G |
| 45 | 2 | 704 | C |
| 45 | 2 | 735 | C |
| 45 | 2 | 737 | A |
| 45 | 2 | 738 | G |
| 45 | 2 | 739 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 741 | C |
| 45 | 2 | 742 | U |
| 45 | 2 | 743 | U |
| 45 | 2 | 754 | A |
| 45 | 2 | 755 | A |
| 45 | 2 | 756 | A |
| 45 | 2 | 762 | A |
| 45 | 2 | 765 | G |
| 45 | 2 | 766 | U |
| 45 | 2 | 770 | A |
| 45 | 2 | 771 | A |
| 45 | 2 | 774 | A |
| 45 | 2 | 775 | G |
| 45 | 2 | 777 | C |
| 45 | 2 | 778 | G |
| 45 | 2 | 779 | U |
| 45 | 2 | 780 | A |
| 45 | 2 | 781 | U |
| 45 | 2 | 782 | U |
| 45 | 2 | 783 | G |
| 45 | 2 | 784 | C |
| 45 | 2 | 789 | A |
| 45 | 2 | 793 | A |
| 45 | 2 | 794 | U |
| 45 | 2 | 795 | U |
| 45 | 2 | 812 | A |
| 45 | 2 | 814 | A |
| 45 | 2 | 815 | G |
| 45 | 2 | 816 | G |
| 45 | 2 | 818 | C |
| 45 | 2 | 820 | U |
| 45 | 2 | 821 | U |
| 45 | 2 | 824 | G |
| 45 | 2 | 827 | C |
| 45 | 2 | 829 | A |
| 45 | 2 | 830 | U |
| 45 | 2 | 831 | U |
| 45 | 2 | 833 | U |
| 45 | 2 | 839 | U |
| 45 | 2 | 840 | U |
| 45 | 2 | 846 | G |
| 45 | 2 | 847 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 855 | A |
| 45 | 2 | 856 | A |
| 45 | 2 | 860 | U |
| 45 | 2 | 863 | A |
| 45 | 2 | 864 | U |
| 45 | 2 | 865 | A |
| 45 | 2 | 873 | U |
| 45 | 2 | 886 | U |
| 45 | 2 | 894 | U |
| 45 | 2 | 895 | G |
| 45 | 2 | 898 | A |
| 45 | 2 | 906 | A |
| 45 | 2 | 911 | U |
| 45 | 2 | 912 | U |
| 45 | 2 | 913 | G |
| 45 | 2 | 914 | G |
| 45 | 2 | 916 | U |
| 45 | 2 | 921 | U |
| 45 | 2 | 927 | C |
| 45 | 2 | 933 | A |
| 45 | 2 | 935 | U |
| 45 | 2 | 942 | G |
| 45 | 2 | 944 | A |
| 45 | 2 | 954 | G |
| 45 | 2 | 960 | U |
| 45 | 2 | 966 | A |
| 45 | 2 | 992 | A |
| 45 | 2 | 993 | A |
| 45 | 2 | 1003 | A |
| 45 | 2 | 1004 | U |
| 45 | 2 | 1005 | A |
| 45 | 2 | 1021 | C |
| 45 | 2 | 1026 | A |
| 45 | 2 | 1028 | C |
| 45 | 2 | 1039 | A |
| 45 | 2 | 1040 | G |
| 45 | 2 | 1042 | G |
| 45 | 2 | 1052 | U |
| 45 | 2 | 1056 | U |
| 45 | 2 | 1057 | U |
| 45 | 2 | 1059 | U |
| 45 | 2 | 1060 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 1061 | A |
| 45 | 2 | 1063 | U |
| 45 | 2 | 1072 | C |
| 45 | 2 | 1075 | C |
| 45 | 2 | 1076 | A |
| 45 | 2 | 1079 | U |
| 45 | 2 | 1081 | A |
| 45 | 2 | 1083 | G |
| 45 | 2 | 1091 | A |
| 45 | 2 | 1092 | A |
| 45 | 2 | 1096 | C |
| 45 | 2 | 1097 | U |
| 45 | 2 | 1100 | G |
| 45 | 2 | 1109 | G |
| 45 | 2 | 1138 | A |
| 45 | 2 | 1146 | G |
| 45 | 2 | 1150 | G |
| 45 | 2 | 1151 | A |
| 45 | 2 | 1155 | G |
| 45 | 2 | 1157 | A |
| 45 | 2 | 1158 | C |
| 45 | 2 | 1160 | A |
| 45 | 2 | 1164 | G |
| 45 | 2 | 1166 | A |
| 45 | 2 | 1167 | G |
| 45 | 2 | 1185 | U |
| 45 | 2 | 1194 | A |
| 45 | 2 | 1196 | A |
| 45 | 2 | 1197 | C |
| 45 | 2 | 1199 | G |
| 45 | 2 | 1200 | G |
| 45 | 2 | 1202 | A |
| 45 | 2 | 1207 | C |
| 45 | 2 | 1208 | A |
| 45 | 2 | 1217 | A |
| 45 | 2 | 1218 | G |
| 45 | 2 | 1227 | A |
| 45 | 2 | 1228 | G |
| 45 | 2 | 1229 | G |
| 45 | 2 | 1230 | A |
| 45 | 2 | 1235 | C |
| 45 | 2 | 1244 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 1245 | G |
| 45 | 2 | 1246 | C |
| 45 | 2 | 1255 | G |
| 45 | 2 | 1256 | A |
| 45 | 2 | 1258 | U |
| 45 | 2 | 1260 | U |
| 45 | 2 | 1261 | G |
| 45 | 2 | 1263 | G |
| 45 | 2 | 1276 | U |
| 45 | 2 | 1287 | A |
| 45 | 2 | 1290 | U |
| 45 | 2 | 1301 | U |
| 45 | 2 | 1314 | U |
| 45 | 2 | 1315 | U |
| 45 | 2 | 1321 | A |
| 45 | 2 | 1325 | A |
| 45 | 2 | 1335 | U |
| 45 | 2 | 1337 | A |
| 45 | 2 | 1339 | C |
| 45 | 2 | 1340 | U |
| 45 | 2 | 1341 | A |
| 45 | 2 | 1343 | U |
| 45 | 2 | 1344 | A |
| 45 | 2 | 1345 | A |
| 45 | 2 | 1346 | A |
| 45 | 2 | 1348 | A |
| 45 | 2 | 1349 | G |
| 45 | 2 | 1361 | U |
| 45 | 2 | 1362 | U |
| 45 | 2 | 1364 | G |
| 45 | 2 | 1369 | U |
| 45 | 2 | 1370 | U |
| 45 | 2 | 1371 | A |
| 45 | 2 | 1372 | U |
| 45 | 2 | 1381 | U |
| 45 | 2 | 1383 | G |
| 45 | 2 | 1385 | G |
| 45 | 2 | 1388 | A |
| 45 | 2 | 1390 | U |
| 45 | 2 | 1398 | U |
| 45 | 2 | 1399 | C |
| 45 | 2 | 1400 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 1412 | G |
| 45 | 2 | 1413 | U |
| 45 | 2 | 1414 | U |
| 45 | 2 | 1415 | U |
| 45 | 2 | 1427 | A |
| 45 | 2 | 1428 | G |
| 45 | 2 | 1432 | U |
| 45 | 2 | 1445 | G |
| 45 | 2 | 1446 | A |
| 45 | 2 | 1447 | C |
| 45 | 2 | 1456 | C |
| 45 | 2 | 1457 | C |
| 45 | 2 | 1458 | G |
| 45 | 2 | 1459 | C |
| 45 | 2 | 1460 | A |
| 45 | 2 | 1461 | C |
| 45 | 2 | 1471 | A |
| 45 | 2 | 1473 | U |
| 45 | 2 | 1474 | G |
| 45 | 2 | 1482 | C |
| 45 | 2 | 1483 | A |
| 45 | 2 | 1485 | C |
| 45 | 2 | 1486 | G |
| 45 | 2 | 1489 | U |
| 45 | 2 | 1490 | C |
| 45 | 2 | 1491 | U |
| 45 | 2 | 1492 | A |
| 45 | 2 | 1493 | A |
| 45 | 2 | 1499 | G |
| 45 | 2 | 1503 | A |
| 45 | 2 | 1506 | G |
| 45 | 2 | 1514 | U |
| 45 | 2 | 1515 | A |
| 45 | 2 | 1516 | A |
| 45 | 2 | 1518 | C |
| 45 | 2 | 1520 | U |
| 45 | 2 | 1521 | G |
| 45 | 2 | 1523 | G |
| 45 | 2 | 1524 | A |
| 45 | 2 | 1535 | U |
| 45 | 2 | 1536 | G |
| 45 | 2 | 1537 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 1538 | U |
| 45 | 2 | 1542 | G |
| 45 | 2 | 1557 | U |
| 45 | 2 | 1559 | A |
| 45 | 2 | 1569 | A |
| 45 | 2 | 1574 | G |
| 45 | 2 | 1575 | G |
| 45 | 2 | 1584 | G |
| 45 | 2 | 1590 | G |
| 45 | 2 | 1601 | G |
| 45 | 2 | 1614 | A |
| 45 | 2 | 1616 | G |
| 45 | 2 | 1619 | C |
| 45 | 2 | 1625 | C |
| 45 | 2 | 1631 | A |
| 45 | 2 | 1634 | C |
| 45 | 2 | 1635 | A |
| 45 | 2 | 1657 | U |
| 45 | 2 | 1658 | G |
| 45 | 2 | 1663 | G |
| 45 | 2 | 1681 | A |
| 45 | 2 | 1682 | U |
| 45 | 2 | 1683 | C |
| 45 | 2 | 1684 | U |
| 45 | 2 | 1715 | G |
| 45 | 2 | 1716 | C |
| 45 | 2 | 1717 | G |
| 45 | 2 | 1755 | A |
| 45 | 2 | 1760 | G |
| 45 | 2 | 1762 | A |
| 45 | 2 | 1766 | A |
| 45 | 2 | 1769 | U |
| 45 | 2 | 1770 | U |
| 45 | 2 | 1780 | G |
| 45 | 2 | 1782 | A |
| 45 | 2 | 1783 | C |
| 45 | 2 | 1792 | G |
| 45 | 2 | 1793 | G |
| 45 | 2 | 1794 | A |
| 45 | 2 | 1796 | C |
| 1 | 5 | 26 | A |
| 1 | 5 | 40 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 43 | A |
| 1 | 5 | 49 | A |
| 1 | 5 | 57 | A |
| 1 | 5 | 60 | A |
| 1 | 5 | 65 | A |
| 1 | 5 | 66 | A |
| 1 | 5 | 73 | C |
| 1 | 5 | 77 | A |
| 1 | 5 | 85 | A |
| 1 | 5 | 92 | G |
| 1 | 5 | 96 | G |
| 1 | 5 | 99 | A |
| 1 | 5 | 108 | A |
| 1 | 5 | 109 | A |
| 1 | 5 | 110 | G |
| 1 | 5 | 113 | C |
| 1 | 5 | 121 | A |
| 1 | 5 | 122 | A |
| 1 | 5 | 127 | G |
| 1 | 5 | 130 | A |
| 1 | 5 | 132 | C |
| 1 | 5 | 133 | U |
| 1 | 5 | 134 | U |
| 1 | 5 | 136 | G |
| 1 | 5 | 138 | U |
| 1 | 5 | 139 | G |
| 1 | 5 | 146 | U |
| 1 | 5 | 150 | A |
| 1 | 5 | 152 | U |
| 1 | 5 | 156 | G |
| 1 | 5 | 157 | A |
| 1 | 5 | 161 | G |
| 1 | 5 | 165 | A |
| 1 | 5 | 170 | G |
| 1 | 5 | 171 | G |
| 1 | 5 | 173 | G |
| 1 | 5 | 174 | C |
| 1 | 5 | 175 | C |
| 1 | 5 | 176 | G |
| 1 | 5 | 180 | C |
| 1 | 5 | 181 | U |
| 1 | 5 | 187 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 190 | U |
| 1 | 5 | 191 | U |
| 1 | 5 | 200 | C |
| 1 | 5 | 210 | U |
| 1 | 5 | 213 | A |
| 1 | 5 | 218 | G |
| 1 | 5 | 219 | A |
| 1 | 5 | 221 | A |
| 1 | 5 | 238 | A |
| 1 | 5 | 239 | G |
| 1 | 5 | 240 | U |
| 1 | 5 | 241 | G |
| 1 | 5 | 242 | C |
| 1 | 5 | 246 | U |
| 1 | 5 | 247 | C |
| 1 | 5 | 249 | U |
| 1 | 5 | 250 | U |
| 1 | 5 | 251 | G |
| 1 | 5 | 252 | U |
| 1 | 5 | 253 | A |
| 1 | 5 | 263 | C |
| 1 | 5 | 269 | G |
| 1 | 5 | 284 | A |
| 1 | 5 | 286 | U |
| 1 | 5 | 295 | A |
| 1 | 5 | 305 | U |
| 1 | 5 | 311 | C |
| 1 | 5 | 323 | A |
| 1 | 5 | 329 | U |
| 1 | 5 | 338 | A |
| 1 | 5 | 339 | C |
| 1 | 5 | 349 | A |
| 1 | 5 | 350 | C |
| 1 | 5 | 351 | A |
| 1 | 5 | 352 | A |
| 1 | 5 | 373 | A |
| 1 | 5 | 376 | G |
| 1 | 5 | 379 | C |
| 1 | 5 | 384 | A |
| 1 | 5 | 390 | G |
| 1 | 5 | 395 | A |
| 1 | 5 | 397 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 399 | A |
| 1 | 5 | 401 | U |
| 1 | 5 | 402 | A |
| 1 | 5 | 403 | C |
| 1 | 5 | 404 | G |
| 1 | 5 | 421 | G |
| 1 | 5 | 422 | A |
| 1 | 5 | 435 | C |
| 1 | 5 | 436 | A |
| 1 | 5 | 439 | C |
| 1 | 5 | 440 | A |
| 1 | 5 | 441 | U |
| 1 | 5 | 442 | G |
| 1 | 5 | 520 | U |
| 1 | 5 | 521 | A |
| 1 | 5 | 524 | U |
| 1 | 5 | 535 | G |
| 1 | 5 | 540 | U |
| 1 | 5 | 542 | G |
| 1 | 5 | 543 | C |
| 1 | 5 | 544 | C |
| 1 | 5 | 545 | U |
| 1 | 5 | 546 | C |
| 1 | 5 | 547 | G |
| 1 | 5 | 548 | G |
| 1 | 5 | 549 | U |
| 1 | 5 | 550 | A |
| 1 | 5 | 551 | A |
| 1 | 5 | 553 | U |
| 1 | 5 | 555 | U |
| 1 | 5 | 557 | A |
| 1 | 5 | 559 | A |
| 1 | 5 | 569 | A |
| 1 | 5 | 578 | A |
| 1 | 5 | 579 | G |
| 1 | 5 | 592 | A |
| 1 | 5 | 594 | U |
| 1 | 5 | 597 | G |
| 1 | 5 | 600 | G |
| 1 | 5 | 604 | G |
| 1 | 5 | 609 | G |
| 1 | 5 | 611 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 618 | C |
| 1 | 5 | 619 | A |
| 1 | 5 | 620 | U |
| 1 | 5 | 621 | A |
| 1 | 5 | 622 | A |
| 1 | 5 | 626 | U |
| 1 | 5 | 636 | C |
| 1 | 5 | 643 | U |
| 1 | 5 | 649 | A |
| 1 | 5 | 660 | A |
| 1 | 5 | 677 | A |
| 1 | 5 | 681 | U |
| 1 | 5 | 691 | A |
| 1 | 5 | 697 | A |
| 1 | 5 | 705 | A |
| 1 | 5 | 708 | G |
| 1 | 5 | 712 | G |
| 1 | 5 | 715 | A |
| 1 | 5 | 716 | A |
| 1 | 5 | 736 | A |
| 1 | 5 | 766 | U |
| 1 | 5 | 768 | C |
| 1 | 5 | 776 | U |
| 1 | 5 | 777 | U |
| 1 | 5 | 780 | A |
| 1 | 5 | 781 | G |
| 1 | 5 | 785 | G |
| 1 | 5 | 786 | A |
| 1 | 5 | 806 | A |
| 1 | 5 | 808 | A |
| 1 | 5 | 816 | A |
| 1 | 5 | 817 | A |
| 1 | 5 | 830 | A |
| 1 | 5 | 837 | A |
| 1 | 5 | 846 | A |
| 1 | 5 | 857 | G |
| 1 | 5 | 861 | C |
| 1 | 5 | 874 | U |
| 1 | 5 | 879 | U |
| 1 | 5 | 882 | A |
| 1 | 5 | 883 | A |
| 1 | 5 | 896 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 907 | G |
| 1 | 5 | 908 | G |
| 1 | 5 | 914 | A |
| 1 | 5 | 916 | G |
| 1 | 5 | 917 | A |
| 1 | 5 | 921 | A |
| 1 | 5 | 924 | G |
| 1 | 5 | 925 | A |
| 1 | 5 | 926 | A |
| 1 | 5 | 937 | G |
| 1 | 5 | 939 | U |
| 1 | 5 | 944 | C |
| 1 | 5 | 953 | G |
| 1 | 5 | 959 | C |
| 1 | 5 | 960 | U |
| 1 | 5 | 964 | G |
| 1 | 5 | 979 | U |
| 1 | 5 | 982 | C |
| 1 | 5 | 994 | G |
| 1 | 5 | 1002 | A |
| 1 | 5 | 1010 | G |
| 1 | 5 | 1015 | U |
| 1 | 5 | 1016 | C |
| 1 | 5 | 1017 | C |
| 1 | 5 | 1018 | G |
| 1 | 5 | 1020 | G |
| 1 | 5 | 1023 | C |
| 1 | 5 | 1024 | G |
| 1 | 5 | 1031 | C |
| 1 | 5 | 1033 | U |
| 1 | 5 | 1035 | G |
| 1 | 5 | 1037 | C |
| 1 | 5 | 1041 | U |
| 1 | 5 | 1047 | A |
| 1 | 5 | 1049 | C |
| 1 | 5 | 1064 | A |
| 1 | 5 | 1065 | A |
| 1 | 5 | 1068 | C |
| 1 | 5 | 1071 | U |
| 1 | 5 | 1072 | G |
| 1 | 5 | 1076 | C |
| 1 | 5 | 1081 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 1082 | U |
| 1 | 5 | 1083 | G |
| 1 | 5 | 1085 | A |
| 1 | 5 | 1093 | A |
| 1 | 5 | 1094 | U |
| 1 | 5 | 1095 | U |
| 1 | 5 | 1097 | G |
| 1 | 5 | 1098 | A |
| 1 | 5 | 1103 | A |
| 1 | 5 | 1104 | G |
| 1 | 5 | 1117 | G |
| 1 | 5 | 1131 | G |
| 1 | 5 | 1144 | U |
| 1 | 5 | 1151 | U |
| 1 | 5 | 1153 | A |
| 1 | 5 | 1159 | A |
| 1 | 5 | 1180 | A |
| 1 | 5 | 1181 | U |
| 1 | 5 | 1182 | A |
| 1 | 5 | 1191 | U |
| 1 | 5 | 1192 | C |
| 1 | 5 | 1196 | C |
| 1 | 5 | 1201 | C |
| 1 | 5 | 1206 | G |
| 1 | 5 | 1209 | G |
| 1 | 5 | 1212 | A |
| 1 | 5 | 1220 | U |
| 1 | 5 | 1222 | G |
| 1 | 5 | 1225 | A |
| 1 | 5 | 1285 | G |
| 1 | 5 | 1308 | A |
| 1 | 5 | 1311 | G |
| 1 | 5 | 1312 | C |
| 1 | 5 | 1313 | G |
| 1 | 5 | 1324 | U |
| 1 | 5 | 1330 | A |
| 1 | 5 | 1332 | A |
| 1 | 5 | 1348 | U |
| 1 | 5 | 1349 | G |
| 1 | 5 | 1350 | A |
| 1 | 5 | 1351 | U |
| 1 | 5 | 1352 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 1353 | U |
| 1 | 5 | 1354 | G |
| 1 | 5 | 1356 | U |
| 1 | 5 | 1357 | G |
| 1 | 5 | 1358 | C |
| 1 | 5 | 1369 | A |
| 1 | 5 | 1380 | G |
| 1 | 5 | 1385 | C |
| 1 | 5 | 1386 | A |
| 1 | 5 | 1392 | G |
| 1 | 5 | 1399 | A |
| 1 | 5 | 1400 | G |
| 1 | 5 | 1416 | C |
| 1 | 5 | 1417 | G |
| 1 | 5 | 1418 | A |
| 1 | 5 | 1419 | A |
| 1 | 5 | 1428 | A |
| 1 | 5 | 1434 | G |
| 1 | 5 | 1437 | C |
| 1 | 5 | 1438 | U |
| 1 | 5 | 1446 | A |
| 1 | 5 | 1450 | G |
| 1 | 5 | 1455 | U |
| 1 | 5 | 1466 | G |
| 1 | 5 | 1481 | A |
| 1 | 5 | 1482 | A |
| 1 | 5 | 1483 | G |
| 1 | 5 | 1488 | G |
| 1 | 5 | 1500 | G |
| 1 | 5 | 1501 | U |
| 1 | 5 | 1503 | A |
| 1 | 5 | 1508 | C |
| 1 | 5 | 1511 | U |
| 1 | 5 | 1524 | A |
| 1 | 5 | 1527 | C |
| 1 | 5 | 1533 | U |
| 1 | 5 | 1539 | A |
| 1 | 5 | 1554 | U |
| 1 | 5 | 1555 | U |
| 1 | 5 | 1556 | C |
| 1 | 5 | 1557 | A |
| 1 | 5 | 1560 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 1561 | G |
| 1 | 5 | 1562 | C |
| 1 | 5 | 1564 | U |
| 1 | 5 | 1565 | G |
| 1 | 5 | 1572 | U |
| 1 | 5 | 1573 | G |
| 1 | 5 | 1574 | C |
| 1 | 5 | 1575 | A |
| 1 | 5 | 1576 | G |
| 1 | 5 | 1577 | G |
| 1 | 5 | 1578 | C |
| 1 | 5 | 1581 | C |
| 1 | 5 | 1582 | C |
| 1 | 5 | 1583 | A |
| 1 | 5 | 1587 | A |
| 1 | 5 | 1589 | A |
| 1 | 5 | 1593 | A |
| 1 | 5 | 1605 | A |
| 1 | 5 | 1607 | U |
| 1 | 5 | 1608 | C |
| 1 | 5 | 1619 | A |
| 1 | 5 | 1628 | C |
| 1 | 5 | 1629 | U |
| 1 | 5 | 1632 | A |
| 1 | 5 | 1636 | U |
| 1 | 5 | 1639 | C |
| 1 | 5 | 1642 | A |
| 1 | 5 | 1643 | A |
| 1 | 5 | 1644 | C |
| 1 | 5 | 1645 | U |
| 1 | 5 | 1655 | G |
| 1 | 5 | 1657 | C |
| 1 | 5 | 1662 | G |
| 1 | 5 | 1687 | U |
| 1 | 5 | 1715 | A |
| 1 | 5 | 1716 | U |
| 1 | 5 | 1724 | U |
| 1 | 5 | 1731 | A |
| 1 | 5 | 1736 | G |
| 1 | 5 | 1746 | U |
| 1 | 5 | 1750 | A |
| 1 | 5 | 1751 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 1759 | C |
| 1 | 5 | 1760 | A |
| 1 | 5 | 1761 | C |
| 1 | 5 | 1762 | C |
| 1 | 5 | 1763 | U |
| 1 | 5 | 1765 | U |
| 1 | 5 | 1766 | G |
| 1 | 5 | 1769 | G |
| 1 | 5 | 1770 | G |
| 1 | 5 | 1775 | G |
| 1 | 5 | 1778 | G |
| 1 | 5 | 1780 | G |
| 1 | 5 | 1788 | C |
| 1 | 5 | 1797 | A |
| 1 | 5 | 1809 | A |
| 1 | 5 | 1810 | A |
| 1 | 5 | 1812 | G |
| 1 | 5 | 1813 | A |
| 1 | 5 | 1814 | A |
| 1 | 5 | 1815 | U |
| 1 | 5 | 1816 | A |
| 1 | 5 | 1817 | G |
| 1 | 5 | 1818 | U |
| 1 | 5 | 1821 | U |
| 1 | 5 | 1835 | A |
| 1 | 5 | 1839 | A |
| 1 | 5 | 1842 | A |
| 1 | 5 | 1846 | C |
| 1 | 5 | 1849 | C |
| 1 | 5 | 1878 | G |
| 1 | 5 | 1879 | A |
| 1 | 5 | 1880 | U |
| 1 | 5 | 1884 | A |
| 1 | 5 | 1886 | A |
| 1 | 5 | 1906 | G |
| 1 | 5 | 1935 | G |
| 1 | 5 | 1948 | G |
| 1 | 5 | 1952 | G |
| 1 | 5 | 2093 | A |
| 1 | 5 | 2100 | A |
| 1 | 5 | 2101 | C |
| 1 | 5 | 2102 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 2112 | U |
| 1 | 5 | 2113 | A |
| 1 | 5 | 2114 | C |
| 1 | 5 | 2121 | G |
| 1 | 5 | 2122 | G |
| 1 | 5 | 2131 | A |
| 1 | 5 | 2140 | U |
| 1 | 5 | 2146 | C |
| 1 | 5 | 2158 | A |
| 1 | 5 | 2168 | A |
| 1 | 5 | 2169 | G |
| 1 | 5 | 2176 | U |
| 1 | 5 | 2179 | C |
| 1 | 5 | 2185 | G |
| 1 | 5 | 2198 | A |
| 1 | 5 | 2201 | G |
| 1 | 5 | 2205 | U |
| 1 | 5 | 2206 | G |
| 1 | 5 | 2210 | G |
| 1 | 5 | 2213 | A |
| 1 | 5 | 2222 | A |
| 1 | 5 | 2223 | A |
| 1 | 5 | 2225 | U |
| 1 | 5 | 2228 | A |
| 1 | 5 | 2244 | A |
| 1 | 5 | 2246 | G |
| 1 | 5 | 2250 | G |
| 1 | 5 | 2251 | G |
| 1 | 5 | 2252 | A |
| 1 | 5 | 2253 | G |
| 1 | 5 | 2255 | A |
| 1 | 5 | 2256 | A |
| 1 | 5 | 2257 | C |
| 1 | 5 | 2266 | U |
| 1 | 5 | 2269 | U |
| 1 | 5 | 2270 | A |
| 1 | 5 | 2273 | G |
| 1 | 5 | 2281 | A |
| 1 | 5 | 2307 | G |
| 1 | 5 | 2310 | U |
| 1 | 5 | 2313 | A |
| 1 | 5 | 2315 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 2334 | U |
| 1 | 5 | 2336 | U |
| 1 | 5 | 2372 | A |
| 1 | 5 | 2373 | A |
| 1 | 5 | 2374 | C |
| 1 | 5 | 2375 | G |
| 1 | 5 | 2388 | U |
| 1 | 5 | 2393 | G |
| 1 | 5 | 2395 | G |
| 1 | 5 | 2397 | A |
| 1 | 5 | 2401 | A |
| 1 | 5 | 2402 | A |
| 1 | 5 | 2403 | G |
| 1 | 5 | 2404 | A |
| 1 | 5 | 2405 | C |
| 1 | 5 | 2411 | U |
| 1 | 5 | 2418 | G |
| 1 | 5 | 2419 | A |
| 1 | 5 | 2420 | C |
| 1 | 5 | 2433 | U |
| 1 | 5 | 2434 | U |
| 1 | 5 | 2435 | G |
| 1 | 5 | 2437 | G |
| 1 | 5 | 2441 | A |
| 1 | 5 | 2442 | G |
| 1 | 5 | 2443 | A |
| 1 | 5 | 2509 | U |
| 1 | 5 | 2510 | U |
| 1 | 5 | 2511 | A |
| 1 | 5 | 2512 | C |
| 1 | 5 | 2514 | U |
| 1 | 5 | 2515 | A |
| 1 | 5 | 2522 | G |
| 1 | 5 | 2523 | A |
| 1 | 5 | 2524 | A |
| 1 | 5 | 2525 | G |
| 1 | 5 | 2535 | A |
| 1 | 5 | 2536 | A |
| 1 | 5 | 2537 | U |
| 1 | 5 | 2538 | U |
| 1 | 5 | 2539 | C |
| 1 | 5 | 2540 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 2541 | U |
| 1 | 5 | 2543 | U |
| 1 | 5 | 2544 | U |
| 1 | 5 | 2545 | C |
| 1 | 5 | 2546 | C |
| 1 | 5 | 2549 | G |
| 1 | 5 | 2552 | C |
| 1 | 5 | 2555 | G |
| 1 | 5 | 2560 | C |
| 1 | 5 | 2562 | A |
| 1 | 5 | 2567 | C |
| 1 | 5 | 2568 | C |
| 1 | 5 | 2569 | A |
| 1 | 5 | 2571 | U |
| 1 | 5 | 2572 | C |
| 1 | 5 | 2573 | G |
| 1 | 5 | 2574 | G |
| 1 | 5 | 2585 | G |
| 1 | 5 | 2593 | A |
| 1 | 5 | 2594 | C |
| 1 | 5 | 2606 | G |
| 1 | 5 | 2607 | G |
| 1 | 5 | 2610 | G |
| 1 | 5 | 2614 | G |
| 1 | 5 | 2619 | G |
| 1 | 5 | 2620 | G |
| 1 | 5 | 2626 | A |
| 1 | 5 | 2629 | U |
| 1 | 5 | 2648 | G |
| 1 | 5 | 2652 | U |
| 1 | 5 | 2656 | A |
| 1 | 5 | 2663 | G |
| 1 | 5 | 2667 | A |
| 1 | 5 | 2673 | A |
| 1 | 5 | 2674 | A |
| 1 | 5 | 2675 | C |
| 1 | 5 | 2676 | A |
| 1 | 5 | 2677 | G |
| 1 | 5 | 2681 | U |
| 1 | 5 | 2689 | A |
| 1 | 5 | 2690 | G |
| 1 | 5 | 2691 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 2694 | A |
| 1 | 5 | 2695 | A |
| 1 | 5 | 2696 | A |
| 1 | 5 | 2714 | G |
| 1 | 5 | 2715 | A |
| 1 | 5 | 2720 | G |
| 1 | 5 | 2728 | G |
| 1 | 5 | 2737 | C |
| 1 | 5 | 2738 | A |
| 1 | 5 | 2740 | A |
| 1 | 5 | 2746 | A |
| 1 | 5 | 2752 | U |
| 1 | 5 | 2753 | G |
| 1 | 5 | 2773 | C |
| 1 | 5 | 2777 | G |
| 1 | 5 | 2778 | G |
| 1 | 5 | 2796 | G |
| 1 | 5 | 2799 | A |
| 1 | 5 | 2800 | G |
| 1 | 5 | 2801 | A |
| 1 | 5 | 2802 | A |
| 1 | 5 | 2810 | C |
| 1 | 5 | 2814 | G |
| 1 | 5 | 2816 | G |
| 1 | 5 | 2817 | A |
| 1 | 5 | 2818 | U |
| 1 | 5 | 2837 | A |
| 1 | 5 | 2843 | U |
| 1 | 5 | 2845 | A |
| 1 | 5 | 2847 | A |
| 1 | 5 | 2853 | A |
| 1 | 5 | 2871 | G |
| 1 | 5 | 2872 | A |
| 1 | 5 | 2875 | U |
| 1 | 5 | 2876 | C |
| 1 | 5 | 2887 | A |
| 1 | 5 | 2889 | C |
| 1 | 5 | 2898 | G |
| 1 | 5 | 2899 | C |
| 1 | 5 | 2910 | A |
| 1 | 5 | 2923 | U |
| 1 | 5 | 2935 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 2936 | A |
| 1 | 5 | 2942 | C |
| 1 | 5 | 2943 | G |
| 1 | 5 | 2947 | G |
| 1 | 5 | 2951 | G |
| 1 | 5 | 2952 | G |
| 1 | 5 | 2967 | A |
| 1 | 5 | 2971 | A |
| 1 | 5 | 2972 | G |
| 1 | 5 | 2979 | U |
| 1 | 5 | 2983 | C |
| 1 | 5 | 2990 | G |
| 1 | 5 | 2994 | A |
| 1 | 5 | 2996 | U |
| 1 | 5 | 2997 | G |
| 1 | 5 | 3012 | A |
| 1 | 5 | 3028 | G |
| 1 | 5 | 3030 | G |
| 1 | 5 | 3039 | C |
| 1 | 5 | 3056 | U |
| 1 | 5 | 3059 | G |
| 1 | 5 | 3062 | G |
| 1 | 5 | 3074 | G |
| 1 | 5 | 3078 | U |
| 1 | 5 | 3080 | G |
| 1 | 5 | 3086 | A |
| 1 | 5 | 3087 | A |
| 1 | 5 | 3092 | C |
| 1 | 5 | 3120 | C |
| 1 | 5 | 3130 | A |
| 1 | 5 | 3131 | U |
| 1 | 5 | 3142 | A |
| 1 | 5 | 3143 | C |
| 1 | 5 | 3153 | U |
| 1 | 5 | 3154 | C |
| 1 | 5 | 3155 | U |
| 1 | 5 | 3156 | U |
| 1 | 5 | 3157 | U |
| 1 | 5 | 3158 | G |
| 1 | 5 | 3164 | C |
| 1 | 5 | 3165 | A |
| 1 | 5 | 3166 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 3168 | A |
| 1 | 5 | 3172 | A |
| 1 | 5 | 3173 | G |
| 1 | 5 | 3174 | A |
| 1 | 5 | 3176 | G |
| 1 | 5 | 3178 | A |
| 1 | 5 | 3180 | A |
| 1 | 5 | 3181 | C |
| 1 | 5 | 3187 | A |
| 1 | 5 | 3188 | G |
| 1 | 5 | 3195 | U |
| 1 | 5 | 3196 | U |
| 1 | 5 | 3207 | U |
| 1 | 5 | 3209 | A |
| 1 | 5 | 3217 | C |
| 1 | 5 | 3218 | A |
| 1 | 5 | 3219 | G |
| 1 | 5 | 3227 | A |
| 1 | 5 | 3229 | G |
| 1 | 5 | 3233 | C |
| 1 | 5 | 3239 | G |
| 1 | 5 | 3244 | A |
| 1 | 5 | 3245 | A |
| 1 | 5 | 3246 | G |
| 1 | 5 | 3247 | G |
| 1 | 5 | 3252 | G |
| 1 | 5 | 3253 | G |
| 1 | 5 | 3254 | G |
| 1 | 5 | 3259 | U |
| 1 | 5 | 3265 | C |
| 1 | 5 | 3270 | U |
| 1 | 5 | 3271 | G |
| 1 | 5 | 3272 | C |
| 1 | 5 | 3275 | U |
| 1 | 5 | 3276 | G |
| 1 | 5 | 3277 | U |
| 1 | 5 | 3279 | A |
| 1 | 5 | 3280 | U |
| 1 | 5 | 3282 | U |
| 1 | 5 | 3284 | G |
| 1 | 5 | 3285 | C |
| 1 | 5 | 3286 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 3287 | U |
| 1 | 5 | 3289 | G |
| 1 | 5 | 3290 | G |
| 1 | 5 | 3294 | A |
| 1 | 5 | 3295 | A |
| 1 | 5 | 3304 | U |
| 1 | 5 | 3313 | U |
| 1 | 5 | 3317 | U |
| 1 | 5 | 3318 | G |
| 1 | 5 | 3319 | U |
| 1 | 5 | 3341 | U |
| 1 | 5 | 3342 | A |
| 1 | 5 | 3345 | G |
| 1 | 5 | 3349 | C |
| 1 | 5 | 3351 | U |
| 1 | 5 | 3352 | U |
| 1 | 5 | 3354 | U |
| 1 | 5 | 3355 | U |
| 1 | 5 | 3358 | U |
| 1 | 5 | 3368 | U |
| 1 | 5 | 3369 | G |
| 1 | 5 | 3378 | C |
| 1 | 5 | 3383 | G |
| 1 | 5 | 3389 | U |
| 1 | 5 | 3396 | U |
| 2 | 7 | 5 | G |
| 2 | 7 | 7 | G |
| 2 | 7 | 21 | G |
| 2 | 7 | 22 | A |
| 2 | 7 | 26 | C |
| 2 | 7 | 27 | A |
| 2 | 7 | 41 | G |
| 2 | 7 | 42 | A |
| 2 | 7 | 52 | G |
| 2 | 7 | 54 | U |
| 2 | 7 | 55 | A |
| 2 | 7 | 65 | G |
| 2 | 7 | 73 | C |
| 2 | 7 | 74 | C |
| 2 | 7 | 76 | A |
| 2 | 7 | 91 | G |
| 2 | 7 | 93 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 7 | 102 | A |
| 2 | 7 | 112 | G |
| 2 | 7 | 121 | U |
| 3 | 8 | 18 | U |
| 3 | 8 | 30 | C |
| 3 | 8 | 34 | U |
| 3 | 8 | 35 | C |
| 3 | 8 | 39 | G |
| 3 | 8 | 50 | C |
| 3 | 8 | 52 | A |
| 3 | 8 | 58 | G |
| 3 | 8 | 59 | A |
| 3 | 8 | 62 | C |
| 3 | 8 | 63 | G |
| 3 | 8 | 79 | A |
| 3 | 8 | 80 | A |
| 3 | 8 | 81 | U |
| 3 | 8 | 82 | U |
| 3 | 8 | 83 | C |
| 3 | 8 | 84 | C |
| 3 | 8 | 85 | G |
| 3 | 8 | 86 | U |
| 3 | 8 | 87 | G |
| 3 | 8 | 90 | U |
| 3 | 8 | 95 | G |
| 3 | 8 | 104 | A |
| 3 | 8 | 106 | C |
| 3 | 8 | 109 | A |
| 3 | 8 | 111 | A |
| 3 | 8 | 113 | U |
| 3 | 8 | 125 | U |
| 3 | 8 | 126 | A |
| 3 | 8 | 127 | U |
| 3 | 8 | 128 | U |
| 3 | 8 | 138 | A |
| 3 | 8 | 155 | A |
| 3 | 8 | 157 | U |
| 3 | 8 | 158 | U |
| 45 | 6 | 2 | A |
| 45 | 6 | 17 | C |
| 45 | 6 | 25 | C |
| 45 | 6 | 26 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 27 | U |
| 45 | 6 | 34 | G |
| 45 | 6 | 42 | G |
| 45 | 6 | 45 | U |
| 45 | 6 | 46 | A |
| 45 | 6 | 47 | A |
| 45 | 6 | 50 | C |
| 45 | 6 | 57 | G |
| 45 | 6 | 60 | U |
| 45 | 6 | 63 | G |
| 45 | 6 | 67 | A |
| 45 | 6 | 68 | A |
| 45 | 6 | 69 | G |
| 45 | 6 | 72 | A |
| 45 | 6 | 73 | U |
| 45 | 6 | 74 | U |
| 45 | 6 | 75 | U |
| 45 | 6 | 76 | A |
| 45 | 6 | 77 | U |
| 45 | 6 | 78 | A |
| 45 | 6 | 104 | A |
| 45 | 6 | 114 | C |
| 45 | 6 | 116 | U |
| 45 | 6 | 121 | U |
| 45 | 6 | 130 | C |
| 45 | 6 | 131 | C |
| 45 | 6 | 138 | A |
| 45 | 6 | 139 | C |
| 45 | 6 | 140 | A |
| 45 | 6 | 141 | U |
| 45 | 6 | 144 | U |
| 45 | 6 | 153 | G |
| 45 | 6 | 158 | U |
| 45 | 6 | 159 | U |
| 45 | 6 | 166 | C |
| 45 | 6 | 170 | U |
| 45 | 6 | 178 | U |
| 45 | 6 | 179 | A |
| 45 | 6 | 185 | U |
| 45 | 6 | 191 | C |
| 45 | 6 | 192 | U |
| 45 | 6 | 193 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 195 | G |
| 45 | 6 | 197 | A |
| 45 | 6 | 198 | A |
| 45 | 6 | 199 | G |
| 45 | 6 | 200 | A |
| 45 | 6 | 201 | G |
| 45 | 6 | 215 | A |
| 45 | 6 | 218 | A |
| 45 | 6 | 222 | A |
| 45 | 6 | 224 | C |
| 45 | 6 | 226 | A |
| 45 | 6 | 227 | U |
| 45 | 6 | 228 | G |
| 45 | 6 | 229 | U |
| 45 | 6 | 231 | U |
| 45 | 6 | 232 | U |
| 45 | 6 | 233 | C |
| 45 | 6 | 234 | G |
| 45 | 6 | 235 | G |
| 45 | 6 | 240 | U |
| 45 | 6 | 241 | U |
| 45 | 6 | 242 | U |
| 45 | 6 | 243 | G |
| 45 | 6 | 249 | U |
| 45 | 6 | 250 | C |
| 45 | 6 | 261 | U |
| 45 | 6 | 262 | U |
| 45 | 6 | 265 | A |
| 45 | 6 | 266 | A |
| 45 | 6 | 267 | U |
| 45 | 6 | 268 | C |
| 45 | 6 | 271 | A |
| 45 | 6 | 272 | U |
| 45 | 6 | 273 | G |
| 45 | 6 | 276 | C |
| 45 | 6 | 277 | U |
| 45 | 6 | 278 | U |
| 45 | 6 | 279 | G |
| 45 | 6 | 280 | U |
| 45 | 6 | 285 | G |
| 45 | 6 | 287 | G |
| 45 | 6 | 299 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 302 | U |
| 45 | 6 | 314 | C |
| 45 | 6 | 316 | A |
| 45 | 6 | 320 | U |
| 45 | 6 | 321 | C |
| 45 | 6 | 322 | G |
| 45 | 6 | 333 | A |
| 45 | 6 | 337 | G |
| 45 | 6 | 338 | C |
| 45 | 6 | 352 | A |
| 45 | 6 | 359 | A |
| 45 | 6 | 360 | A |
| 45 | 6 | 361 | C |
| 45 | 6 | 369 | A |
| 45 | 6 | 370 | A |
| 45 | 6 | 379 | U |
| 45 | 6 | 380 | U |
| 45 | 6 | 393 | C |
| 45 | 6 | 400 | A |
| 45 | 6 | 401 | A |
| 45 | 6 | 402 | C |
| 45 | 6 | 403 | G |
| 45 | 6 | 404 | G |
| 45 | 6 | 416 | A |
| 45 | 6 | 418 | G |
| 45 | 6 | 419 | G |
| 45 | 6 | 424 | C |
| 45 | 6 | 425 | A |
| 45 | 6 | 426 | G |
| 45 | 6 | 428 | A |
| 45 | 6 | 434 | G |
| 45 | 6 | 437 | A |
| 45 | 6 | 439 | U |
| 45 | 6 | 444 | C |
| 45 | 6 | 448 | C |
| 45 | 6 | 449 | C |
| 45 | 6 | 452 | A |
| 45 | 6 | 454 | U |
| 45 | 6 | 455 | C |
| 45 | 6 | 468 | A |
| 45 | 6 | 474 | A |
| 45 | 6 | 475 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 480 | G |
| 45 | 6 | 485 | A |
| 45 | 6 | 486 | G |
| 45 | 6 | 487 | G |
| 45 | 6 | 488 | G |
| 45 | 6 | 500 | C |
| 45 | 6 | 501 | U |
| 45 | 6 | 504 | U |
| 45 | 6 | 505 | A |
| 45 | 6 | 506 | A |
| 45 | 6 | 507 | U |
| 45 | 6 | 508 | U |
| 45 | 6 | 510 | G |
| 45 | 6 | 511 | A |
| 45 | 6 | 512 | A |
| 45 | 6 | 513 | U |
| 45 | 6 | 515 | A |
| 45 | 6 | 519 | C |
| 45 | 6 | 527 | A |
| 45 | 6 | 534 | A |
| 45 | 6 | 538 | A |
| 45 | 6 | 539 | G |
| 45 | 6 | 540 | G |
| 45 | 6 | 541 | A |
| 45 | 6 | 542 | A |
| 45 | 6 | 543 | C |
| 45 | 6 | 544 | A |
| 45 | 6 | 554 | C |
| 45 | 6 | 555 | A |
| 45 | 6 | 556 | A |
| 45 | 6 | 557 | G |
| 45 | 6 | 558 | U |
| 45 | 6 | 564 | G |
| 45 | 6 | 565 | C |
| 45 | 6 | 566 | C |
| 45 | 6 | 570 | A |
| 45 | 6 | 574 | G |
| 45 | 6 | 579 | A |
| 45 | 6 | 580 | A |
| 45 | 6 | 582 | U |
| 45 | 6 | 583 | C |
| 45 | 6 | 585 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 594 | A |
| 45 | 6 | 595 | G |
| 45 | 6 | 596 | C |
| 45 | 6 | 606 | A |
| 45 | 6 | 610 | G |
| 45 | 6 | 611 | U |
| 45 | 6 | 619 | A |
| 45 | 6 | 620 | A |
| 45 | 6 | 622 | A |
| 45 | 6 | 623 | A |
| 45 | 6 | 624 | G |
| 45 | 6 | 639 | U |
| 45 | 6 | 647 | G |
| 45 | 6 | 648 | G |
| 45 | 6 | 649 | U |
| 45 | 6 | 650 | U |
| 45 | 6 | 685 | A |
| 45 | 6 | 745 | U |
| 45 | 6 | 746 | A |
| 45 | 6 | 754 | A |
| 45 | 6 | 755 | A |
| 45 | 6 | 756 | A |
| 45 | 6 | 758 | U |
| 45 | 6 | 765 | G |
| 45 | 6 | 766 | U |
| 45 | 6 | 774 | A |
| 45 | 6 | 775 | G |
| 45 | 6 | 778 | G |
| 45 | 6 | 780 | A |
| 45 | 6 | 781 | U |
| 45 | 6 | 782 | U |
| 45 | 6 | 783 | G |
| 45 | 6 | 789 | A |
| 45 | 6 | 793 | A |
| 45 | 6 | 794 | U |
| 45 | 6 | 803 | A |
| 45 | 6 | 811 | A |
| 45 | 6 | 812 | A |
| 45 | 6 | 813 | U |
| 45 | 6 | 815 | G |
| 45 | 6 | 819 | G |
| 45 | 6 | 820 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 821 | U |
| 45 | 6 | 823 | G |
| 45 | 6 | 825 | U |
| 45 | 6 | 826 | U |
| 45 | 6 | 829 | A |
| 45 | 6 | 830 | U |
| 45 | 6 | 831 | U |
| 45 | 6 | 832 | U |
| 45 | 6 | 834 | G |
| 45 | 6 | 835 | U |
| 45 | 6 | 839 | U |
| 45 | 6 | 842 | C |
| 45 | 6 | 843 | U |
| 45 | 6 | 845 | G |
| 45 | 6 | 849 | C |
| 45 | 6 | 856 | A |
| 45 | 6 | 863 | A |
| 45 | 6 | 864 | U |
| 45 | 6 | 876 | G |
| 45 | 6 | 877 | G |
| 45 | 6 | 886 | U |
| 45 | 6 | 898 | A |
| 45 | 6 | 906 | A |
| 45 | 6 | 913 | G |
| 45 | 6 | 914 | G |
| 45 | 6 | 916 | U |
| 45 | 6 | 926 | A |
| 45 | 6 | 929 | A |
| 45 | 6 | 933 | A |
| 45 | 6 | 935 | U |
| 45 | 6 | 942 | G |
| 45 | 6 | 944 | A |
| 45 | 6 | 945 | U |
| 45 | 6 | 951 | A |
| 45 | 6 | 957 | G |
| 45 | 6 | 959 | U |
| 45 | 6 | 960 | U |
| 45 | 6 | 966 | A |
| 45 | 6 | 969 | C |
| 45 | 6 | 971 | A |
| 45 | 6 | 984 | G |
| 45 | 6 | 992 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 993 | A |
| 45 | 6 | 995 | A |
| 45 | 6 | 996 | U |
| 45 | 6 | 997 | G |
| 45 | 6 | 1003 | A |
| 45 | 6 | 1004 | U |
| 45 | 6 | 1005 | A |
| 45 | 6 | 1024 | U |
| 45 | 6 | 1025 | A |
| 45 | 6 | 1026 | A |
| 45 | 6 | 1028 | C |
| 45 | 6 | 1030 | A |
| 45 | 6 | 1039 | A |
| 45 | 6 | 1040 | G |
| 45 | 6 | 1042 | G |
| 45 | 6 | 1043 | A |
| 45 | 6 | 1051 | G |
| 45 | 6 | 1052 | U |
| 45 | 6 | 1053 | G |
| 45 | 6 | 1058 | U |
| 45 | 6 | 1059 | U |
| 45 | 6 | 1060 | U |
| 45 | 6 | 1061 | A |
| 45 | 6 | 1062 | A |
| 45 | 6 | 1063 | U |
| 45 | 6 | 1071 | U |
| 45 | 6 | 1076 | A |
| 45 | 6 | 1081 | A |
| 45 | 6 | 1082 | C |
| 45 | 6 | 1083 | G |
| 45 | 6 | 1092 | A |
| 45 | 6 | 1096 | C |
| 45 | 6 | 1097 | U |
| 45 | 6 | 1098 | U |
| 45 | 6 | 1100 | G |
| 45 | 6 | 1109 | G |
| 45 | 6 | 1112 | G |
| 45 | 6 | 1138 | A |
| 45 | 6 | 1140 | G |
| 45 | 6 | 1150 | G |
| 45 | 6 | 1155 | G |
| 45 | 6 | 1158 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 1160 | A |
| 45 | 6 | 1163 | A |
| 45 | 6 | 1167 | G |
| 45 | 6 | 1185 | U |
| 45 | 6 | 1186 | U |
| 45 | 6 | 1194 | A |
| 45 | 6 | 1196 | A |
| 45 | 6 | 1199 | G |
| 45 | 6 | 1200 | G |
| 45 | 6 | 1202 | A |
| 45 | 6 | 1208 | A |
| 45 | 6 | 1212 | G |
| 45 | 6 | 1217 | A |
| 45 | 6 | 1218 | G |
| 45 | 6 | 1225 | U |
| 45 | 6 | 1226 | A |
| 45 | 6 | 1228 | G |
| 45 | 6 | 1229 | G |
| 45 | 6 | 1230 | A |
| 45 | 6 | 1235 | C |
| 45 | 6 | 1240 | U |
| 45 | 6 | 1243 | G |
| 45 | 6 | 1244 | A |
| 45 | 6 | 1245 | G |
| 45 | 6 | 1249 | U |
| 45 | 6 | 1252 | C |
| 45 | 6 | 1254 | U |
| 45 | 6 | 1256 | A |
| 45 | 6 | 1257 | U |
| 45 | 6 | 1258 | U |
| 45 | 6 | 1261 | G |
| 45 | 6 | 1263 | G |
| 45 | 6 | 1285 | U |
| 45 | 6 | 1312 | A |
| 45 | 6 | 1314 | U |
| 45 | 6 | 1315 | U |
| 45 | 6 | 1316 | G |
| 45 | 6 | 1321 | A |
| 45 | 6 | 1337 | A |
| 45 | 6 | 1341 | A |
| 45 | 6 | 1344 | A |
| 45 | 6 | 1345 | A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 1346 | A |
| 45 | 6 | 1347 | U |
| 45 | 6 | 1349 | G |
| 45 | 6 | 1354 | G |
| 45 | 6 | 1356 | U |
| 45 | 6 | 1357 | A |
| 45 | 6 | 1360 | A |
| 45 | 6 | 1361 | U |
| 45 | 6 | 1362 | U |
| 45 | 6 | 1363 | U |
| 45 | 6 | 1364 | G |
| 45 | 6 | 1366 | U |
| 45 | 6 | 1371 | A |
| 45 | 6 | 1372 | U |
| 45 | 6 | 1385 | G |
| 45 | 6 | 1388 | A |
| 45 | 6 | 1390 | U |
| 45 | 6 | 1398 | U |
| 45 | 6 | 1399 | C |
| 45 | 6 | 1400 | A |
| 45 | 6 | 1402 | G |
| 45 | 6 | 1406 | A |
| 45 | 6 | 1413 | U |
| 45 | 6 | 1414 | U |
| 45 | 6 | 1415 | U |
| 45 | 6 | 1427 | A |
| 45 | 6 | 1428 | G |
| 45 | 6 | 1433 | G |
| 45 | 6 | 1435 | G |
| 45 | 6 | 1437 | U |
| 45 | 6 | 1445 | G |
| 45 | 6 | 1446 | A |
| 45 | 6 | 1447 | C |
| 45 | 6 | 1459 | C |
| 45 | 6 | 1460 | A |
| 45 | 6 | 1461 | C |
| 45 | 6 | 1469 | A |
| 45 | 6 | 1471 | A |
| 45 | 6 | 1477 | G |
| 45 | 6 | 1481 | C |
| 45 | 6 | 1482 | C |
| 45 | 6 | 1486 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 1489 | U |
| 45 | 6 | 1490 | C |
| 45 | 6 | 1491 | U |
| 45 | 6 | 1492 | A |
| 45 | 6 | 1493 | A |
| 45 | 6 | 1506 | G |
| 45 | 6 | 1510 | U |
| 45 | 6 | 1511 | U |
| 45 | 6 | 1514 | U |
| 45 | 6 | 1516 | A |
| 45 | 6 | 1518 | C |
| 45 | 6 | 1520 | U |
| 45 | 6 | 1521 | G |
| 45 | 6 | 1523 | G |
| 45 | 6 | 1524 | A |
| 45 | 6 | 1533 | C |
| 45 | 6 | 1535 | U |
| 45 | 6 | 1536 | G |
| 45 | 6 | 1537 | C |
| 45 | 6 | 1538 | U |
| 45 | 6 | 1542 | G |
| 45 | 6 | 1554 | U |
| 45 | 6 | 1557 | U |
| 45 | 6 | 1559 | A |
| 45 | 6 | 1569 | A |
| 45 | 6 | 1571 | C |
| 45 | 6 | 1574 | G |
| 45 | 6 | 1575 | G |
| 45 | 6 | 1584 | G |
| 45 | 6 | 1590 | G |
| 45 | 6 | 1597 | A |
| 45 | 6 | 1600 | A |
| 45 | 6 | 1601 | G |
| 45 | 6 | 1610 | G |
| 45 | 6 | 1616 | G |
| 45 | 6 | 1625 | C |
| 45 | 6 | 1629 | G |
| 45 | 6 | 1637 | C |
| 45 | 6 | 1638 | G |
| 45 | 6 | 1656 | U |
| 45 | 6 | 1657 | U |
| 45 | 6 | 1658 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 1678 | A |
| 45 | 6 | 1680 | G |
| 45 | 6 | 1683 | C |
| 45 | 6 | 1685 | G |
| 45 | 6 | 1713 | G |
| 45 | 6 | 1715 | G |
| 45 | 6 | 1716 | C |
| 45 | 6 | 1717 | G |
| 45 | 6 | 1736 | G |
| 45 | 6 | 1750 | A |
| 45 | 6 | 1755 | A |
| 45 | 6 | 1756 | A |
| 45 | 6 | 1760 | G |
| 45 | 6 | 1762 | A |
| 45 | 6 | 1763 | A |
| 45 | 6 | 1766 | A |
| 45 | 6 | 1767 | G |
| 45 | 6 | 1769 | U |
| 45 | 6 | 1780 | G |
| 45 | 6 | 1782 | A |
| 45 | 6 | 1783 | C |
| 45 | 6 | 1789 | G |
| 45 | 6 | 1791 | A |
| 45 | 6 | 1792 | G |
| 45 | 6 | 1793 | G |
| 45 | 6 | 1794 | A |
| 45 | 6 | 1795 | U |
| 45 | 6 | 1796 | C |
| 45 | 6 | 1799 | U |

All (193) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 25 | U |
| 1 | 1 | 239 | G |
| 1 | 1 | 594 | U |
| 1 | 1 | 637 | C |
| 1 | 1 | 763 | G |
| 1 | 1 | 816 | A |
| 1 | 1 | 873 | C |
| 1 | 1 | 916 | G |
| 1 | 1 | 978 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 981 | U |
| 1 | 1 | 993 | G |
| 1 | 1 | 1064 | A |
| 1 | 1 | 1095 | U |
| 1 | 1 | 1097 | G |
| 1 | 1 | 1103 | A |
| 1 | 1 | 1190 | A |
| 1 | 1 | 1329 | U |
| 1 | 1 | 1331 | U |
| 1 | 1 | 1355 | A |
| 1 | 1 | 1399 | A |
| 1 | 1 | 1481 | A |
| 1 | 1 | 1482 | A |
| 1 | 1 | 1484 | U |
| 1 | 1 | 1556 | C |
| 1 | 1 | 1563 | C |
| 1 | 1 | 1580 | A |
| 1 | 1 | 1716 | U |
| 1 | 1 | 1815 | U |
| 1 | 1 | 2101 | C |
| 1 | 1 | 2112 | U |
| 1 | 1 | 2205 | U |
| 1 | 1 | 2209 | U |
| 1 | 1 | 2249 | G |
| 1 | 1 | 2372 | A |
| 1 | 1 | 2405 | C |
| 1 | 1 | 2418 | G |
| 1 | 1 | 2537 | U |
| 1 | 1 | 2540 | A |
| 1 | 1 | 2541 | U |
| 1 | 1 | 2571 | U |
| 1 | 1 | 2585 | G |
| 1 | 1 | 2656 | A |
| 1 | 1 | 2728 | G |
| 1 | 1 | 2801 | A |
| 1 | 1 | 2817 | A |
| 1 | 1 | 2818 | U |
| 1 | 1 | 2872 | A |
| 1 | 1 | 2970 | C |
| 1 | 1 | 3121 | U |
| 1 | 1 | 3169 | U |
| 1 | 1 | 3195 | U |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 3218 | A |
| 1 | 1 | 3228 | C |
| 1 | 1 | 3269 | U |
| 1 | 1 | 3350 | C |
| 1 | 1 | 3393 | U |
| 2 | 3 | 52 | G |
| 3 | 4 | 80 | A |
| 3 | 4 | 82 | U |
| 3 | 4 | 89 | A |
| 3 | 4 | 125 | U |
| 45 | 2 | 1 | U |
| 45 | 2 | 68 | A |
| 45 | 2 | 77 | U |
| 45 | 2 | 103 | A |
| 45 | 2 | 130 | C |
| 45 | 2 | 136 | C |
| 45 | 2 | 139 | C |
| 45 | 2 | 158 | U |
| 45 | 2 | 218 | A |
| 45 | 2 | 232 | U |
| 45 | 2 | 278 | U |
| 45 | 2 | 280 | U |
| 45 | 2 | 320 | U |
| 45 | 2 | 417 | A |
| 45 | 2 | 503 | G |
| 45 | 2 | 512 | A |
| 45 | 2 | 555 | A |
| 45 | 2 | 558 | U |
| 45 | 2 | 685 | A |
| 45 | 2 | 782 | U |
| 45 | 2 | 829 | A |
| 45 | 2 | 1150 | G |
| 45 | 2 | 1157 | A |
| 45 | 2 | 1196 | A |
| 45 | 2 | 1244 | A |
| 45 | 2 | 1344 | A |
| 45 | 2 | 1369 | U |
| 45 | 2 | 1370 | U |
| 45 | 2 | 1481 | C |
| 45 | 2 | 1568 | C |
| 45 | 2 | 1573 | A |
| 45 | 2 | 1615 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 2 | 1761 | U |
| 1 | 5 | 65 | A |
| 1 | 5 | 151 | A |
| 1 | 5 | 252 | U |
| 1 | 5 | 441 | U |
| 1 | 5 | 558 | U |
| 1 | 5 | 618 | C |
| 1 | 5 | 873 | C |
| 1 | 5 | 916 | G |
| 1 | 5 | 979 | U |
| 1 | 5 | 1081 | U |
| 1 | 5 | 1093 | A |
| 1 | 5 | 1096 | U |
| 1 | 5 | 1284 | C |
| 1 | 5 | 1307 | G |
| 1 | 5 | 1329 | U |
| 1 | 5 | 1348 | U |
| 1 | 5 | 1352 | A |
| 1 | 5 | 1355 | A |
| 1 | 5 | 1368 | U |
| 1 | 5 | 1481 | A |
| 1 | 5 | 1560 | G |
| 1 | 5 | 1573 | G |
| 1 | 5 | 1589 | A |
| 1 | 5 | 1715 | A |
| 1 | 5 | 1814 | A |
| 1 | 5 | 1815 | U |
| 1 | 5 | 1816 | A |
| 1 | 5 | 2101 | C |
| 1 | 5 | 2112 | U |
| 1 | 5 | 2144 | A |
| 1 | 5 | 2204 | C |
| 1 | 5 | 2205 | U |
| 1 | 5 | 2209 | U |
| 1 | 5 | 2249 | G |
| 1 | 5 | 2255 | A |
| 1 | 5 | 2281 | A |
| 1 | 5 | 2372 | A |
| 1 | 5 | 2404 | A |
| 1 | 5 | 2513 | U |
| 1 | 5 | 2662 | G |
| 1 | 5 | 2772 | C |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 2801 | A |
| 1 | 5 | 2818 | U |
| 1 | 5 | 2971 | A |
| 1 | 5 | 3154 | C |
| 1 | 5 | 3218 | A |
| 1 | 5 | 3228 | C |
| 1 | 5 | 3269 | U |
| 1 | 5 | 3289 | G |
| 1 | 5 | 3303 | G |
| 1 | 5 | 3317 | U |
| 1 | 5 | 3340 | G |
| 1 | 5 | 3357 | U |
| 3 | 8 | 79 | A |
| 3 | 8 | 80 | A |
| 3 | 8 | 81 | U |
| 3 | 8 | 82 | U |
| 3 | 8 | 83 | C |
| 3 | 8 | 84 | C |
| 3 | 8 | 126 | A |
| 45 | 6 | 25 | C |
| 45 | 6 | 76 | A |
| 45 | 6 | 103 | A |
| 45 | 6 | 114 | C |
| 45 | 6 | 139 | C |
| 45 | 6 | 158 | U |
| 45 | 6 | 217 | A |
| 45 | 6 | 233 | C |
| 45 | 6 | 272 | U |
| 45 | 6 | 321 | C |
| 45 | 6 | 417 | A |
| 45 | 6 | 487 | G |
| 45 | 6 | 506 | A |
| 45 | 6 | 512 | A |
| 45 | 6 | 540 | G |
| 45 | 6 | 542 | A |
| 45 | 6 | 555 | A |
| 45 | 6 | 744 | U |
| 45 | 6 | 745 | U |
| 45 | 6 | 755 | A |
| 45 | 6 | 841 | U |
| 45 | 6 | 968 | U |
| 45 | 6 | 1051 | G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | 6 | 1058 | U |
| 45 | 6 | 1097 | U |
| 45 | 6 | 1207 | C |
| 45 | 6 | 1244 | A |
| 45 | 6 | 1255 | G |
| 45 | 6 | 1344 | A |
| 45 | 6 | 1346 | A |
| 45 | 6 | 1363 | U |
| 45 | 6 | 1413 | U |
| 45 | 6 | 1481 | C |
| 45 | 6 | 1535 | U |
| 45 | 6 | 1568 | C |
| 45 | 6 | 1573 | A |
| 45 | 6 | 1600 | A |
| 45 | 6 | 1615 | C |
| 45 | 6 | 1657 | U |

## 5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 2242 ligands modelled in this entry, 2155 are monoatomic - leaving 87 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 80 | PAR | 1 | 3421 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.93 | 2 (3%) |
| 80 | PAR | 5 | 3413 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 1.40 | 6 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 80 | PAR | 1 | 3433 | - | 45,45,45 | 0.27 | 0 | 64,67,67 | 1.24 | 6 (9%) |
| 80 | PAR | 5 | 3419 | - | 45,45,45 | 0.33 | 0 | 64,67,67 | 1.27 | 8 (12%) |
| 80 | PAR | 3 | 201 | - | 45,45,45 | 0.26 | 0 | 64,67,67 | 1.46 | 5 (7%) |
| 80 | PAR | 1 | 3431 | - | 45,45,45 | 0.19 | 0 | 64,67,67 | 1.13 | 3 (4%) |
| 80 | PAR | 1 | 3405 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 0.89 | 2 (3%) |
| 80 | PAR | 5 | 3408 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.91 | 3 (4%) |
| 80 | PAR | 1 | 3406 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.89 | 4 (6%) |
| 80 | PAR | 7 | 201 | - | 45,45,45 | 0.17 | 0 | 64,67,67 | 0.75 | 2 (3%) |
| 80 | PAR | 1 | 3434 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.89 | 5 (7%) |
| 80 | PAR | 2 | 1904 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 1.42 | 4 (6%) |
| 80 | PAR | 5 | 3425 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.98 | 4 (6%) |
| 80 | PAR | 2 | 1902 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 1.34 | 5 (7%) |
| 80 | PAR | 1 | 3414 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 1.05 | 4 (6%) |
| 80 | PAR | 1 | 3422 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 1.05 | 3 (4%) |
| 80 | PAR | n3 | 201 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 1.07 | 4 (6%) |
| 80 | PAR | 5 | 3423 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.96 | 4 (6%) |
| 80 | PAR | 6 | 1905 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 1.05 | 4 (6%) |
| 80 | PAR | 6 | 1906 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.75 | 2 (3%) |
| 80 | PAR | 5 | 3410 | - | 45,45,45 | 0.17 | 0 | 64,67,67 | 0.87 | 2 (3%) |
| 80 | PAR | 1 | 3427 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.83 | 3 (4%) |
| 80 | PAR | 3 | 203 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.99 | 3 (4%) |
| 80 | PAR | 5 | 3416 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.91 | 3 (4%) |
| 80 | PAR | 1 | 3408 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 1.07 | 5 (7%) |
| 80 | PAR | 1 | 3403 | 81 | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.92 | 1 (1%) |
| 80 | PAR | 1 | 3426 | - | 45,45,45 | 0.25 | 0 | 64,67,67 | 1.02 | 3 (4%) |
| 80 | PAR | 1 | 3432 | - | 45,45,45 | 0.25 | 0 | 64,67,67 | 1.11 | 2 (3%) |
| 80 | PAR | 5 | 3426 | - | 45,45,45 | 0.23 | 0 | 64,67,67 | 0.89 | 1 (1%) |
| 80 | PAR | 5 | 3404 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 1.22 | 4 (6%) |
| 80 | PAR | 1 | 3418 | - | 45,45,45 | 0.26 | 0 | 64,67,67 | 0.87 | 2 (3%) |
| 80 | PAR | 1 | 3424 | - | 45,45,45 | 0.16 | 0 | 64,67,67 | 0.71 | 2 (3%) |
| 80 | PAR | 2 | 1901 | - | 45,45,45 | 0.19 | 0 | 64,67,67 | 0.74 | 2 (3%) |
| 80 | PAR | 6 | 1902 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 0.98 | 3 (4%) |
| 80 | PAR | 5 | 3402 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 1.05 | 2 (3%) |
| 80 | PAR | 8 | 202 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.88 | 1 (1%) |
| 80 | PAR | 5 | 3428 | 81 | 45,45,45 | 0.39 | 0 | 64,67,67 | 1.21 | 5 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 80 | PAR | 1 | 3417 | - | 45,45,45 | 0.17 | 0 | 64,67,67 | 0.88 | 2 (3%) |
| 80 | PAR | 1 | 3412 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 1.23 | 8 (12%) |
| 80 | PAR | 1 | 3411 | - | 45,45,45 | 0.32 | 0 | 64,67,67 | 1.68 | 5 (7%) |
| 80 | PAR | 5 | 3421 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 1.25 | 2 (3%) |
| 80 | PAR | 2 | 1903 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.84 | 3 (4%) |
| 80 | PAR | 1 | 3401 | - | 45,45,45 | 0.18 | 0 | 64,67,67 | 1.22 | 2 (3%) |
| 80 | PAR | 6 | 1904 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.90 | 3 (4%) |
| 80 | PAR | 5 | 3415 | - | 45,45,45 | 0.26 | 0 | 64,67,67 | 1.01 | 2 (3%) |
| 80 | PAR | 5 | 3409 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.98 | 4 (6%) |
| 80 | PAR | 1 | 3425 | - | 45,45,45 | 0.28 | 0 | 64,67,67 | 1.17 | 5 (7%) |
| 80 | PAR | 1 | 3410 | - | 45,45,45 | 0.36 | 0 | 64,67,67 | 1.38 | 8 (12%) |
| 80 | PAR | 5 | 3427 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 1.05 | 3 (4%) |
| 80 | PAR | 2 | 1905 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.79 | 4 (6%) |
| 80 | PAR | 5 | 3417 | - | 45,45,45 | 0.16 | 0 | 64,67,67 | 0.78 | 2 (3%) |
| 80 | PAR | 1 | 3429 | - | 45,45,45 | 0.23 | 0 | 64,67,67 | 1.26 | 4 (6%) |
| 80 | PAR | 5 | 3420 | - | 45,45,45 | 0.23 | 0 | 64,67,67 | 1.30 | 7 (10%) |
| 80 | PAR | 4 | 201 | - | 45,45,45 | 0.29 | 0 | 64,67,67 | 1.21 | 5 (7%) |
| 80 | PAR | 5 | 3407 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.81 | 3 (4%) |
| 80 | PAR | 1 | 3419 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 1.15 | 5 (7%) |
| 80 | PAR | 5 | 3418 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 1.08 | 3 (4%) |
| 80 | PAR | 1 | 3420 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.99 | 3 (4%) |
| 80 | PAR | 6 | 1901 | - | 45,45,45 | 0.25 | 0 | 64,67,67 | 0.92 | 2 (3%) |
| 80 | PAR | 5 | 3401 | - | 45,45,45 | 0.27 | 0 | 64,67,67 | 1.01 | 2 (3%) |
| 80 | PAR | 1 | 3415 | - | 45,45,45 | 0.25 | 0 | 64,67,67 | 0.88 | 3 (4%) |
| 80 | PAR | 1 | 3407 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.95 | 3 (4%) |
| 80 | PAR | 1 | 3435 | - | 45,45,45 | 0.38 | 0 | 64,67,67 | 1.31 | 4 (6%) |
| 80 | PAR | 8 | 201 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 1.01 | 5 (7%) |
| 80 | PAR | 7 | 202 | - | 45,45,45 | 0.18 | 0 | 64,67,67 | 0.87 | 3 (4%) |
| 80 | PAR | 1 | 3409 | - | 45,45,45 | 0.29 | 0 | 64,67,67 | 1.45 | 4 (6%) |
| 80 | PAR | 5 | 3403 | - | 45,45,45 | 0.25 | 0 | 64,67,67 | 1.02 | 3 (4%) |
| 80 | PAR | 1 | 3430 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 0.95 | 3 (4%) |
| 80 | PAR | 5 | 3422 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.91 | 4 (6%) |
| 80 | PAR | 1 | 3413 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.66 | 1 (1%) |
| 80 | PAR | 1 | 3437 | 1 | 45,45,45 | 0.19 | 0 | 64,67,67 | 0.73 | 2 (3%) |
| 80 | PAR | 1 | 3402 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.78 | 2 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 80 | PAR | 3 | 202 | 81 | 45,45,45 | 0.21 | 0 | 64,67,67 | 1.06 | 3 (4%) |
| 80 | PAR | 4 | 202 | - | 45,45,45 | 0.26 | 0 | 64,67,67 | 1.06 | 4 (6%) |
| 80 | PAR | 5 | 3424 | - | 45,45,45 | 0.23 | 0 | 64,67,67 | 1.02 | 3 (4%) |
| 80 | PAR | 5 | 3405 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.80 | 2 (3%) |
| 80 | PAR | o2 | 201 | - | 45,45,45 | 0.28 | 0 | 64,67,67 | 1.17 | 4 (6%) |
| 80 | PAR | 5 | 3406 | 81 | 45,45,45 | 0.27 | 0 | 64,67,67 | 0.95 | 5 (7%) |
| 80 | PAR | 5 | 3414 | - | 45,45,45 | 0.19 | 0 | 64,67,67 | 0.80 | 4 (6%) |
| 80 | PAR | 1 | 3423 | - | 45,45,45 | 0.20 | 0 | 64,67,67 | 0.75 | 1 (1%) |
| 80 | PAR | 1 | 3416 | - | 45,45,45 | 0.28 | 0 | 64,67,67 | 1.13 | 5 (7%) |
| 80 | PAR | 1 | 3404 | - | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.92 | 2 (3%) |
| 80 | PAR | 1 | 3436 | - | 45,45,45 | 0.23 | 0 | 64,67,67 | 1.01 | 3 (4%) |
| 80 | PAR | 6 | 1903 | - | 45,45,45 | 0.18 | 0 | 64,67,67 | 0.88 | 1 (1%) |
| 80 | PAR | 1 | 3428 | 81 | 45,45,45 | 0.22 | 0 | 64,67,67 | 0.99 | 2 (3%) |
| 80 | PAR | 5 | 3412 | - | 45,45,45 | 0.21 | 0 | 64,67,67 | 0.89 | 2 (3%) |
| 80 | PAR | 5 | 3411 | - | 45,45,45 | 0.24 | 0 | 64,67,67 | 1.13 | 5 (7%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 80 | PAR | 1 | 3421 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3413 | - | - | 2/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3433 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3419 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 3 | 201 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3431 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3405 | - | - | 11/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3408 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3406 | - | - | 2/18/94/94 | 0/4/4/4 |
| 80 | PAR | 7 | 201 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3434 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 2 | 1904 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3425 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 2 | 1902 | - | - | 3/18/94/94 | 0/4/4/4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 80 | PAR | 1 | 3414 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3422 | - | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | n3 | 201 | - | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3423 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 6 | 1905 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 6 | 1906 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3410 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3427 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 3 | 203 | - | - | 4/18/94/94 | 1/4/4/4 |
| 80 | PAR | 5 | 3416 | - | - | 2/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3408 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3403 | 81 | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3426 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3432 | - | - | 3/18/94/94 | 1/4/4/4 |
| 80 | PAR | 5 | 3426 | - | - | 4/18/94/94 | 1/4/4/4 |
| 80 | PAR | 5 | 3404 | - | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3418 | - | - | 7/18/94/94 | 1/4/4/4 |
| 80 | PAR | 1 | 3424 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 2 | 1901 | - | - | 1/18/94/94 | 0/4/4/4 |
| 80 | PAR | 6 | 1902 | - | - | 9/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3402 | - | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | 8 | 202 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3428 | 81 | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3417 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3412 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3411 | - | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3421 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 2 | 1903 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3401 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 6 | 1904 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3415 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3409 | - | - | 9/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3425 | - | - | 10/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3410 | - | - | 6/18/94/94 | 0/4/4/4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 80 | PAR | 5 | 3427 | - | - | 3/18/94/94 | 1/4/4/4 |
| 80 | PAR | 2 | 1905 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3417 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3429 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3420 | - | - | 3/18/94/94 | 1/4/4/4 |
| 80 | PAR | 4 | 201 | - | - | 6/18/94/94 | 1/4/4/4 |
| 80 | PAR | 5 | 3407 | - | - | 9/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3419 | - | - | 7/18/94/94 | 1/4/4/4 |
| 80 | PAR | 5 | 3418 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3420 | - | - | 1/18/94/94 | 0/4/4/4 |
| 80 | PAR | 6 | 1901 | - | - | 2/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3401 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3415 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3407 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3435 | - | - | 11/18/94/94 | 0/4/4/4 |
| 80 | PAR | 8 | 201 | - | - | 1/18/94/94 | 0/4/4/4 |
| 80 | PAR | 7 | 202 | - | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3409 | - | - | 9/18/94/94 | 1/4/4/4 |
| 80 | PAR | 5 | 3403 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3430 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3422 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3413 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3437 | 1 | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3402 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | 3 | 202 | 81 | - | 8/18/94/94 | 0/4/4/4 |
| 80 | PAR | 4 | 202 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3424 | - | - | 4/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3405 | - | - | 7/18/94/94 | 0/4/4/4 |
| 80 | PAR | o2 | 201 | - | - | 10/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3406 | 81 | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3414 | - | - | 1/18/94/94 | 1/4/4/4 |
| 80 | PAR | 1 | 3423 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3416 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3404 | - | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3436 | - | - | 9/18/94/94 | 0/4/4/4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 80 | PAR | 6 | 1903 | - | - | 5/18/94/94 | 0/4/4/4 |
| 80 | PAR | 1 | 3428 | 81 | - | 3/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3412 | - | - | 6/18/94/94 | 0/4/4/4 |
| 80 | PAR | 5 | 3411 | - | - | 7/18/94/94 | 0/4/4/4 |

There are no bond length outliers.

All (294) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 1 | 3409 | PAR | O11-C11-C21 | 8.93 | 123.60 | 108.22 |
| 80 | 5 | 3421 | PAR | O52-C13-O43 | -8.23 | 102.52 | 111.43 |
| 80 | 2 | 1904 | PAR | O52-C13-O43 | -7.82 | 102.97 | 111.43 |
| 80 | 1 | 3431 | PAR | O52-C13-O43 | -7.17 | 103.67 | 111.43 |
| 80 | 5 | 3413 | PAR | O11-C11-C21 | 6.84 | 120.00 | 108.22 |
| 80 | 1 | 3411 | PAR | O33-C14-C24 | 6.81 | 119.95 | 108.22 |
| 80 | 1 | 3435 | PAR | O52-C13-O43 | -6.78 | 104.09 | 111.43 |
| 80 | 1 | 3411 | PAR | C14-C24-N24 | 6.69 | 122.25 | 110.20 |
| 80 | 1 | 3411 | PAR | O52-C13-O43 | -6.59 | 104.29 | 111.43 |
| 80 | 3 | 201 | PAR | O52-C13-O43 | -6.41 | 104.49 | 111.43 |
| 80 | 5 | 3402 | PAR | O52-C13-O43 | -6.30 | 104.61 | 111.43 |
| 80 | 1 | 3401 | PAR | O33-C14-C24 | 6.29 | 119.05 | 108.22 |
| 80 | 1 | 3429 | PAR | O52-C13-O43 | -6.00 | 104.93 | 111.43 |
| 80 | 5 | 3404 | PAR | O11-C11-C21 | 5.93 | 118.43 | 108.22 |
| 80 | 1 | 3425 | PAR | O11-C11-C21 | 5.85 | 118.29 | 108.22 |
| 80 | 5 | 3425 | PAR | O52-C13-O43 | -5.81 | 105.15 | 111.43 |
| 80 | o2 | 201 | PAR | O52-C13-O43 | -5.74 | 105.22 | 111.43 |
| 80 | 4 | 202 | PAR | O52-C13-O43 | -5.57 | 105.41 | 111.43 |
| 80 | 5 | 3410 | PAR | O52-C13-O43 | -5.53 | 105.44 | 111.43 |
| 80 | 4 | 201 | PAR | O11-C11-C21 | 5.45 | 117.61 | 108.22 |
| 80 | 1 | 3421 | PAR | O52-C13-O43 | -5.44 | 105.54 | 111.43 |
| 80 | 5 | 3401 | PAR | O52-C13-O43 | -5.42 | 105.56 | 111.43 |
| 80 | 6 | 1901 | PAR | O52-C13-O43 | -5.40 | 105.58 | 111.43 |
| 80 | 3 | 201 | PAR | O11-C11-C21 | 5.40 | 117.52 | 108.22 |
| 80 | 6 | 1903 | PAR | O52-C13-O43 | -5.37 | 105.62 | 111.43 |
| 80 | 1 | 3422 | PAR | O52-C13-O43 | -5.29 | 105.70 | 111.43 |
| 80 | 5 | 3428 | PAR | O11-C11-C21 | 5.28 | 117.31 | 108.22 |
| 80 | 5 | 3427 | PAR | O11-C11-C21 | 5.26 | 117.28 | 108.22 |
| 80 | 6 | 1905 | PAR | O52-C13-O43 | -5.24 | 105.75 | 111.43 |
| 80 | 1 | 3432 | PAR | O11-C11-C21 | 5.16 | 117.10 | 108.22 |
| 80 | 5 | 3416 | PAR | O52-C13-O43 | -5.15 | 105.85 | 111.43 |
| 80 | 3 | 202 | PAR | O52-C13-O43 | -5.12 | 105.89 | 111.43 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 5 | 3420 | PAR | O52-C13-O43 | -5.09 | 105.92 | 111.43 |
| 80 | 2 | 1902 | PAR | O52-C52-C62 | 5.09 | 120.81 | 107.28 |
| 80 | 5 | 3403 | PAR | O52-C13-O43 | -5.08 | 105.93 | 111.43 |
| 80 | 5 | 3415 | PAR | O52-C13-O43 | -5.08 | 105.93 | 111.43 |
| 80 | 5 | 3418 | PAR | O52-C13-O43 | -5.06 | 105.95 | 111.43 |
| 80 | 1 | 3420 | PAR | O52-C13-O43 | -5.04 | 105.98 | 111.43 |
| 80 | 2 | 1902 | PAR | O33-C33-C23 | 5.03 | 127.48 | 111.32 |
| 80 | 6 | 1902 | PAR | O52-C13-O43 | -5.01 | 106.00 | 111.43 |
| 80 | 1 | 3436 | PAR | O52-C13-O43 | -4.89 | 106.13 | 111.43 |
| 80 | 8 | 202 | PAR | O52-C13-O43 | -4.86 | 106.17 | 111.43 |
| 80 | 1 | 3401 | PAR | O52-C13-O43 | -4.85 | 106.19 | 111.43 |
| 80 | 5 | 3412 | PAR | O52-C13-O43 | -4.72 | 106.32 | 111.43 |
| 80 | 1 | 3432 | PAR | O52-C13-O43 | -4.66 | 106.39 | 111.43 |
| 80 | 2 | 1904 | PAR | O11-C11-C21 | 4.61 | 116.15 | 108.22 |
| 80 | 5 | 3413 | PAR | O52-C13-O43 | -4.59 | 106.46 | 111.43 |
| 80 | n3 | 201 | PAR | O52-C13-O43 | -4.59 | 106.46 | 111.43 |
| 80 | 1 | 3412 | PAR | C13-C23-C33 | -4.50 | 96.69 | 102.10 |
| 80 | 1 | 3408 | PAR | O52-C13-O43 | -4.47 | 106.59 | 111.43 |
| 80 | 1 | 3433 | PAR | C14-C24-N24 | 4.46 | 118.25 | 110.20 |
| 80 | 1 | 3412 | PAR | O33-C14-C24 | -4.45 | 100.55 | 108.22 |
| 80 | 5 | 3417 | PAR | O52-C13-O43 | -4.43 | 106.64 | 111.43 |
| 80 | 1 | 3414 | PAR | O52-C52-C62 | 4.40 | 118.98 | 107.28 |
| 80 | 3 | 203 | PAR | O33-C14-C24 | 4.40 | 115.79 | 108.22 |
| 80 | 1 | 3417 | PAR | O52-C13-O43 | -4.39 | 106.68 | 111.43 |
| 80 | 1 | 3416 | PAR | O52-C52-C62 | 4.39 | 118.95 | 107.28 |
| 80 | 5 | 3411 | PAR | O11-C42-C32 | -4.33 | 98.85 | 109.18 |
| 80 | 1 | 3403 | PAR | O11-C11-C21 | 4.32 | 115.65 | 108.22 |
| 80 | 5 | 3424 | PAR | O52-C13-O43 | -4.32 | 106.76 | 111.43 |
| 80 | 1 | 3419 | PAR | O11-C42-C32 | -4.31 | 98.89 | 109.18 |
| 80 | 7 | 202 | PAR | O52-C13-O43 | -4.28 | 106.80 | 111.43 |
| 80 | 5 | 3426 | PAR | O52-C13-O43 | -4.25 | 106.83 | 111.43 |
| 80 | 1 | 3433 | PAR | O33-C14-C24 | 4.24 | 115.53 | 108.22 |
| 80 | n3 | 201 | PAR | O11-C11-C21 | 4.24 | 115.52 | 108.22 |
| 80 | 5 | 3409 | PAR | O52-C13-O43 | -4.21 | 106.87 | 111.43 |
| 80 | 1 | 3410 | PAR | O52-C52-C62 | 4.19 | 118.42 | 107.28 |
| 80 | 8 | 201 | PAR | O52-C13-O43 | -4.15 | 106.94 | 111.43 |
| 80 | 1 | 3405 | PAR | O33-C14-C24 | 4.14 | 115.35 | 108.22 |
| 80 | 6 | 1905 | PAR | O11-C11-C21 | 4.11 | 115.30 | 108.22 |
| 80 | 5 | 3427 | PAR | O52-C13-O43 | -4.11 | 106.98 | 111.43 |
| 80 | 1 | 3430 | PAR | O52-C13-O43 | -4.11 | 106.98 | 111.43 |
| 80 | 1 | 3404 | PAR | O52-C13-O43 | -4.08 | 107.02 | 111.43 |
| 80 | 5 | 3428 | PAR | C13-C23-C33 | -4.07 | 97.21 | 102.10 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 5 | 3418 | PAR | O11-C11-C21 | 4.06 | 115.21 | 108.22 |
| 80 | 1 | 3426 | PAR | O11-C11-C21 | 4.01 | 115.12 | 108.22 |
| 80 | 5 | 3420 | PAR | O33-C14-C24 | 4.00 | 115.10 | 108.22 |
| 80 | 5 | 3419 | PAR | O52-C52-C62 | 3.98 | 117.87 | 107.28 |
| 80 | 1 | 3410 | PAR | O11-C11-C21 | 3.96 | 115.03 | 108.22 |
| 80 | 1 | 3422 | PAR | O33-C14-C24 | -3.91 | 101.47 | 108.22 |
| 80 | 5 | 3413 | PAR | O33-C14-C24 | -3.88 | 101.53 | 108.22 |
| 80 | 5 | 3423 | PAR | C13-C23-C33 | -3.87 | 97.45 | 102.10 |
| 80 | 1 | 3424 | PAR | O52-C13-O43 | -3.87 | 107.25 | 111.43 |
| 80 | 1 | 3415 | PAR | O11-C11-C21 | 3.82 | 114.80 | 108.22 |
| 80 | 1 | 3433 | PAR | O52-C13-O43 | -3.82 | 107.29 | 111.43 |
| 80 | 1 | 3429 | PAR | O33-C14-C24 | 3.81 | 114.78 | 108.22 |
| 80 | 6 | 1902 | PAR | O11-C11-C21 | 3.80 | 114.77 | 108.22 |
| 80 | 1 | 3407 | PAR | O52-C13-O43 | -3.80 | 107.32 | 111.43 |
| 80 | 1 | 3428 | PAR | O33-C14-C24 | -3.78 | 101.70 | 108.22 |
| 80 | 2 | 1904 | PAR | O33-C14-C24 | -3.77 | 101.72 | 108.22 |
| 80 | 5 | 3420 | PAR | O52-C13-C23 | 3.77 | 115.77 | 107.96 |
| 80 | 1 | 3416 | PAR | C13-C23-C33 | -3.76 | 97.58 | 102.10 |
| 80 | 5 | 3422 | PAR | O52-C13-O43 | -3.75 | 107.37 | 111.43 |
| 80 | 1 | 3406 | PAR | O52-C13-O43 | -3.75 | 107.37 | 111.43 |
| 80 | 5 | 3421 | PAR | O11-C11-C21 | 3.73 | 114.65 | 108.22 |
| 80 | 5 | 3419 | PAR | C32-C22-C12 | 3.73 | 118.85 | 111.18 |
| 80 | 5 | 3409 | PAR | O11-C11-C21 | 3.70 | 114.59 | 108.22 |
| 80 | 1 | 3429 | PAR | C13-C23-C33 | -3.68 | 97.67 | 102.10 |
| 80 | 1 | 3425 | PAR | C14-C24-N24 | 3.68 | 116.83 | 110.20 |
| 80 | 1 | 3410 | PAR | O11-C42-C32 | 3.62 | 117.81 | 109.18 |
| 80 | 1 | 3419 | PAR | O52-C13-O43 | -3.62 | 107.52 | 111.43 |
| 80 | 3 | 202 | PAR | O52-C52-C62 | 3.62 | 116.90 | 107.28 |
| 80 | 1 | 3404 | PAR | O52-C52-C62 | 3.58 | 116.79 | 107.28 |
| 80 | 1 | 3410 | PAR | O52-C13-O43 | -3.56 | 107.57 | 111.43 |
| 80 | 1 | 3423 | PAR | O52-C13-O43 | -3.48 | 107.66 | 111.43 |
| 80 | 2 | 1903 | PAR | O33-C14-C24 | -3.47 | 102.23 | 108.22 |
| 80 | 1 | 3413 | PAR | O52-C13-O43 | -3.44 | 107.71 | 111.43 |
| 80 | 5 | 3411 | PAR | O52-C13-O43 | -3.43 | 107.72 | 111.43 |
| 80 | 5 | 3424 | PAR | O11-C11-C21 | 3.41 | 114.09 | 108.22 |
| 80 | 5 | 3408 | PAR | O11-C11-C21 | 3.41 | 114.08 | 108.22 |
| 80 | 1 | 3434 | PAR | O52-C13-O43 | -3.40 | 107.75 | 111.43 |
| 80 | 7 | 201 | PAR | O52-C13-O43 | -3.37 | 107.78 | 111.43 |
| 80 | 1 | 3427 | PAR | O52-C13-O43 | -3.36 | 107.80 | 111.43 |
| 80 | 1 | 3420 | PAR | O33-C14-C24 | -3.35 | 102.44 | 108.22 |
| 80 | 5 | 3413 | PAR | O11-C42-C32 | 3.34 | 117.15 | 109.18 |
| 80 | 1 | 3426 | PAR | O33-C33-C23 | -3.31 | 100.66 | 111.32 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 2 | 1902 | PAR | O33-C14-C24 | -3.30 | 102.53 | 108.22 |
| 80 | 1 | 3431 | PAR | O11-C11-C21 | 3.29 | 113.89 | 108.22 |
| 80 | 3 | 201 | PAR | O33-C33-C23 | 3.28 | 121.87 | 111.32 |
| 80 | 1 | 3427 | PAR | O11-C11-C21 | 3.27 | 113.85 | 108.22 |
| 80 | 1 | 3436 | PAR | O11-C11-C21 | 3.24 | 113.80 | 108.22 |
| 80 | 5 | 3422 | PAR | O33-C33-C23 | 3.23 | 121.70 | 111.32 |
| 80 | 5 | 3411 | PAR | O33-C33-C23 | 3.22 | 121.66 | 111.32 |
| 80 | 5 | 3415 | PAR | O11-C42-C52 | 3.20 | 115.61 | 107.48 |
| 80 | 5 | 3419 | PAR | O33-C14-C24 | -3.19 | 102.72 | 108.22 |
| 80 | 1 | 3419 | PAR | O33-C14-C24 | -3.18 | 102.75 | 108.22 |
| 80 | 8 | 201 | PAR | O11-C42-C32 | -3.15 | 101.65 | 109.18 |
| 80 | 1 | 3422 | PAR | O11-C11-C21 | 3.12 | 113.59 | 108.22 |
| 80 | 1 | 3428 | PAR | O11-C11-C21 | 3.12 | 113.59 | 108.22 |
| 80 | 1 | 3406 | PAR | O33-C14-C24 | -3.11 | 102.85 | 108.22 |
| 80 | 5 | 3416 | PAR | O11-C11-C21 | 3.11 | 113.58 | 108.22 |
| 80 | 1 | 3426 | PAR | C13-C23-C33 | -3.11 | 98.36 | 102.10 |
| 80 | 3 | 201 | PAR | O33-C14-C24 | -3.10 | 102.88 | 108.22 |
| 80 | 5 | 3408 | PAR | O33-C14-C24 | 3.09 | 113.55 | 108.22 |
| 80 | 5 | 3404 | PAR | O52-C52-C62 | 3.08 | 115.46 | 107.28 |
| 80 | 5 | 3420 | PAR | O11-C11-C21 | 3.06 | 113.49 | 108.22 |
| 80 | 5 | 3405 | PAR | O11-C11-C21 | 3.06 | 113.49 | 108.22 |
| 80 | 1 | 3433 | PAR | O11-C42-C32 | -3.05 | 101.90 | 109.18 |
| 80 | 7 | 202 | PAR | O11-C11-C21 | 3.05 | 113.47 | 108.22 |
| 80 | 5 | 3407 | PAR | O52-C13-O43 | -3.03 | 108.15 | 111.43 |
| 80 | 2 | 1902 | PAR | O23-C23-C33 | 3.03 | 119.76 | 111.17 |
| 80 | 5 | 3428 | PAR | C11-C21-N21 | 3.02 | 115.64 | 110.20 |
| 80 | 4 | 202 | PAR | O33-C14-C24 | -3.01 | 103.02 | 108.22 |
| 80 | 5 | 3428 | PAR | O33-C33-C23 | -3.01 | 101.63 | 111.32 |
| 80 | 5 | 3414 | PAR | O52-C13-O43 | -2.96 | 108.22 | 111.43 |
| 80 | 1 | 3410 | PAR | C32-C22-C12 | 2.96 | 117.25 | 111.18 |
| 80 | 5 | 3408 | PAR | O52-C13-O43 | -2.94 | 108.25 | 111.43 |
| 80 | 5 | 3406 | PAR | C13-C23-C33 | -2.91 | 98.60 | 102.10 |
| 80 | 4 | 201 | PAR | O52-C13-C23 | 2.91 | 113.99 | 107.96 |
| 80 | 1 | 3425 | PAR | C11-C21-N21 | 2.91 | 115.44 | 110.20 |
| 80 | 1 | 3402 | PAR | O11-C42-C32 | -2.90 | 102.26 | 109.18 |
| 80 | 5 | 3419 | PAR | O11-C11-C21 | 2.89 | 113.20 | 108.22 |
| 80 | 1 | 3408 | PAR | C11-C21-N21 | -2.87 | 105.03 | 110.20 |
| 80 | 1 | 3410 | PAR | C62-C52-C42 | -2.86 | 105.12 | 111.66 |
| 80 | 8 | 201 | PAR | C32-C22-C12 | -2.86 | 105.31 | 111.18 |
| 80 | n3 | 201 | PAR | O11-C42-C32 | 2.83 | 115.94 | 109.18 |
| 80 | 6 | 1904 | PAR | O11-C42-C32 | -2.82 | 102.44 | 109.18 |
| 80 | 3 | 203 | PAR | O11-C11-C21 | 2.80 | 113.04 | 108.22 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 1 | 3429 | PAR | C14-C24-N24 | 2.79 | 115.23 | 110.20 |
| 80 | 5 | 3406 | PAR | C14-O54-C54 | 2.76 | 119.11 | 113.69 |
| 80 | 7 | 201 | PAR | O11-C11-C21 | 2.76 | 112.97 | 108.22 |
| 80 | 2 | 1901 | PAR | O11-C11-C21 | 2.76 | 112.97 | 108.22 |
| 80 | 1 | 3409 | PAR | O33-C14-C24 | -2.73 | 103.51 | 108.22 |
| 80 | 1 | 3434 | PAR | C13-C23-C33 | 2.71 | 105.36 | 102.10 |
| 80 | 1 | 3412 | PAR | O52-C13-C23 | 2.70 | 113.57 | 107.96 |
| 80 | 1 | 3411 | PAR | O11-C42-C32 | -2.70 | 102.75 | 109.18 |
| 80 | 2 | 1905 | PAR | O11-C42-C32 | -2.69 | 102.75 | 109.18 |
| 80 | 5 | 3420 | PAR | C14-C24-N24 | 2.69 | 115.05 | 110.20 |
| 80 | 1 | 3437 | PAR | O52-C13-O43 | -2.69 | 108.52 | 111.43 |
| 80 | 5 | 3409 | PAR | C11-C21-N21 | 2.64 | 114.97 | 110.20 |
| 80 | 2 | 1903 | PAR | O11-C11-C21 | 2.64 | 112.77 | 108.22 |
| 80 | 1 | 3412 | PAR | O33-C33-C23 | -2.63 | 102.84 | 111.32 |
| 80 | 5 | 3420 | PAR | O33-C33-C23 | 2.63 | 119.78 | 111.32 |
| 80 | 1 | 3436 | PAR | C13-C23-C33 | -2.63 | 98.94 | 102.10 |
| 80 | 5 | 3417 | PAR | O11-C11-C21 | 2.62 | 112.72 | 108.22 |
| 80 | 5 | 3409 | PAR | O33-C14-C24 | -2.61 | 103.71 | 108.22 |
| 80 | 5 | 3406 | PAR | O52-C13-O43 | -2.61 | 108.60 | 111.43 |
| 80 | 1 | 3416 | PAR | O33-C33-C23 | -2.59 | 102.98 | 111.32 |
| 80 | 6 | 1906 | PAR | O11-C11-C21 | 2.59 | 112.67 | 108.22 |
| 80 | 1 | 3434 | PAR | O52-C52-C62 | 2.59 | 114.16 | 107.28 |
| 80 | 4 | 201 | PAR | O11-C42-C32 | 2.58 | 115.34 | 109.18 |
| 80 | 2 | 1905 | PAR | O52-C13-O43 | -2.58 | 108.63 | 111.43 |
| 80 | o2 | 201 | PAR | C32-C22-C12 | -2.57 | 105.90 | 111.18 |
| 80 | 1 | 3407 | PAR | O11-C11-C21 | 2.53 | 112.58 | 108.22 |
| 80 | 1 | 3417 | PAR | O11-C11-C21 | 2.53 | 112.58 | 108.22 |
| 80 | 5 | 3404 | PAR | O11-C42-C32 | 2.53 | 115.22 | 109.18 |
| 80 | 1 | 3409 | PAR | O11-C11-O51 | 2.52 | 117.72 | 110.67 |
| 80 | 6 | 1902 | PAR | C13-C23-C33 | 2.51 | 105.12 | 102.10 |
| 80 | 5 | 3411 | PAR | C14-C24-N24 | 2.48 | 114.68 | 110.20 |
| 80 | 1 | 3414 | PAR | O52-C13-O43 | -2.48 | 108.75 | 111.43 |
| 80 | 5 | 3422 | PAR | O23-C23-C33 | 2.48 | 118.20 | 111.17 |
| 80 | 5 | 3407 | PAR | C13-C23-C33 | -2.47 | 99.13 | 102.10 |
| 80 | 5 | 3414 | PAR | O33-C14-C24 | -2.47 | 103.97 | 108.22 |
| 80 | 2 | 1905 | PAR | O11-C11-C21 | 2.47 | 112.46 | 108.22 |
| 80 | 3 | 202 | PAR | C13-C23-C33 | 2.46 | 105.06 | 102.10 |
| 80 | 5 | 3419 | PAR | C14-C24-N24 | 2.45 | 114.63 | 110.20 |
| 80 | 1 | 3434 | PAR | O33-C33-C23 | 2.45 | 119.19 | 111.32 |
| 80 | 1 | 3416 | PAR | O52-C13-O43 | -2.45 | 108.78 | 111.43 |
| 80 | 1 | 3427 | PAR | O33-C14-C24 | 2.45 | 112.43 | 108.22 |
| 80 | 5 | 3422 | PAR | O11-C11-C21 | 2.42 | 112.39 | 108.22 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 1 | 3421 | PAR | O33-C14-C24 | -2.42 | 104.04 | 108.22 |
| 80 | 1 | 3416 | PAR | O43-C13-C23 | -2.41 | 101.87 | 104.98 |
| 80 | 1 | 3430 | PAR | O11-C11-C21 | 2.38 | 112.32 | 108.22 |
| 80 | 5 | 3401 | PAR | O33-C14-C24 | -2.38 | 104.11 | 108.22 |
| 80 | 1 | 3406 | PAR | O11-C11-C21 | 2.38 | 112.32 | 108.22 |
| 80 | 5 | 3425 | PAR | O33-C14-C24 | -2.38 | 104.12 | 108.22 |
| 80 | 5 | 3413 | PAR | C11-C21-N21 | 2.37 | 114.47 | 110.20 |
| 80 | 2 | 1901 | PAR | O52-C13-O43 | -2.37 | 108.87 | 111.43 |
| 80 | 1 | 3410 | PAR | O33-C14-C24 | 2.37 | 112.29 | 108.22 |
| 80 | 5 | 3425 | PAR | O11-C11-C21 | 2.35 | 112.27 | 108.22 |
| 80 | o2 | 201 | PAR | O33-C33-C23 | 2.35 | 118.88 | 111.32 |
| 80 | 1 | 3437 | PAR | O11-C11-C21 | 2.35 | 112.26 | 108.22 |
| 80 | 1 | 3405 | PAR | O52-C52-C62 | 2.35 | 113.52 | 107.28 |
| 80 | 5 | 3419 | PAR | C62-C52-C42 | -2.34 | 106.31 | 111.66 |
| 80 | 4 | 201 | PAR | O33-C14-C24 | 2.34 | 112.25 | 108.22 |
| 80 | 1 | 3420 | PAR | O11-C42-C32 | -2.33 | 103.61 | 109.18 |
| 80 | 5 | 3423 | PAR | O52-C13-O43 | -2.33 | 108.91 | 111.43 |
| 80 | 4 | 201 | PAR | C13-C23-C33 | 2.33 | 104.90 | 102.10 |
| 80 | 1 | 3418 | PAR | C13-C23-C33 | -2.33 | 99.30 | 102.10 |
| 80 | 1 | 3412 | PAR | O52-C13-O43 | -2.31 | 108.93 | 111.43 |
| 80 | 5 | 3403 | PAR | O11-C11-C21 | -2.31 | 104.24 | 108.22 |
| 80 | 5 | 3405 | PAR | C32-C22-C12 | -2.29 | 106.48 | 111.18 |
| 80 | 8 | 201 | PAR | C52-C42-C32 | 2.28 | 115.42 | 111.16 |
| 80 | 5 | 3414 | PAR | C32-C22-C12 | 2.27 | 115.85 | 111.18 |
| 80 | 5 | 3419 | PAR | C22-C12-C62 | 2.26 | 113.46 | 110.04 |
| 80 | 1 | 3425 | PAR | O52-C13-O43 | -2.26 | 108.98 | 111.43 |
| 80 | 2 | 1902 | PAR | O11-C11-C21 | 2.26 | 112.11 | 108.22 |
| 80 | o2 | 201 | PAR | O23-C23-C33 | 2.23 | 117.51 | 111.17 |
| 80 | 7 | 202 | PAR | O11-C42-C32 | -2.23 | 103.87 | 109.18 |
| 80 | 2 | 1905 | PAR | O33-C14-C24 | -2.22 | 104.39 | 108.22 |
| 80 | 1 | 3415 | PAR | C13-C23-C33 | -2.21 | 99.44 | 102.10 |
| 80 | 6 | 1905 | PAR | O33-C14-C24 | 2.21 | 112.02 | 108.22 |
| 80 | 8 | 201 | PAR | O33-C14-C24 | -2.21 | 104.41 | 108.22 |
| 80 | 1 | 3433 | PAR | C52-C42-C32 | 2.20 | 115.28 | 111.16 |
| 80 | 1 | 3414 | PAR | O11-C42-C32 | -2.20 | 103.92 | 109.18 |
| 80 | 1 | 3411 | PAR | O54-C54-C64 | 2.20 | 110.11 | 106.01 |
| 80 | 2 | 1903 | PAR | C13-O43-C43 | -2.20 | 97.98 | 106.13 |
| 80 | 5 | 3412 | PAR | O11-C11-C21 | 2.20 | 112.00 | 108.22 |
| 80 | 5 | 3425 | PAR | C13-C23-C33 | 2.20 | 104.74 | 102.10 |
| 80 | 1 | 3414 | PAR | C13-C23-C33 | -2.19 | 99.46 | 102.10 |
| 80 | 1 | 3419 | PAR | O52-C52-C42 | 2.19 | 113.03 | 107.48 |
| 80 | 2 | 1904 | PAR | C14-O54-C54 | 2.17 | 117.96 | 113.69 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 5 | 3423 | PAR | O11-C11-C21 | 2.17 | 111.96 | 108.22 |
| 80 | 1 | 3408 | PAR | O11-C11-C21 | 2.16 | 111.94 | 108.22 |
| 80 | 1 | 3412 | PAR | C23-C33-C43 | -2.16 | 99.40 | 103.22 |
| 80 | 5 | 3424 | PAR | C13-O43-C43 | -2.16 | 98.13 | 106.13 |
| 80 | 6 | 1904 | PAR | O52-C13-O43 | -2.15 | 109.10 | 111.43 |
| 80 | 1 | 3412 | PAR | O11-C42-C32 | -2.15 | 104.04 | 109.18 |
| 80 | 5 | 3407 | PAR | O33-C14-C24 | 2.15 | 111.91 | 108.22 |
| 80 | 5 | 3406 | PAR | O54-C54-C64 | 2.14 | 110.00 | 106.01 |
| 80 | 1 | 3425 | PAR | O33-C33-C23 | -2.14 | 104.43 | 111.32 |
| 80 | 4 | 202 | PAR | O33-C33-C23 | -2.14 | 104.45 | 111.32 |
| 80 | 3 | 203 | PAR | C32-C22-C12 | 2.13 | 115.57 | 111.18 |
| 80 | 5 | 3406 | PAR | O52-C13-C23 | 2.13 | 112.38 | 107.96 |
| 80 | 5 | 3404 | PAR | C62-C52-C42 | -2.13 | 106.81 | 111.66 |
| 80 | 1 | 3433 | PAR | O54-C54-C64 | 2.12 | 109.96 | 106.01 |
| 80 | 1 | 3402 | PAR | O52-C13-O43 | -2.12 | 109.13 | 111.43 |
| 80 | 5 | 3423 | PAR | O52-C52-C42 | -2.11 | 102.11 | 107.48 |
| 80 | 5 | 3414 | PAR | O11-C11-C21 | 2.11 | 111.85 | 108.22 |
| 80 | 6 | 1906 | PAR | C11-C21-N21 | 2.11 | 114.01 | 110.20 |
| 80 | 1 | 3435 | PAR | C41-C31-C21 | -2.11 | 107.44 | 111.07 |
| 80 | 1 | 3408 | PAR | O51-C11-C21 | 2.11 | 114.80 | 110.06 |
| 80 | 6 | 1901 | PAR | O33-C14-C24 | -2.11 | 104.58 | 108.22 |
| 80 | 1 | 3406 | PAR | O11-C42-C32 | -2.09 | 104.18 | 109.18 |
| 80 | 3 | 201 | PAR | O23-C23-C33 | 2.09 | 117.10 | 111.17 |
| 80 | 1 | 3418 | PAR | C23-C33-C43 | -2.09 | 99.52 | 103.22 |
| 80 | 1 | 3407 | PAR | C14-O54-C54 | 2.09 | 117.78 | 113.69 |
| 80 | 1 | 3434 | PAR | O33-C14-C24 | -2.08 | 104.63 | 108.22 |
| 80 | 5 | 3402 | PAR | O11-C42-C32 | -2.08 | 104.22 | 109.18 |
| 80 | 1 | 3424 | PAR | O11-C11-C21 | 2.08 | 111.80 | 108.22 |
| 80 | 1 | 3419 | PAR | O11-C11-C21 | 2.07 | 111.79 | 108.22 |
| 80 | n3 | 201 | PAR | O11-C42-C52 | -2.07 | 102.21 | 107.48 |
| 80 | 1 | 3408 | PAR | O33-C33-C23 | 2.07 | 117.97 | 111.32 |
| 80 | 5 | 3411 | PAR | O52-C52-C62 | 2.07 | 112.78 | 107.28 |
| 80 | 5 | 3419 | PAR | O43-C43-C33 | -2.07 | 100.44 | 104.87 |
| 80 | 5 | 3413 | PAR | C62-C52-C42 | -2.07 | 106.94 | 111.66 |
| 80 | 4 | 202 | PAR | O11-C42-C32 | -2.06 | 104.26 | 109.18 |
| 80 | 1 | 3430 | PAR | O33-C14-C24 | 2.06 | 111.76 | 108.22 |
| 80 | 1 | 3431 | PAR | O52-C52-C62 | 2.06 | 112.76 | 107.28 |
| 80 | 5 | 3428 | PAR | O52-C13-O43 | -2.06 | 109.20 | 111.43 |
| 80 | 5 | 3420 | PAR | C13-C23-C33 | -2.06 | 99.63 | 102.10 |
| 80 | 1 | 3409 | PAR | C62-C52-C42 | -2.05 | 106.98 | 111.66 |
| 80 | 5 | 3416 | PAR | C11-C21-N21 | 2.05 | 113.89 | 110.20 |
| 80 | 1 | 3435 | PAR | O23-C23-C33 | -2.05 | 105.36 | 111.17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 80 | 1 | 3415 | PAR | O33-C14-C24 | 2.04 | 111.73 | 108.22 |
| 80 | 1 | 3412 | PAR | C14-O33-C33 | 2.04 | 123.02 | 117.96 |
| 80 | 5 | 3427 | PAR | C13-C23-C33 | 2.04 | 104.55 | 102.10 |
| 80 | 6 | 1904 | PAR | C52-C42-C32 | 2.04 | 114.96 | 111.16 |
| 80 | 6 | 1905 | PAR | C14-C24-N24 | 2.03 | 113.87 | 110.20 |
| 80 | 5 | 3403 | PAR | O52-C52-C62 | 2.03 | 112.67 | 107.28 |
| 80 | 5 | 3418 | PAR | C13-C23-C33 | -2.02 | 99.67 | 102.10 |
| 80 | 5 | 3410 | PAR | O11-C11-C21 | 2.02 | 111.70 | 108.22 |
| 80 | 1 | 3435 | PAR | O33-C14-C24 | -2.01 | 104.76 | 108.22 |
| 80 | 1 | 3410 | PAR | O62-C62-C52 | 2.00 | 115.25 | 109.94 |

There are no chirality outliers.

All (474) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 5 | 3413 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3431 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3414 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3418 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3418 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3406 | PAR | C23-C13-O52-C52 |
| 80 | o2 | 201 | PAR | C23-C33-O33-C14 |
| 80 | 2 | 1902 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3404 | PAR | C21-C11-O11-C42 |
| 80 | 5 | 3404 | PAR | C24-C14-O33-C33 |
| 80 | 7 | 202 | PAR | C23-C13-O52-C52 |
| 80 | 7 | 202 | PAR | O43-C13-O52-C52 |
| 80 | 7 | 202 | PAR | C24-C14-O33-C33 |
| 80 | 3 | 202 | PAR | C23-C13-O52-C52 |
| 80 | 3 | 202 | PAR | C44-C54-C64-N64 |
| 80 | 3 | 202 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3422 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3422 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3422 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3422 | PAR | O54-C54-C64-N64 |
| 80 | 6 | 1905 | PAR | C23-C13-O52-C52 |
| 80 | 6 | 1905 | PAR | O43-C13-O52-C52 |
| 80 | 6 | 1905 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3432 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3432 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3435 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3435 | PAR | O54-C54-C64-N64 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 1 | 3436 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3436 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3423 | PAR | C21-C11-O11-C42 |
| 80 | 5 | 3423 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3423 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3421 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3407 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3407 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3407 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3407 | PAR | O54-C54-C64-N64 |
| 80 | 6 | 1901 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3407 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3407 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3407 | PAR | C23-C33-O33-C14 |
| 80 | 6 | 1904 | PAR | C23-C13-O52-C52 |
| 80 | 6 | 1904 | PAR | C24-C14-O33-C33 |
| 80 | 6 | 1904 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3402 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3419 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3409 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3409 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3409 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3403 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3403 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3403 | PAR | O54-C54-C64-N64 |
| 80 | 3 | 201 | PAR | C23-C13-O52-C52 |
| 80 | 3 | 201 | PAR | C23-C33-O33-C14 |
| 80 | 6 | 1906 | PAR | C21-C11-O11-C42 |
| 80 | 5 | 3410 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3410 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3417 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3410 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3410 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3410 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3410 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3420 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3420 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3405 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3405 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3405 | PAR | C43-C33-O33-C14 |
| 80 | 5 | 3405 | PAR | C24-C14-O33-C33 |
| 80 | 6 | 1903 | PAR | C23-C13-O52-C52 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 5 | 3425 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3403 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3403 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3403 | PAR | O43-C13-O52-C52 |
| 80 | 8 | 202 | PAR | C23-C13-O52-C52 |
| 80 | 8 | 202 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3411 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3411 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3411 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3411 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3411 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3437 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3437 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3437 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3437 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3437 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3433 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3433 | PAR | C24-C14-O33-C33 |
| 80 | 3 | 203 | PAR | C24-C14-O33-C33 |
| 80 | 6 | 1902 | PAR | C21-C11-O11-C42 |
| 80 | 6 | 1902 | PAR | C43-C33-O33-C14 |
| 80 | 6 | 1902 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3428 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3428 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3401 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3401 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3412 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3412 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3401 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3401 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3424 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3427 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3427 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3427 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3417 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3417 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3426 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3426 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3426 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3425 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3425 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3425 | PAR | C43-C33-O33-C14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 1 | 3425 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3422 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3422 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3421 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3421 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3405 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3405 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3405 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3405 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3405 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3405 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3408 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3408 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3408 | PAR | C24-C14-O33-C33 |
| 80 | n3 | 201 | PAR | C21-C11-O11-C42 |
| 80 | n3 | 201 | PAR | C32-C42-O11-C11 |
| 80 | n3 | 201 | PAR | C23-C13-O52-C52 |
| 80 | n3 | 201 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3418 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3418 | PAR | C23-C33-O33-C14 |
| 80 | 2 | 1903 | PAR | C23-C13-O52-C52 |
| 80 | 2 | 1903 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3415 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3411 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3424 | PAR | C43-C33-O33-C14 |
| 80 | 5 | 3427 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3427 | PAR | O43-C13-O52-C52 |
| 80 | 4 | 201 | PAR | C23-C13-O52-C52 |
| 80 | 4 | 201 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3409 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3409 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3409 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3416 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3408 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3429 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3429 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3430 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3430 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3430 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3413 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3414 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3434 | PAR | C62-C52-O52-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 5 | 3411 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3415 | PAR | C52-C42-O11-C11 |
| 80 | 6 | 1904 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3403 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3405 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3433 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3424 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3415 | PAR | O54-C14-O33-C33 |
| 80 | 3 | 201 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3401 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3416 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3409 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3420 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3401 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3412 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3413 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3431 | PAR | C62-C52-O52-C13 |
| 80 | 2 | 1902 | PAR | C62-C52-O52-C13 |
| 80 | 3 | 202 | PAR | C62-C52-O52-C13 |
| 80 | 3 | 203 | PAR | C42-C52-O52-C13 |
| 80 | 7 | 202 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3435 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3406 | PAR | O51-C11-O11-C42 |
| 80 | 2 | 1905 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3403 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3410 | PAR | O54-C14-O33-C33 |
| 80 | 2 | 1904 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3403 | PAR | O51-C11-O11-C42 |
| 80 | 8 | 202 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3426 | PAR | O54-C14-O33-C33 |
| 80 | n3 | 201 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3415 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3414 | PAR | O54-C14-O33-C33 |
| 80 | 2 | 1901 | PAR | O51-C11-O11-C42 |
| 80 | 6 | 1902 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3426 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3425 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3404 | PAR | O54-C14-O33-C33 |
| 80 | 6 | 1905 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3411 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3412 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3404 | PAR | C62-C52-O52-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 5 | 3415 | PAR | C42-C52-O52-C13 |
| 80 | 1 | 3402 | PAR | O54-C14-O33-C33 |
| 80 | n3 | 201 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3401 | PAR | O43-C43-C53-O53 |
| 80 | 5 | 3427 | PAR | O51-C11-O11-C42 |
| 80 | 6 | 1906 | PAR | C52-C42-O11-C11 |
| 80 | 6 | 1902 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3402 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3417 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3405 | PAR | O43-C43-C53-O53 |
| 80 | 3 | 202 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3419 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3401 | PAR | C33-C43-C53-O53 |
| 80 | 1 | 3419 | PAR | C42-C52-O52-C13 |
| 80 | 1 | 3422 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3436 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3419 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3419 | PAR | O43-C43-C53-O53 |
| 80 | 5 | 3423 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3404 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3425 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3435 | PAR | C41-C51-C61-O61 |
| 80 | 1 | 3425 | PAR | O43-C43-C53-O53 |
| 80 | 1 | 3430 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3417 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3405 | PAR | C33-C43-C53-O53 |
| 80 | 5 | 3408 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3402 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3419 | PAR | C33-C43-C53-O53 |
| 80 | 5 | 3409 | PAR | C33-C43-C53-O53 |
| 80 | 5 | 3410 | PAR | C41-C51-C61-O61 |
| 80 | 1 | 3430 | PAR | O51-C11-O11-C42 |
| 80 | 3 | 202 | PAR | C41-C51-C61-O61 |
| 80 | 1 | 3402 | PAR | C41-C51-C61-O61 |
| 80 | 5 | 3423 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3425 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3405 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3420 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3422 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3409 | PAR | O43-C43-C53-O53 |
| 80 | 6 | 1903 | PAR | C33-C43-C53-O53 |
| 80 | 1 | 3401 | PAR | C42-C52-O52-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 1 | 3435 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3411 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3419 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3401 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3408 | PAR | O51-C11-O11-C42 |
| 80 | o2 | 201 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3428 | PAR | O43-C43-C53-O53 |
| 80 | 1 | 3422 | PAR | C41-C51-C61-O61 |
| 80 | o2 | 201 | PAR | O54-C14-O33-C33 |
| 80 | 7 | 201 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3417 | PAR | O51-C11-O11-C42 |
| 80 | 7 | 202 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3412 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3405 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3413 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3431 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3418 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3406 | PAR | O43-C13-O52-C52 |
| 80 | o2 | 201 | PAR | O43-C13-O52-C52 |
| 80 | 3 | 202 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3422 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3435 | PAR | O43-C13-O52-C52 |
| 80 | 6 | 1901 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3402 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3423 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3409 | PAR | O43-C13-O52-C52 |
| 80 | 3 | 201 | PAR | O43-C13-O52-C52 |
| 80 | 6 | 1903 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3425 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3433 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3401 | PAR | O43-C13-O52-C52 |
| 80 | 4 | 202 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3427 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3418 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3424 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3408 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3415 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3410 | PAR | O51-C51-C61-O61 |
| 80 | 8 | 201 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3406 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3411 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3436 | PAR | O51-C11-O11-C42 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 6 | 1906 | PAR | C42-C52-O52-C13 |
| 80 | o2 | 201 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3409 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3419 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3434 | PAR | O51-C51-C61-O61 |
| 80 | 6 | 1906 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3418 | PAR | C42-C52-O52-C13 |
| 80 | 1 | 3405 | PAR | C42-C52-O52-C13 |
| 80 | 1 | 3404 | PAR | O54-C14-O33-C33 |
| 80 | 2 | 1905 | PAR | C44-C54-C64-N64 |
| 80 | 3 | 201 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3434 | PAR | C23-C33-O33-C14 |
| 80 | 2 | 1903 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3430 | PAR | C43-C33-O33-C14 |
| 80 | 6 | 1903 | PAR | O43-C43-C53-O53 |
| 80 | 1 | 3425 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3418 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3411 | PAR | C42-C52-O52-C13 |
| 80 | n3 | 201 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3424 | PAR | O51-C11-O11-C42 |
| 80 | 7 | 202 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3436 | PAR | C41-C51-C61-O61 |
| 80 | 1 | 3425 | PAR | C33-C43-C53-O53 |
| 80 | o2 | 201 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3425 | PAR | C41-C51-C61-O61 |
| 80 | 5 | 3402 | PAR | C42-C52-O52-C13 |
| 80 | 1 | 3423 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3409 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3404 | PAR | O43-C43-C53-O53 |
| 80 | 5 | 3407 | PAR | O54-C14-O33-C33 |
| 80 | 7 | 201 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3421 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3419 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3417 | PAR | O43-C13-O52-C52 |
| 80 | 5 | 3424 | PAR | O43-C13-O52-C52 |
| 80 | 1 | 3411 | PAR | C62-C52-O52-C13 |
| 80 | 6 | 1902 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3428 | PAR | O51-C11-O11-C42 |
| 80 | 1 | 3417 | PAR | C23-C13-O52-C52 |
| 80 | 4 | 202 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3424 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3416 | PAR | O51-C11-O11-C42 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 5 | 3402 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3425 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3411 | PAR | C32-C42-O11-C11 |
| 80 | 1 | 3409 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3415 | PAR | C62-C52-O52-C13 |
| 80 | o2 | 201 | PAR | O54-C54-C64-N64 |
| 80 | 2 | 1902 | PAR | O54-C54-C64-N64 |
| 80 | 6 | 1905 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3402 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3436 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3421 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3419 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3410 | PAR | O54-C54-C64-N64 |
| 80 | 2 | 1904 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3434 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3412 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3404 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3417 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3422 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3418 | PAR | O54-C54-C64-N64 |
| 80 | 2 | 1903 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3415 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3416 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3412 | PAR | O54-C54-C64-N64 |
| 80 | 4 | 201 | PAR | O54-C54-C64-N64 |
| 80 | 5 | 3426 | PAR | O54-C54-C64-N64 |
| 80 | 1 | 3428 | PAR | C52-C42-O11-C11 |
| 80 | 4 | 201 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3421 | PAR | O51-C11-O11-C42 |
| 80 | 6 | 1902 | PAR | C42-C52-O52-C13 |
| 80 | 6 | 1904 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3418 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3435 | PAR | C42-C52-O52-C13 |
| 80 | 1 | 3409 | PAR | C52-C42-O11-C11 |
| 80 | 2 | 1904 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3426 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3408 | PAR | C41-C51-C61-O61 |
| 80 | 5 | 3428 | PAR | C42-C52-O52-C13 |
| 80 | o2 | 201 | PAR | O43-C43-C53-O53 |
| 80 | 3 | 202 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3432 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3402 | PAR | C23-C33-O33-C14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 5 | 3406 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3436 | PAR | C43-C33-O33-C14 |
| 80 | 5 | 3419 | PAR | C44-C54-C64-N64 |
| 80 | 8 | 202 | PAR | C43-C33-O33-C14 |
| 80 | 3 | 203 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3405 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3415 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3413 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3422 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3418 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3411 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3416 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3429 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3407 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3409 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3428 | PAR | O51-C51-C61-O61 |
| 80 | 2 | 1905 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3407 | PAR | C42-C52-O52-C13 |
| 80 | 4 | 202 | PAR | O43-C43-C53-O53 |
| 80 | 1 | 3435 | PAR | C62-C52-O52-C13 |
| 80 | 1 | 3419 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3412 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3407 | PAR | O43-C43-C53-O53 |
| 80 | 1 | 3433 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3407 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3409 | PAR | C41-C51-C61-O61 |
| 80 | 1 | 3402 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3426 | PAR | C62-C52-O52-C13 |
| 80 | 7 | 202 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3428 | PAR | C62-C52-O52-C13 |
| 80 | 5 | 3408 | PAR | O51-C51-C61-O61 |
| 80 | 1 | 3407 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3419 | PAR | O51-C51-C61-O61 |
| 80 | 5 | 3407 | PAR | C62-C52-O52-C13 |
| 80 | 3 | 201 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3410 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3414 | PAR | C52-C42-O11-C11 |
| 80 | 4 | 201 | PAR | O51-C51-C61-O61 |
| 80 | 2 | 1904 | PAR | C62-C52-O52-C13 |
| 80 | 2 | 1903 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3431 | PAR | C23-C13-O52-C52 |
| 80 | 7 | 201 | PAR | C23-C13-O52-C52 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | o2 | 201 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3402 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3435 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3421 | PAR | C23-C13-O52-C52 |
| 80 | 1 | 3423 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3424 | PAR | C23-C13-O52-C52 |
| 80 | 5 | 3415 | PAR | C23-C13-O52-C52 |
| 80 | o2 | 201 | PAR | C32-C42-O11-C11 |
| 80 | 1 | 3427 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3421 | PAR | O54-C14-O33-C33 |
| 80 | 5 | 3426 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3430 | PAR | C52-C42-O11-C11 |
| 80 | 1 | 3436 | PAR | O43-C43-C53-O53 |
| 80 | 1 | 3408 | PAR | C42-C52-O52-C13 |
| 80 | 2 | 1905 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3418 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3418 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3428 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3404 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3404 | PAR | C43-C33-O33-C14 |
| 80 | 7 | 202 | PAR | C23-C33-O33-C14 |
| 80 | 6 | 1905 | PAR | C23-C33-O33-C14 |
| 80 | 6 | 1905 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3402 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3435 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3406 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3406 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3436 | PAR | C23-C33-O33-C14 |
| 80 | 5 | 3421 | PAR | C43-C33-O33-C14 |
| 80 | 5 | 3407 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3407 | PAR | C44-C54-C64-N64 |
| 80 | 6 | 1904 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3402 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3423 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3423 | PAR | C43-C33-O33-C14 |
| 80 | 5 | 3419 | PAR | C23-C33-O33-C14 |
| 80 | 6 | 1906 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3410 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3417 | PAR | C43-C33-O33-C14 |
| 80 | 6 | 1903 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3425 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3403 | PAR | C23-C33-O33-C14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 8 | 202 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3434 | PAR | C43-C33-O33-C14 |
| 80 | 3 | 203 | PAR | C43-C33-O33-C14 |
| 80 | 6 | 1902 | PAR | C23-C33-O33-C14 |
| 80 | 6 | 1902 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3412 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3417 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3421 | PAR | C43-C33-O33-C14 |
| 80 | n3 | 201 | PAR | C43-C33-O33-C14 |
| 80 | 1 | 3415 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3412 | PAR | C43-C33-O33-C14 |
| 80 | 4 | 201 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3409 | PAR | C44-C54-C64-N64 |
| 80 | 5 | 3426 | PAR | C44-C54-C64-N64 |
| 80 | 1 | 3413 | PAR | C23-C33-O33-C14 |
| 80 | 1 | 3431 | PAR | C24-C14-O33-C33 |
| 80 | 5 | 3403 | PAR | C24-C14-O33-C33 |
| 80 | 1 | 3434 | PAR | C21-C11-O11-C42 |
| 80 | 5 | 3428 | PAR | C21-C11-O11-C42 |
| 80 | 5 | 3411 | PAR | C21-C11-O11-C42 |
| 80 | 1 | 3413 | PAR | C21-C11-O11-C42 |
| 80 | 5 | 3410 | PAR | O54-C14-O33-C33 |
| 80 | 1 | 3435 | PAR | O51-C11-O11-C42 |
| 80 | 5 | 3402 | PAR | C52-C42-O11-C11 |
| 80 | 5 | 3404 | PAR | C41-C51-C61-O61 |
| 80 | 5 | 3405 | PAR | C42-C52-O52-C13 |
| 80 | 5 | 3409 | PAR | O51-C51-C61-O61 |

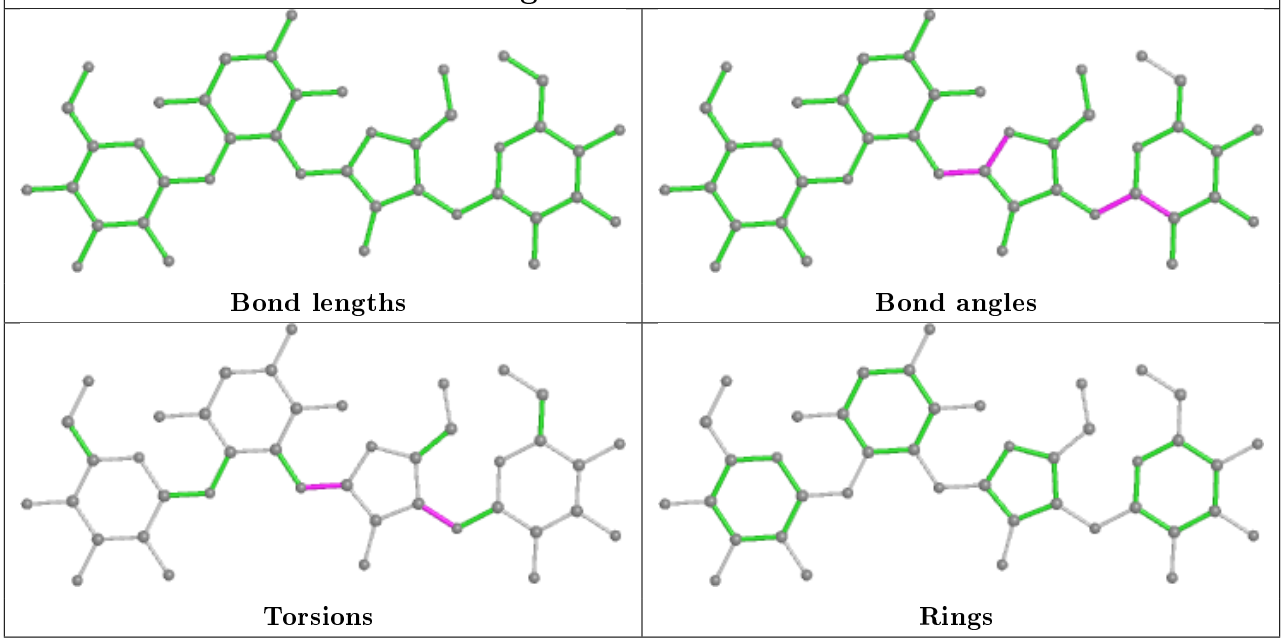
All (10) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 80 | 1 | 3409 | PAR | C12-C22-C32-C42-C52-C62 |
| 80 | 5 | 3414 | PAR | C12-C22-C32-C42-C52-C62 |
| 80 | 4 | 201 | PAR | C12-C22-C32-C42-C52-C62 |
| 80 | 3 | 203 | PAR | C12-C22-C32-C42-C52-C62 |
| 80 | 1 | 3418 | PAR | C14-C24-C34-C44-C54-O54 |
| 80 | 1 | 3432 | PAR | C12-C22-C32-C42-C52-C62 |
| 80 | 5 | 3426 | PAR | C14-C24-C34-C44-C54-O54 |
| 80 | 1 | 3419 | PAR | C14-C24-C34-C44-C54-O54 |
| 80 | 5 | 3427 | PAR | C12-C22-C32-C42-C52-C62 |
| 80 | 5 | 3420 | PAR | C12-C22-C32-C42-C52-C62 |

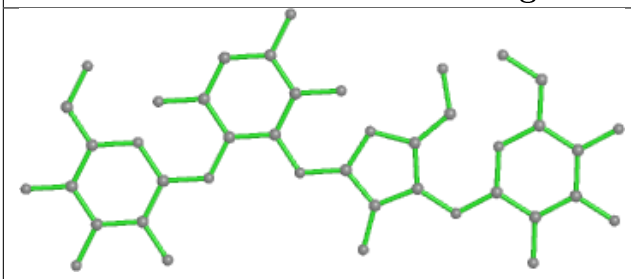
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

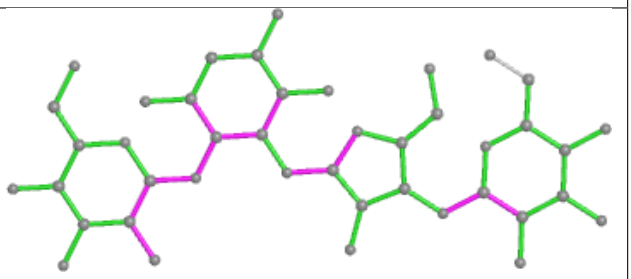
**Ligand PAR 1 3421**



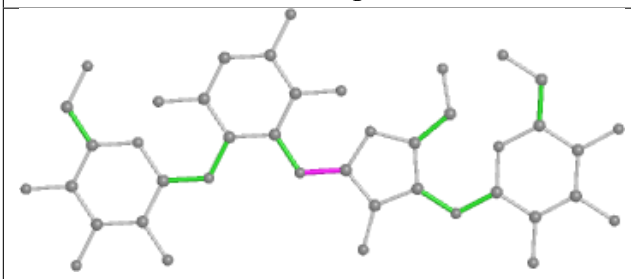
### Ligand PAR 5 3413



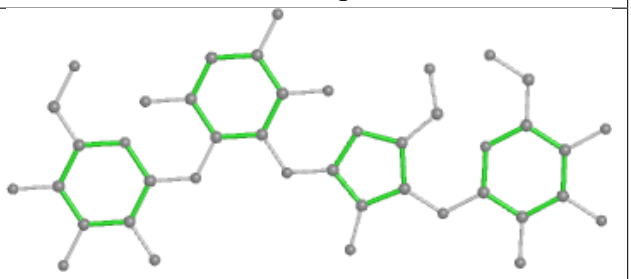
Bond lengths



Bond angles

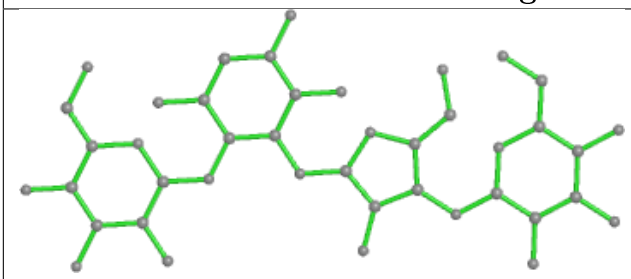


Torsions

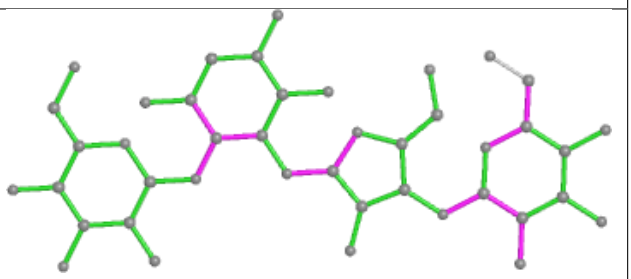


Rings

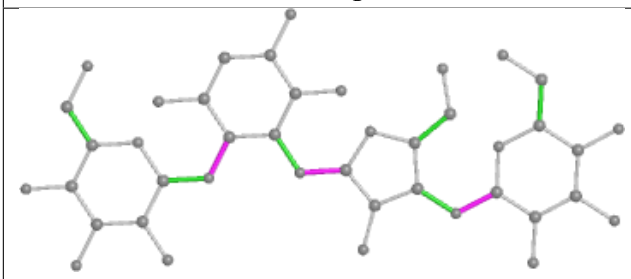
### Ligand PAR 1 3433



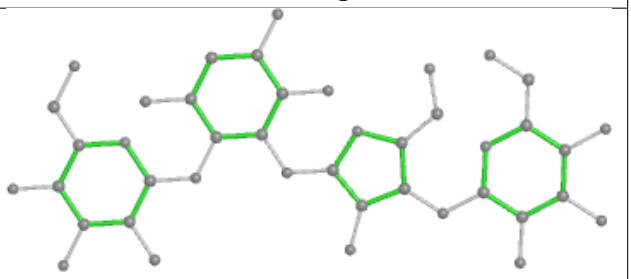
Bond lengths



Bond angles

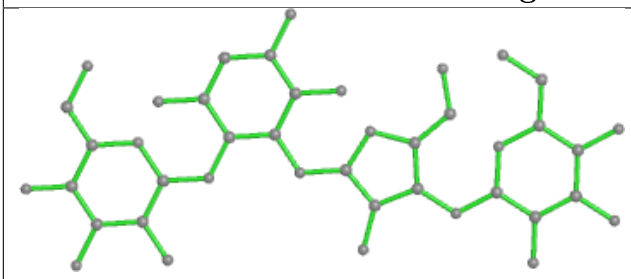


Torsions

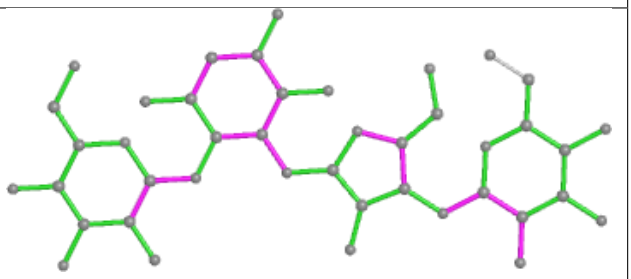


Rings

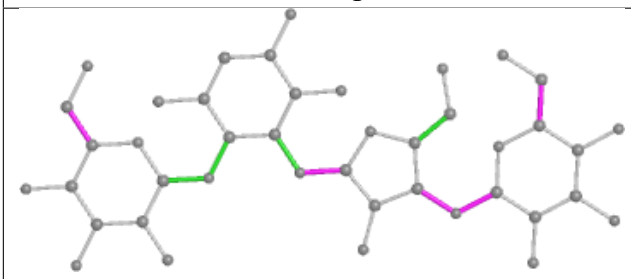
**Ligand PAR 5 3419**



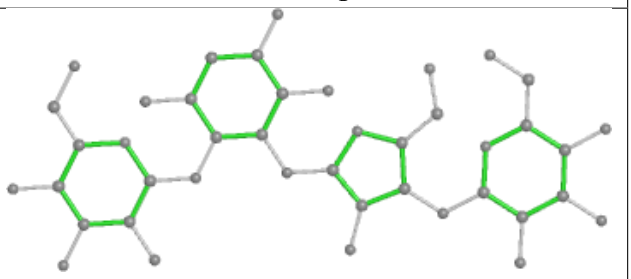
Bond lengths



Bond angles

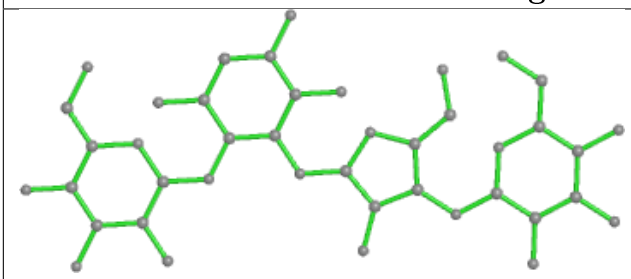


Torsions

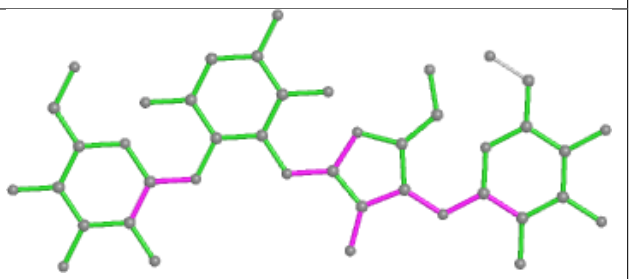


Rings

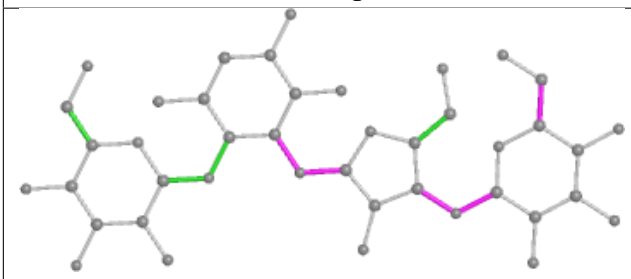
**Ligand PAR 3 201**



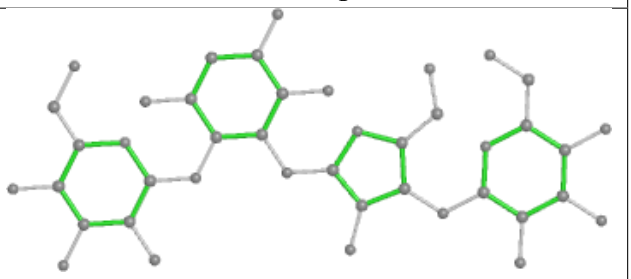
Bond lengths



Bond angles

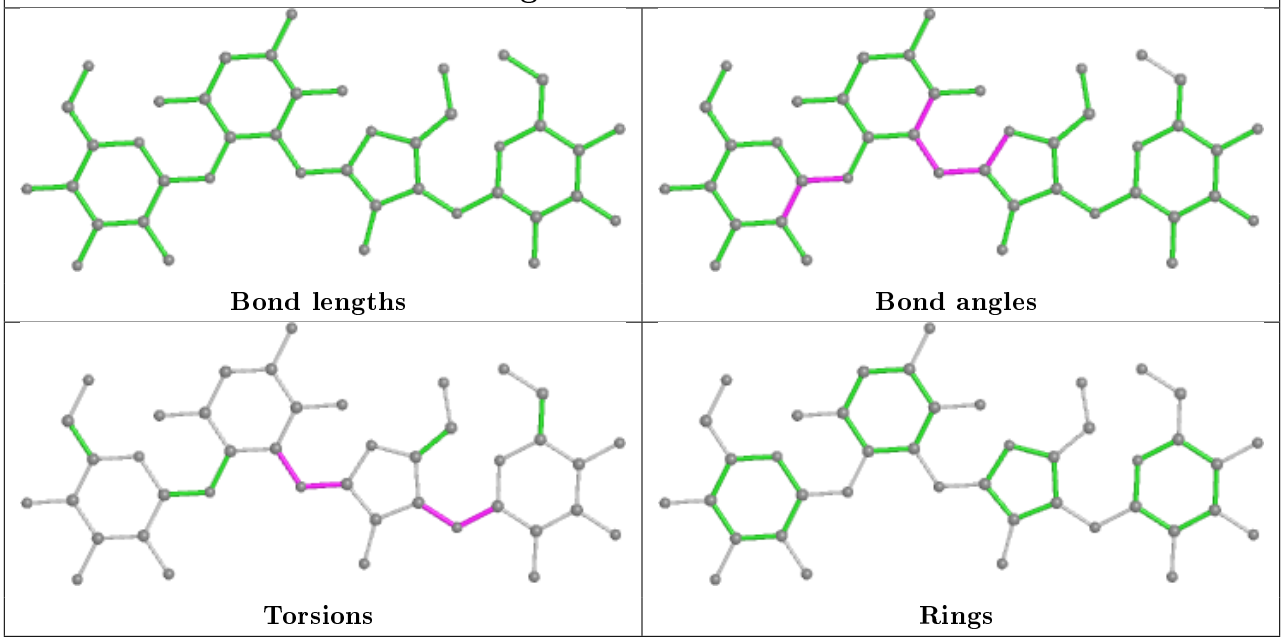


Torsions

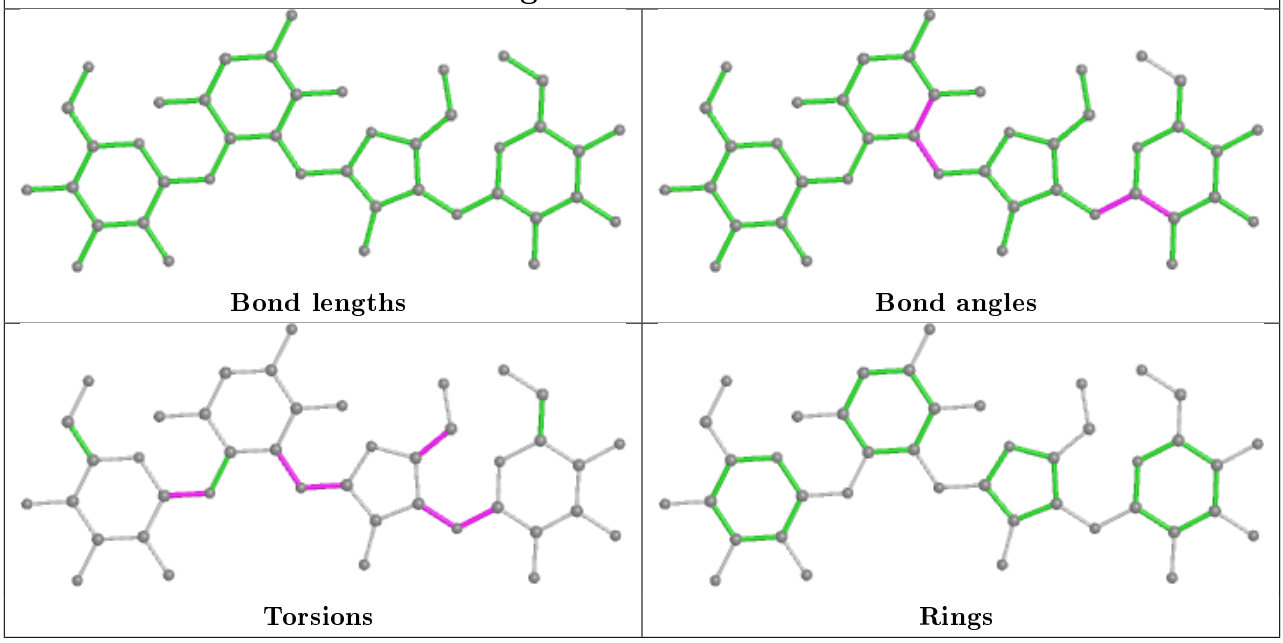


Rings

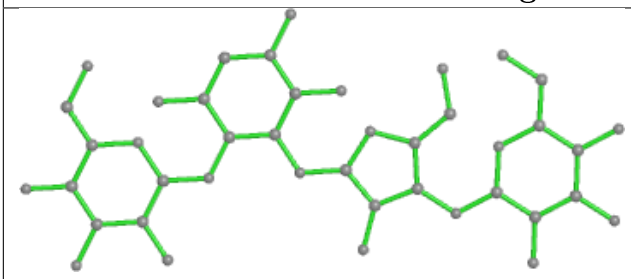
**Ligand PAR 1 3431**



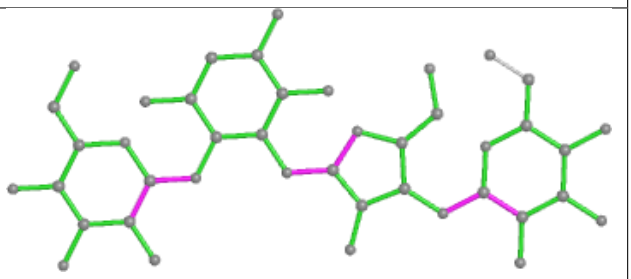

**Ligand PAR 1 3405**



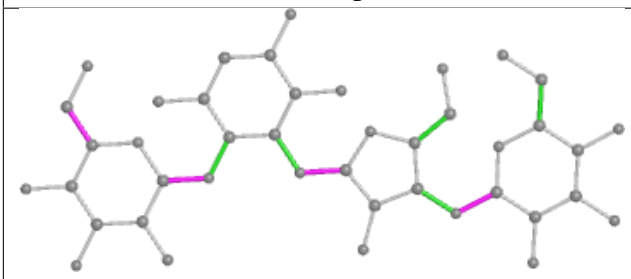
**Ligand PAR 5 3408**



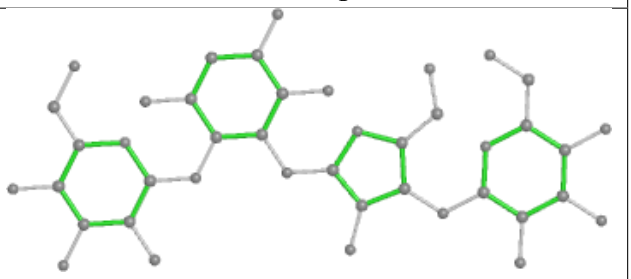
Bond lengths



Bond angles

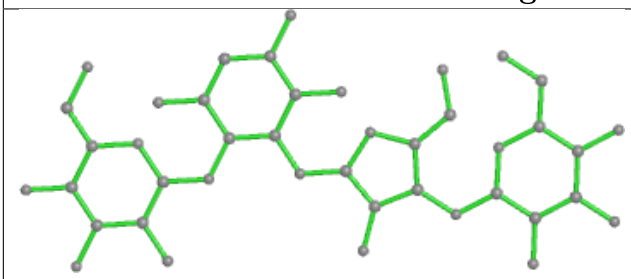


Torsions

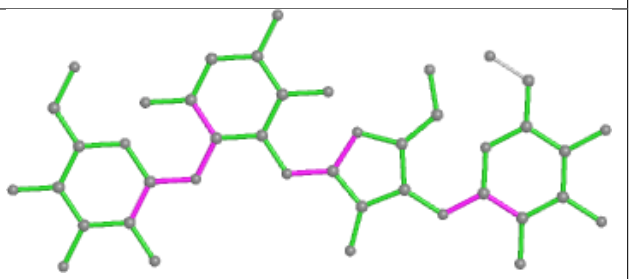


Rings

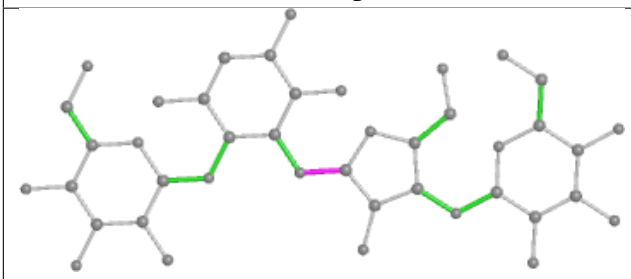
**Ligand PAR 1 3406**



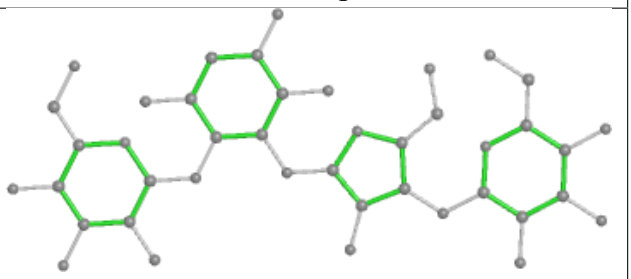
Bond lengths



Bond angles

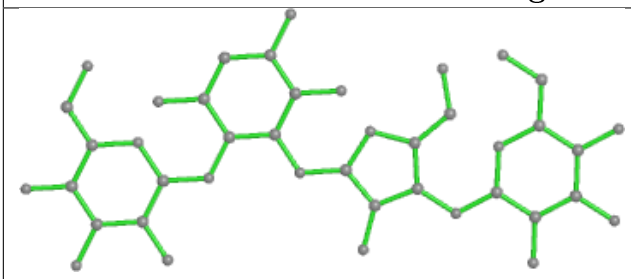


Torsions

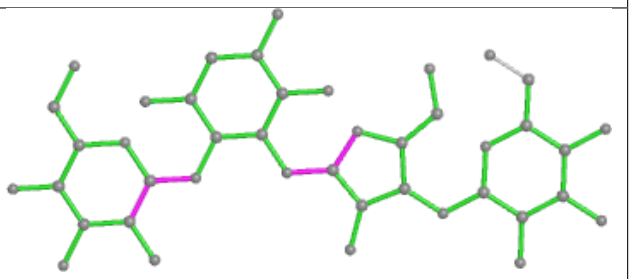


Rings

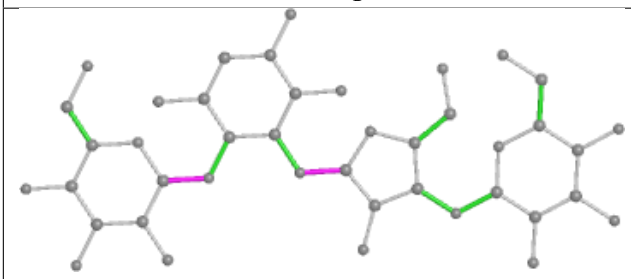
**Ligand PAR 7 201**



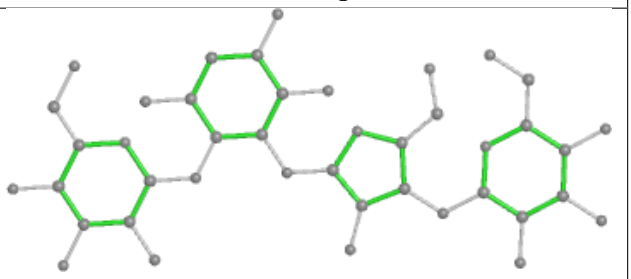
Bond lengths



Bond angles

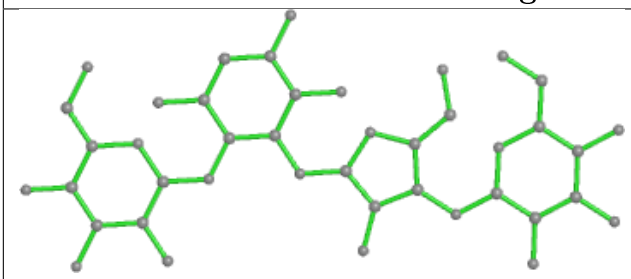


Torsions

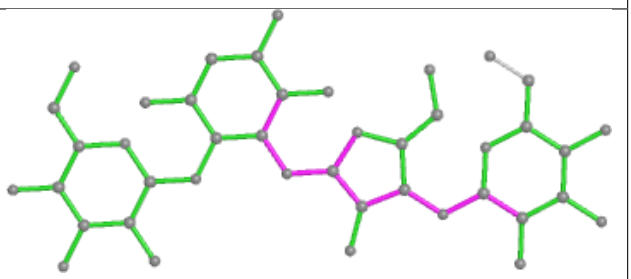


Rings

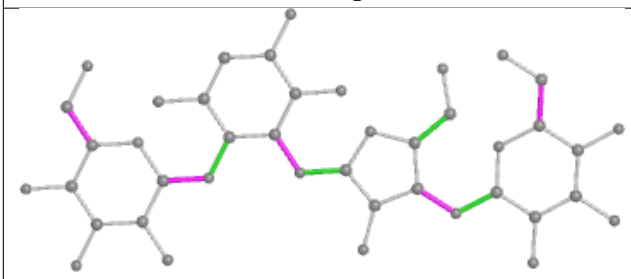
**Ligand PAR 1 3434**



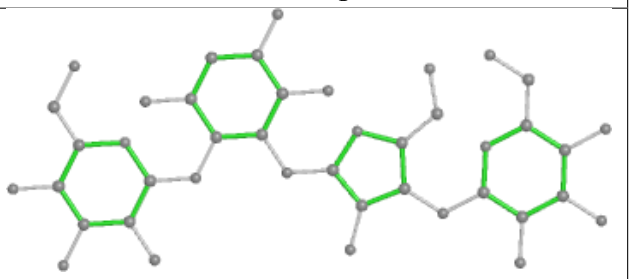
Bond lengths



Bond angles

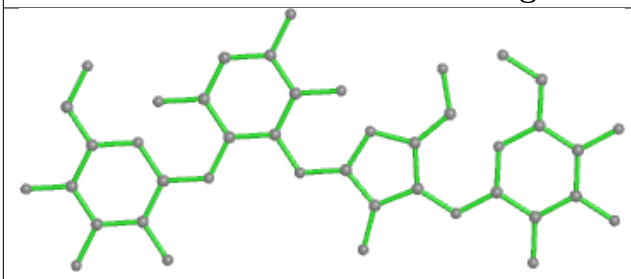


Torsions

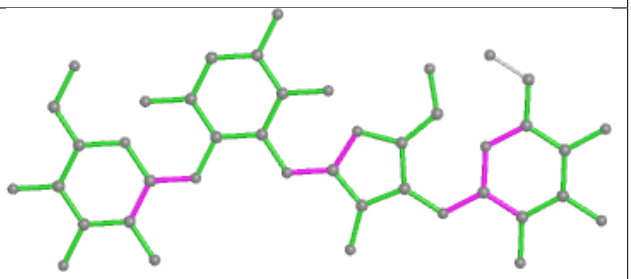


Rings

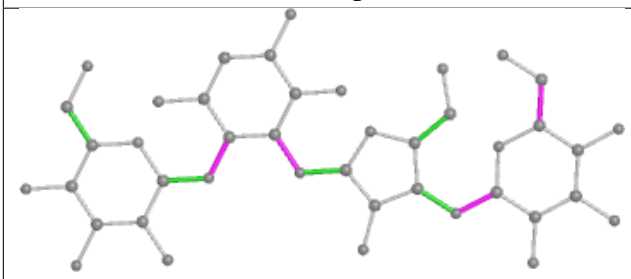
**Ligand PAR 2 1904**



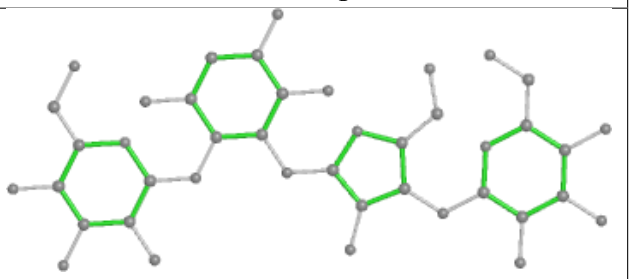
Bond lengths



Bond angles

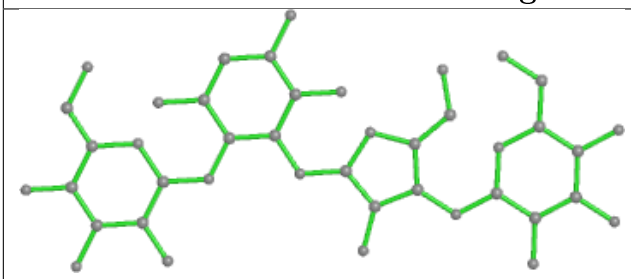


Torsions

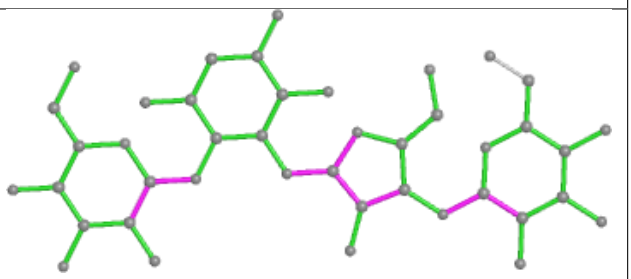


Rings

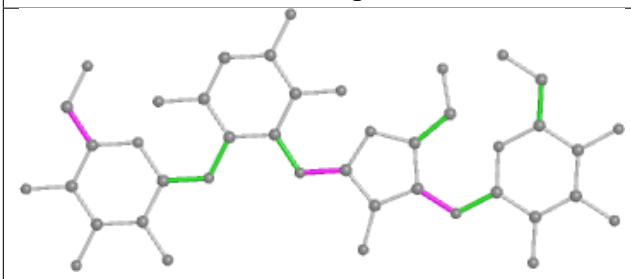
**Ligand PAR 5 3425**



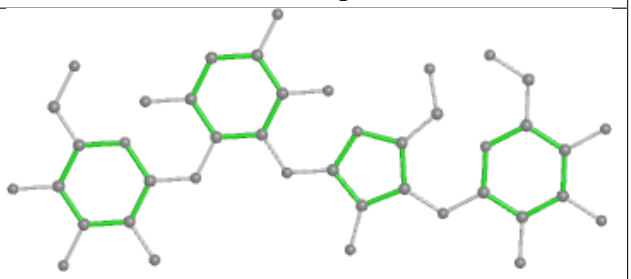
Bond lengths



Bond angles

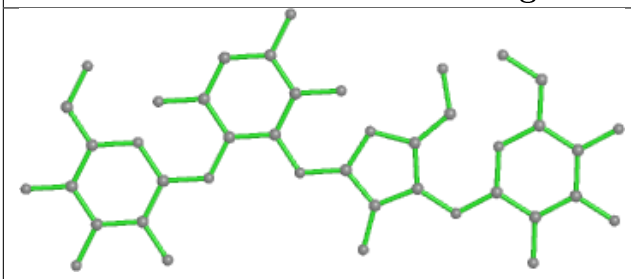


Torsions

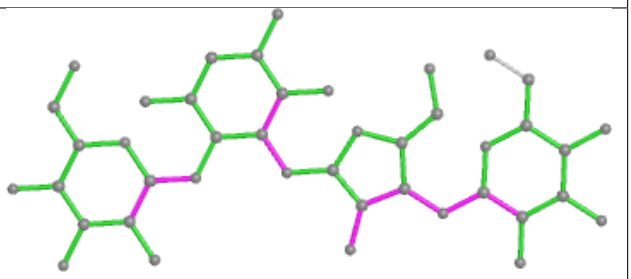


Rings

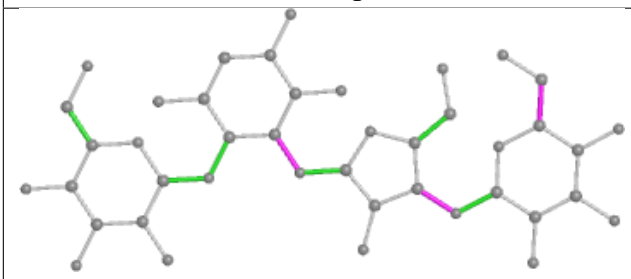
**Ligand PAR 2 1902**



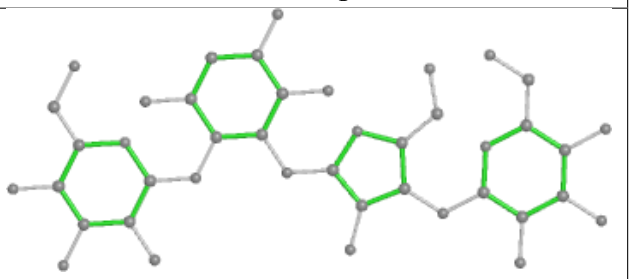
Bond lengths



Bond angles

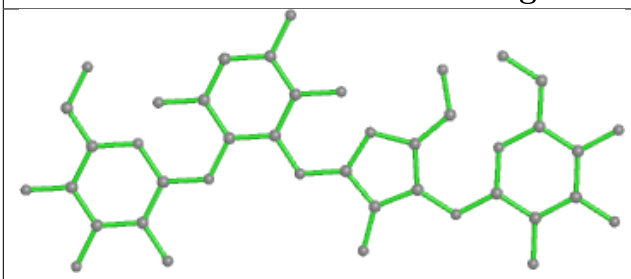


Torsions

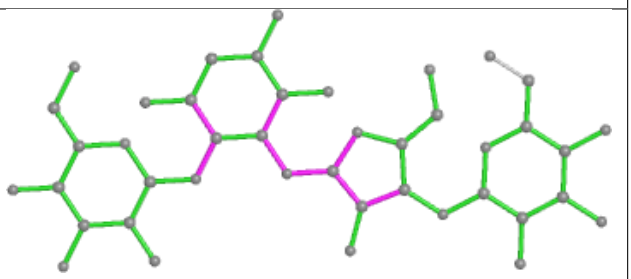


Rings

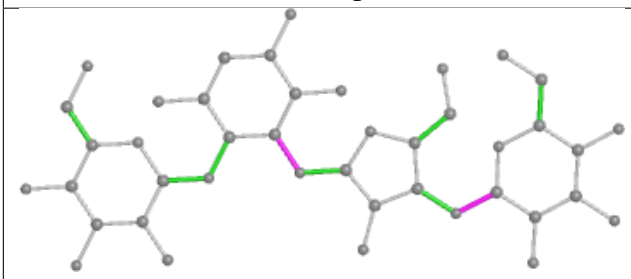
**Ligand PAR 1 3414**



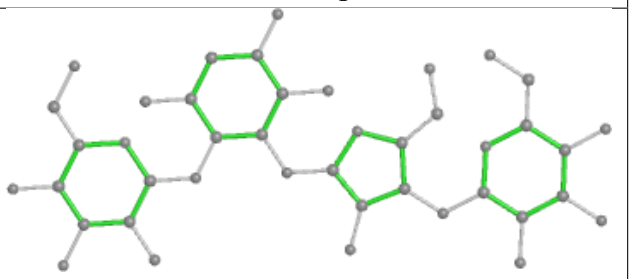
Bond lengths



Bond angles

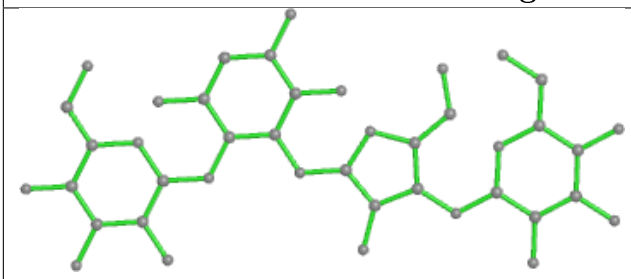


Torsions

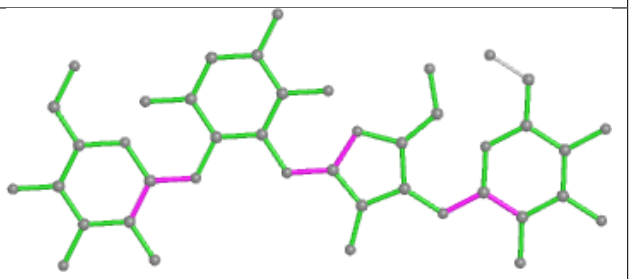


Rings

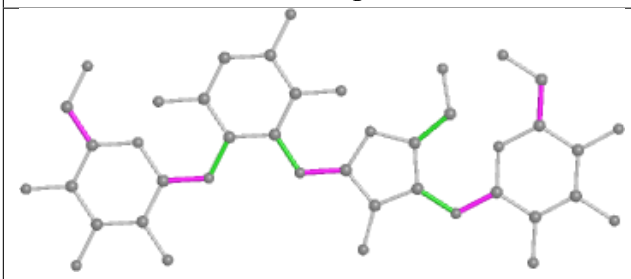
**Ligand PAR 1 3422**



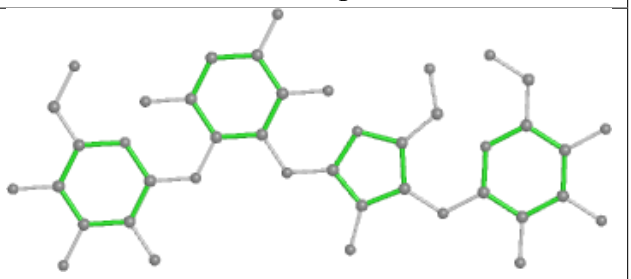
Bond lengths



Bond angles

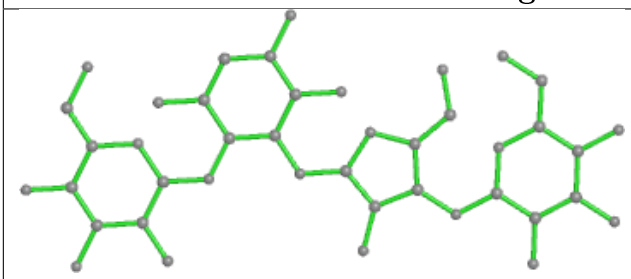


Torsions

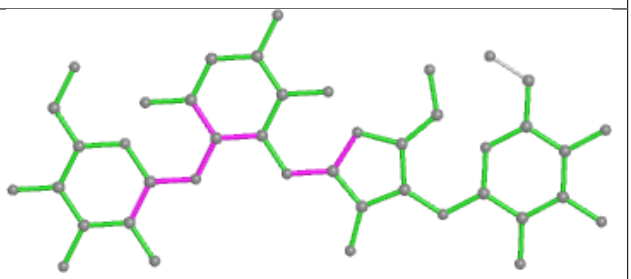


Rings

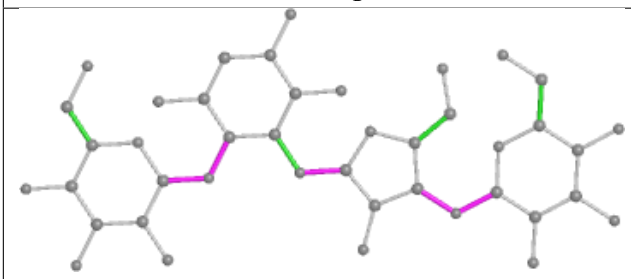
**Ligand PAR n3 201**



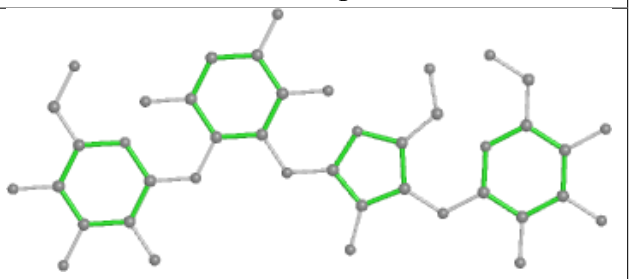
Bond lengths



Bond angles

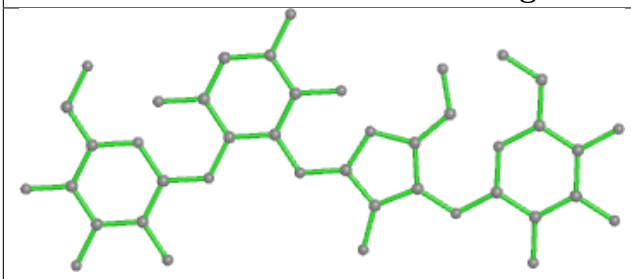


Torsions

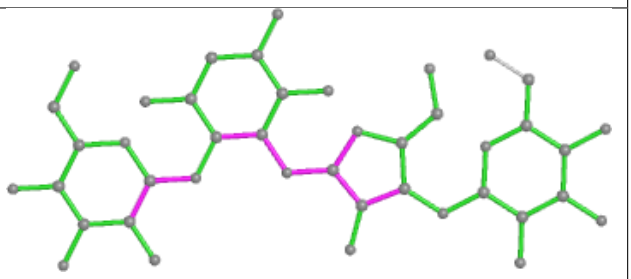


Rings

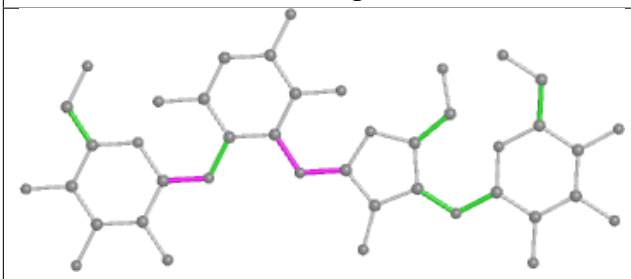
### Ligand PAR 5 3423



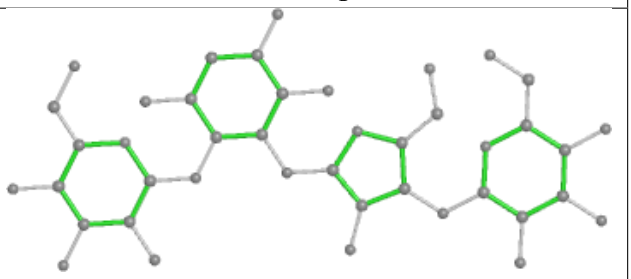
Bond lengths



Bond angles

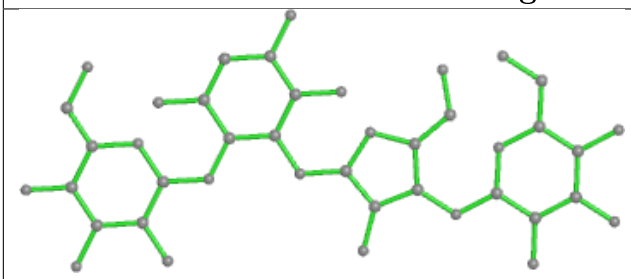


Torsions

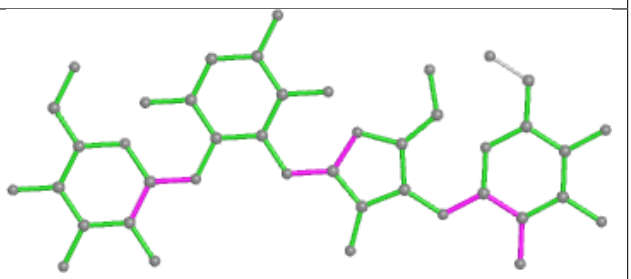


Rings

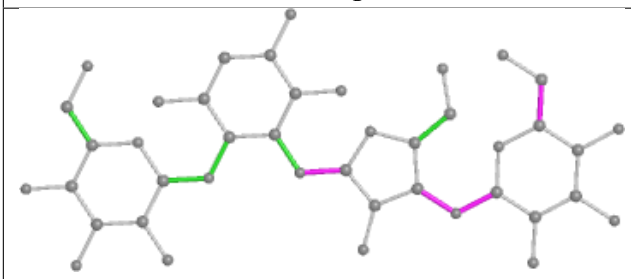
### Ligand PAR 6 1905



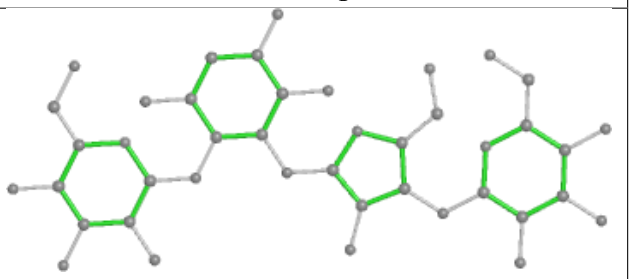
Bond lengths



Bond angles

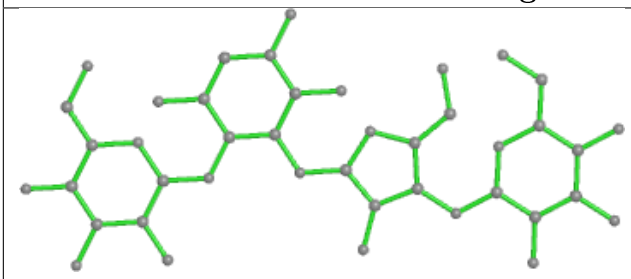


Torsions

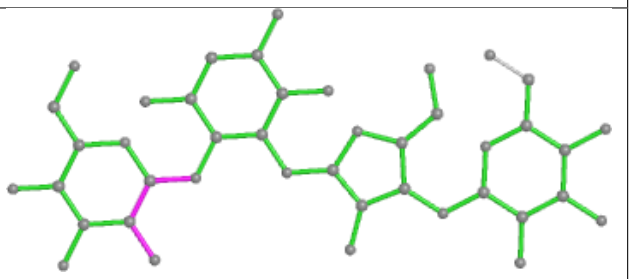


Rings

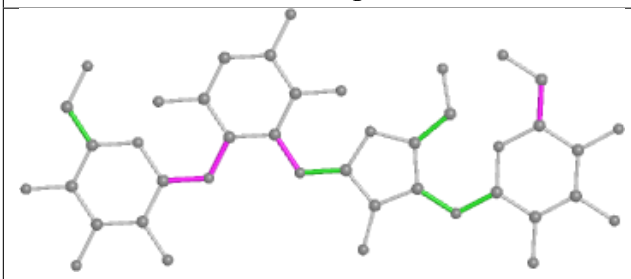
**Ligand PAR 6 1906**



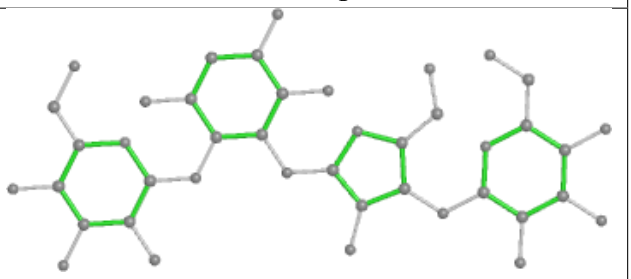
Bond lengths



Bond angles

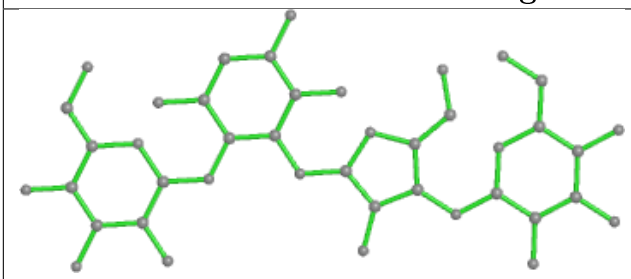


Torsions

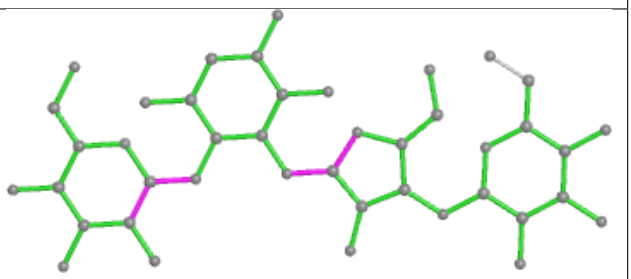


Rings

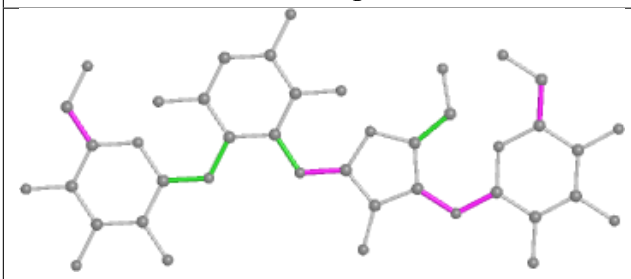
**Ligand PAR 5 3410**



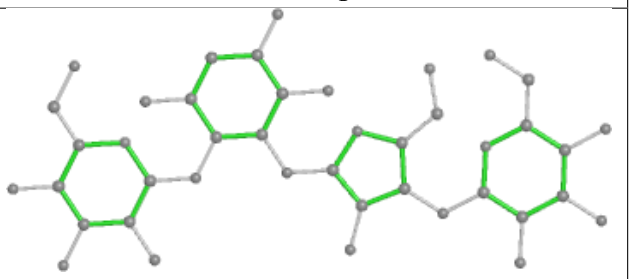
Bond lengths



Bond angles

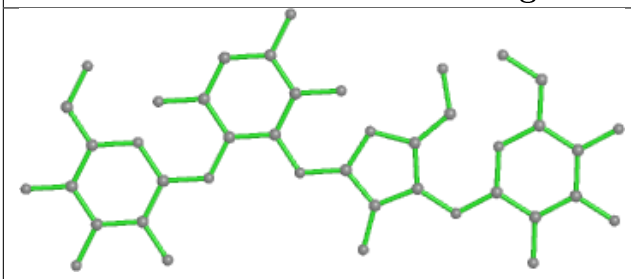


Torsions

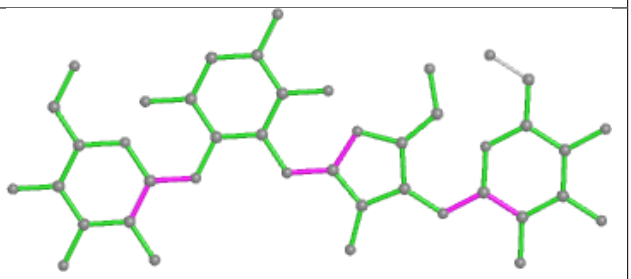


Rings

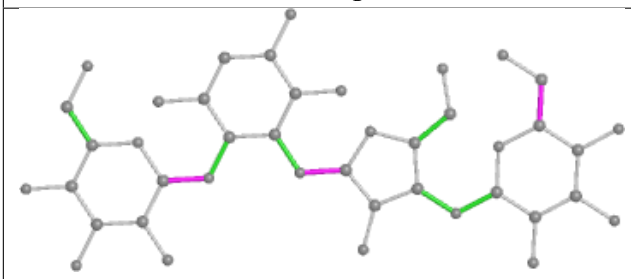
**Ligand PAR 1 3427**



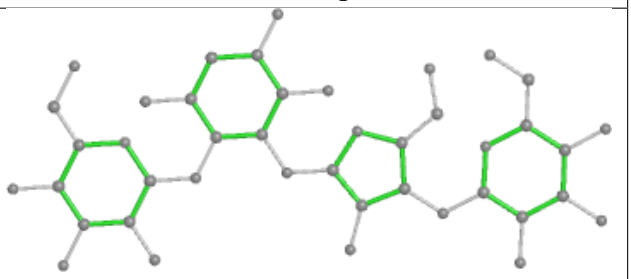
Bond lengths



Bond angles

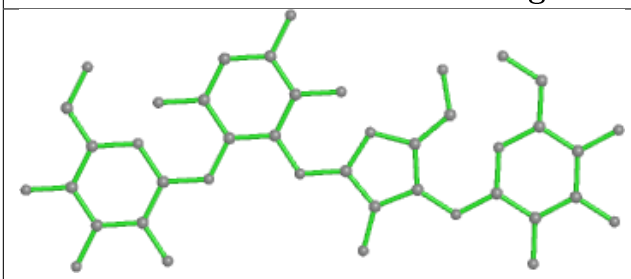


Torsions

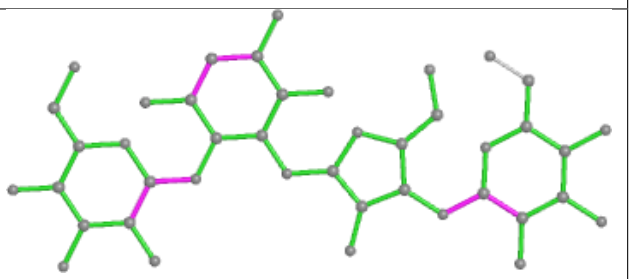


Rings

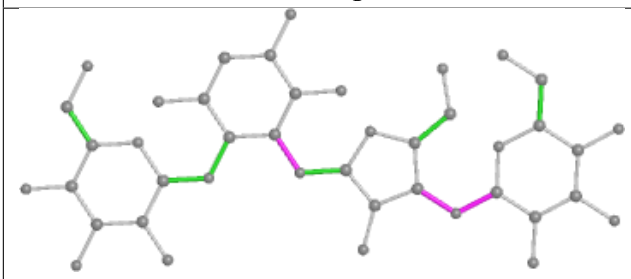
**Ligand PAR 3 203**



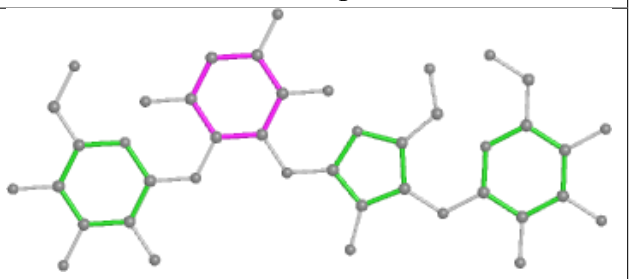
Bond lengths



Bond angles

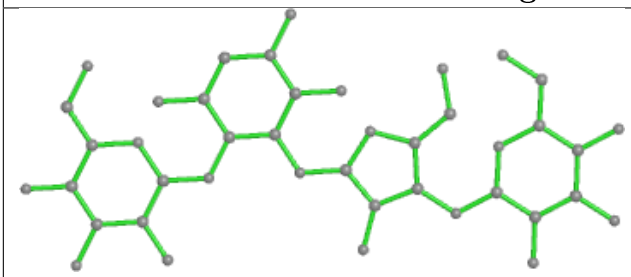


Torsions

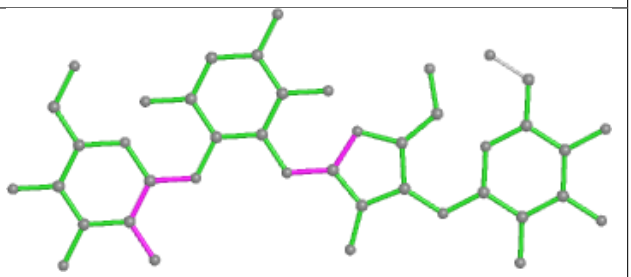


Rings

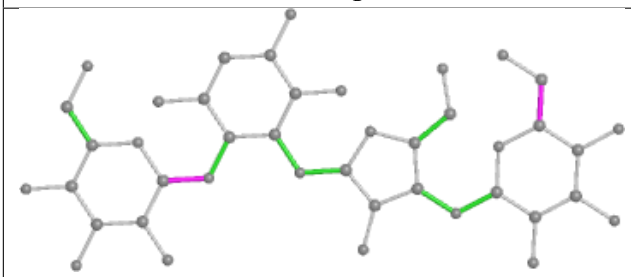
**Ligand PAR 5 3416**



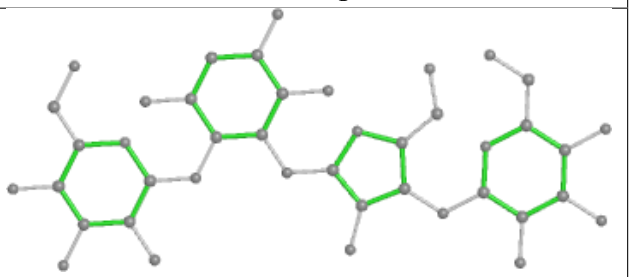
Bond lengths



Bond angles

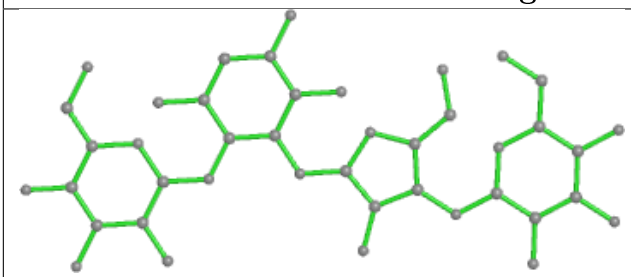


Torsions

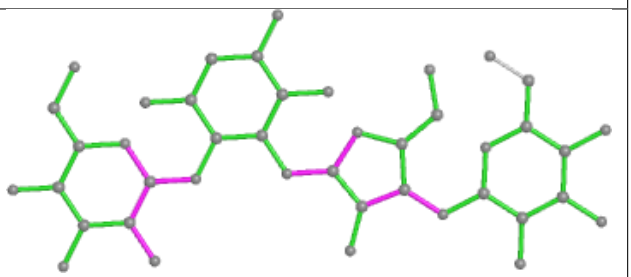


Rings

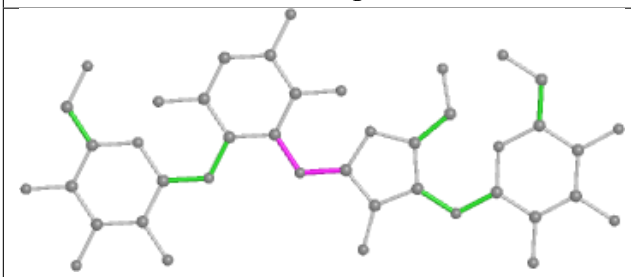
**Ligand PAR 1 3408**



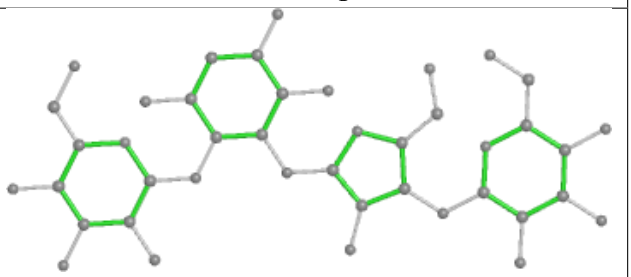
Bond lengths



Bond angles

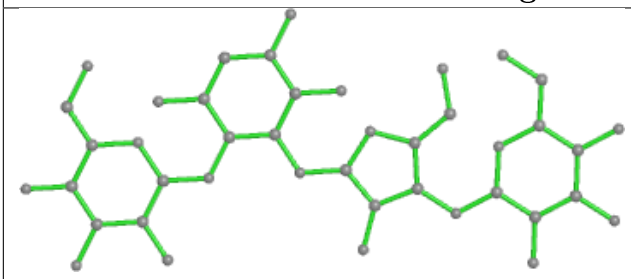


Torsions

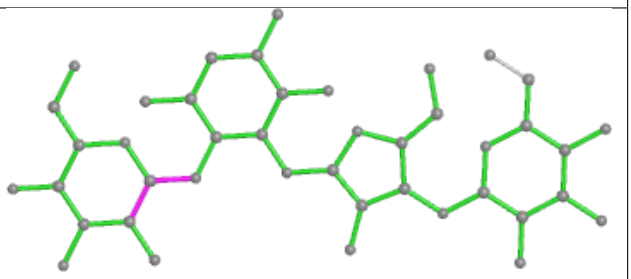


Rings

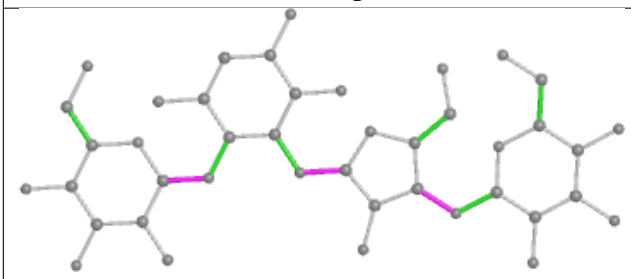
**Ligand PAR 1 3403**



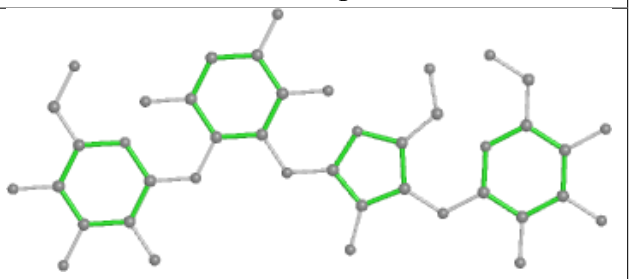
Bond lengths



Bond angles

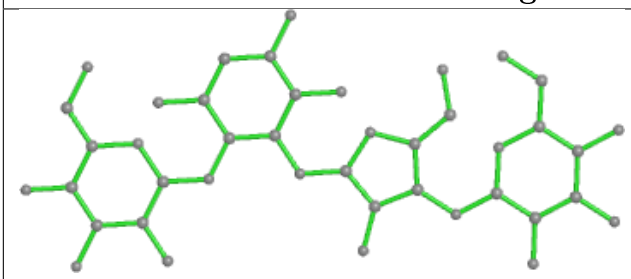


Torsions

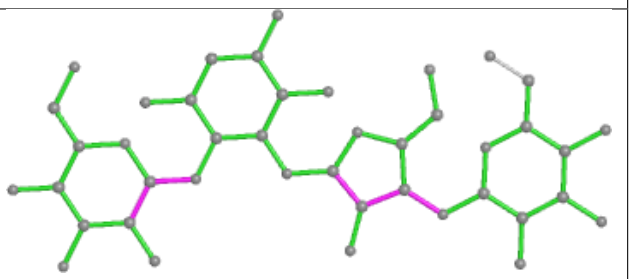


Rings

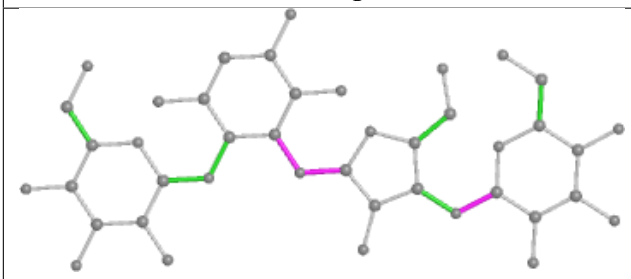
**Ligand PAR 1 3426**



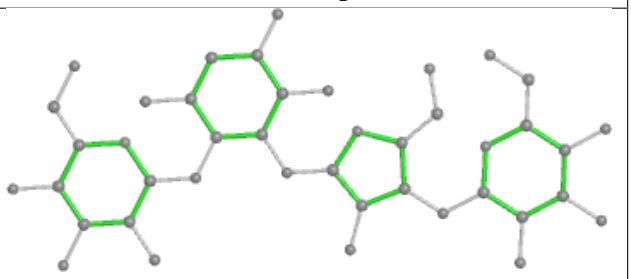
Bond lengths



Bond angles

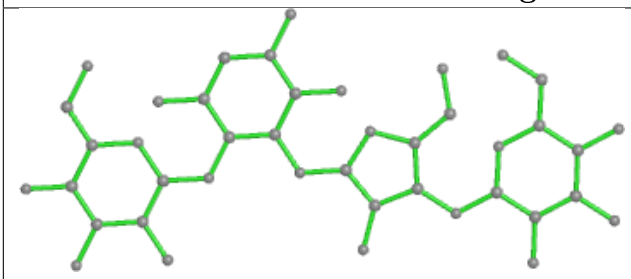


Torsions

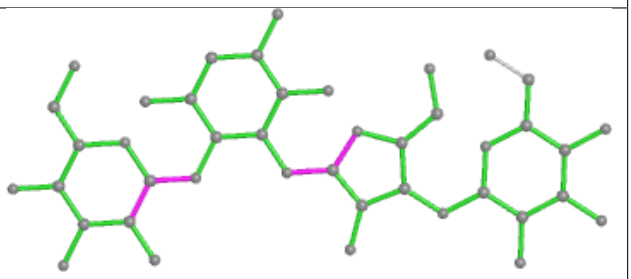


Rings

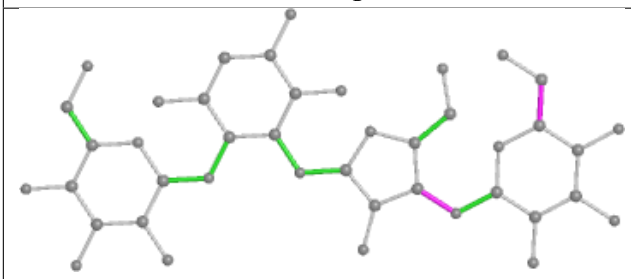
**Ligand PAR 1 3432**



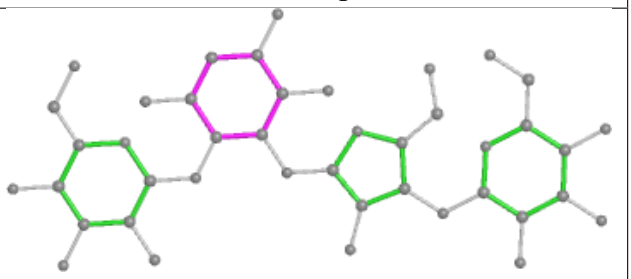
Bond lengths



Bond angles

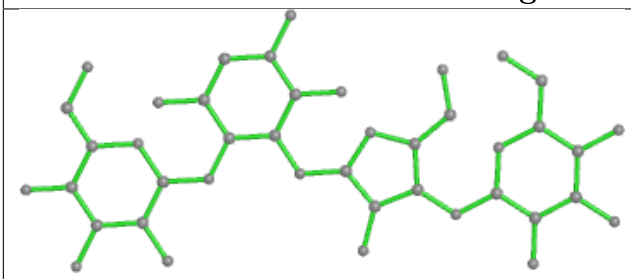


Torsions

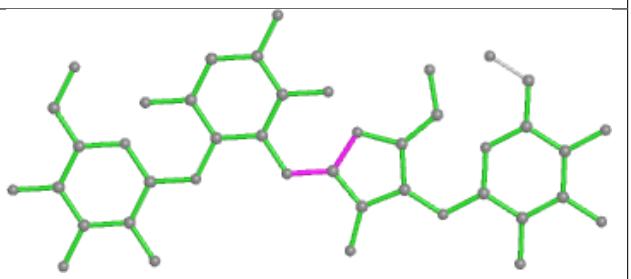


Rings

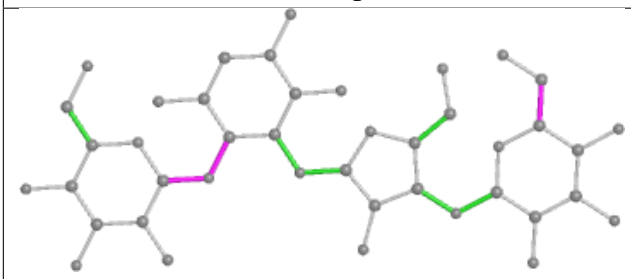
**Ligand PAR 5 3426**



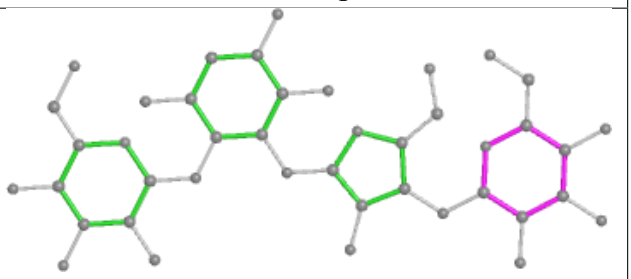
Bond lengths



Bond angles

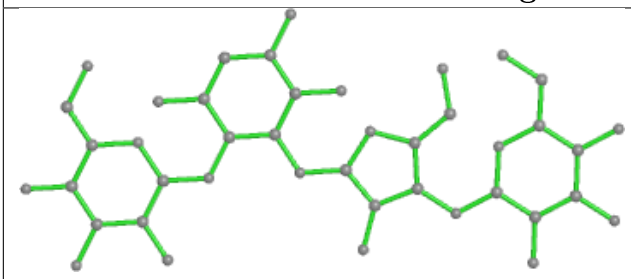


Torsions

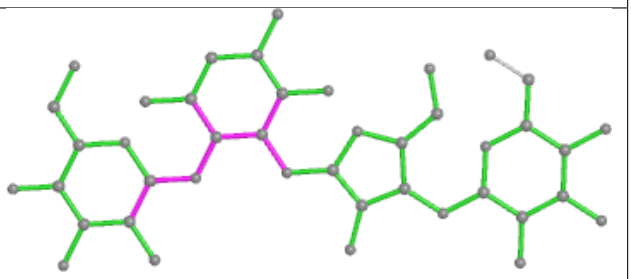


Rings

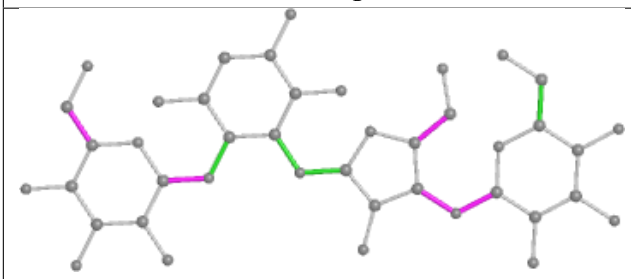
**Ligand PAR 5 3404**



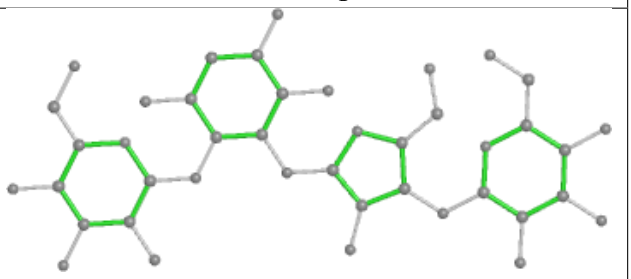
Bond lengths



Bond angles

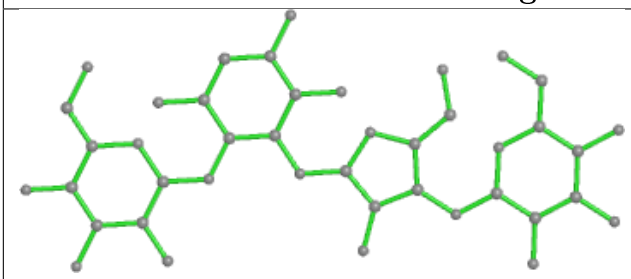


Torsions

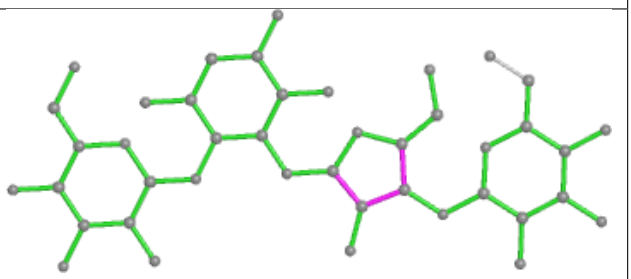


Rings

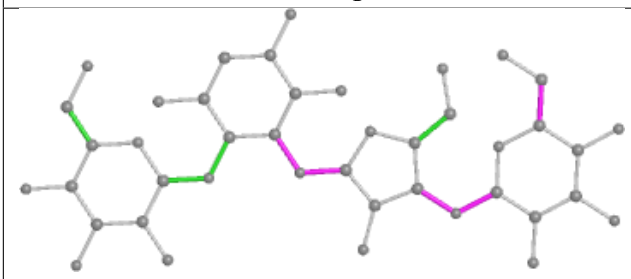
**Ligand PAR 1 3418**



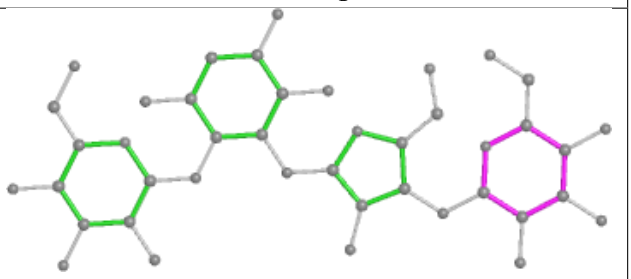
Bond lengths



Bond angles

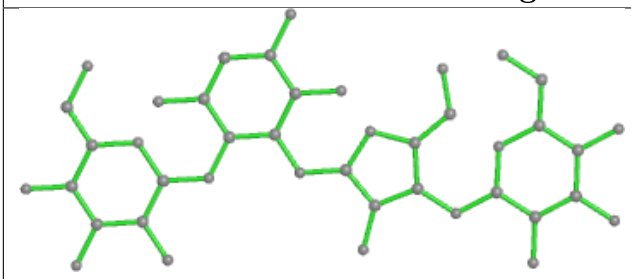


Torsions

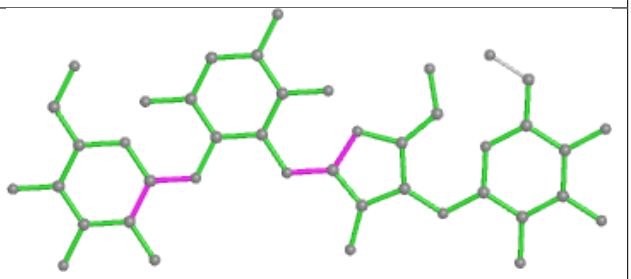


Rings

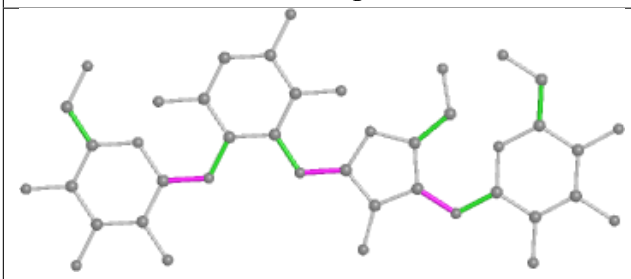
**Ligand PAR 1 3424**



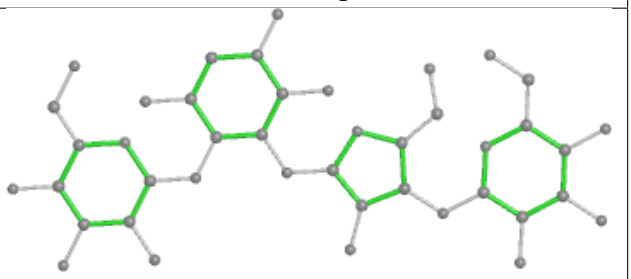
Bond lengths



Bond angles

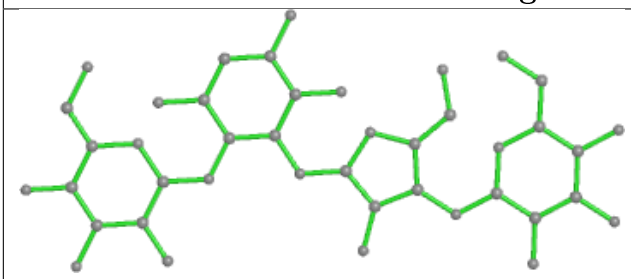


Torsions

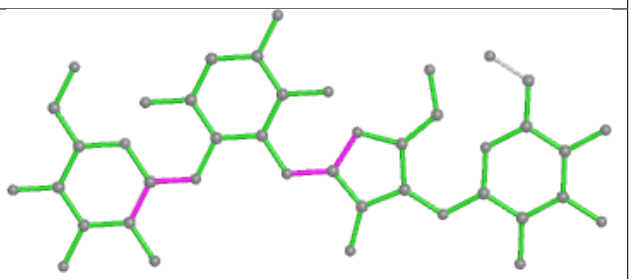


Rings

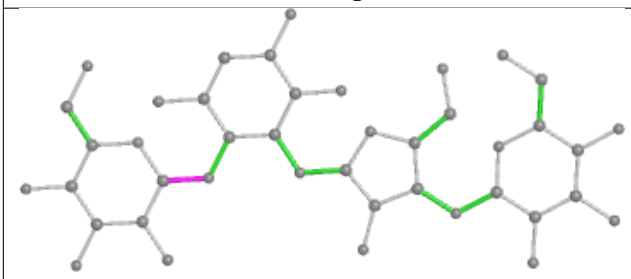
**Ligand PAR 2 1901**



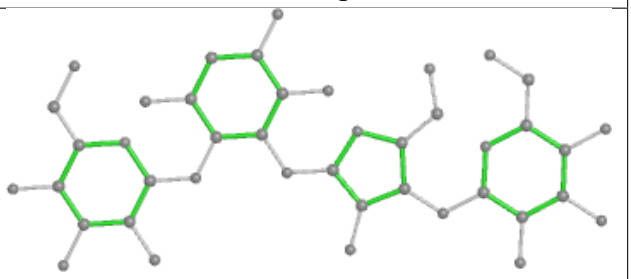
Bond lengths



Bond angles

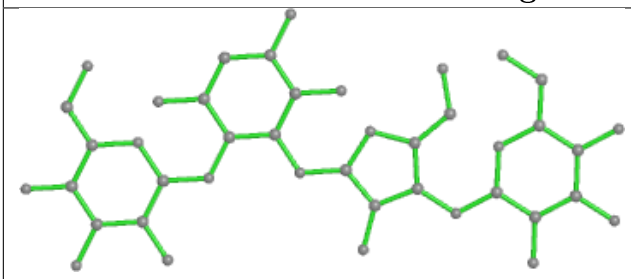


Torsions

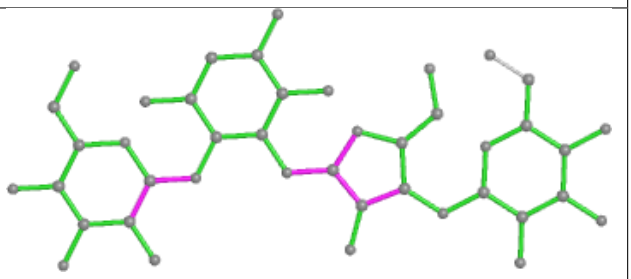


Rings

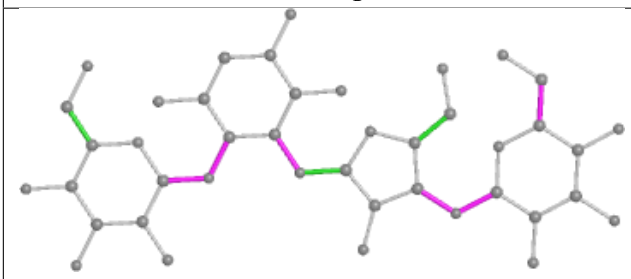
### Ligand PAR 6 1902



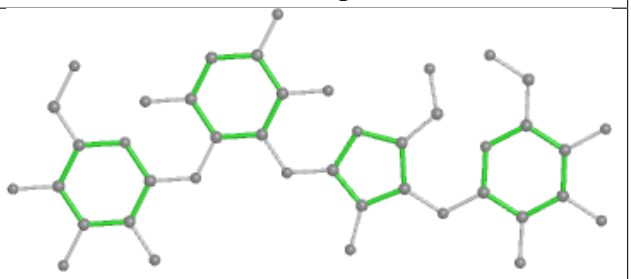
Bond lengths



Bond angles

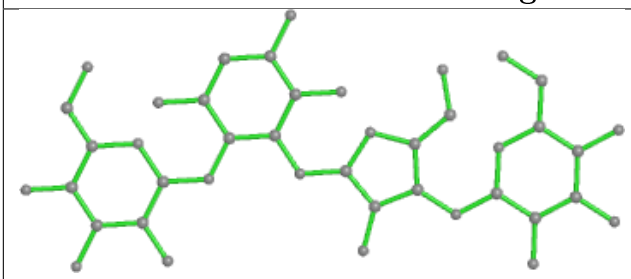


Torsions

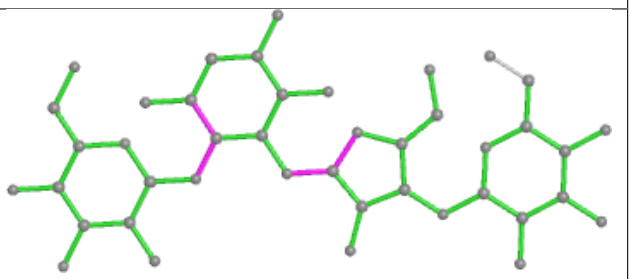


Rings

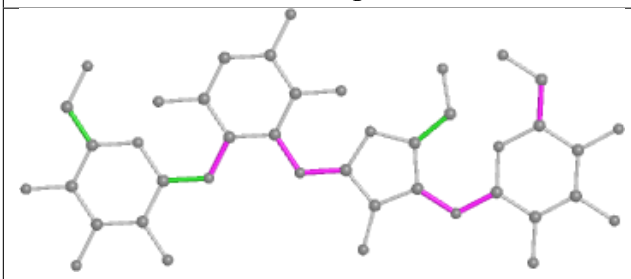
### Ligand PAR 5 3402



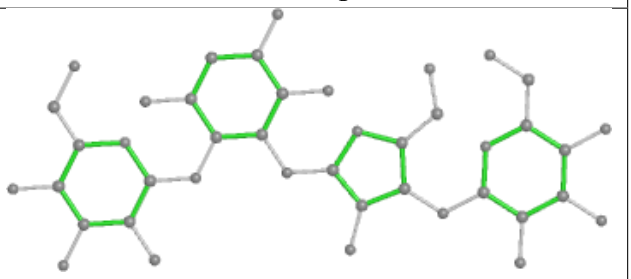
Bond lengths



Bond angles

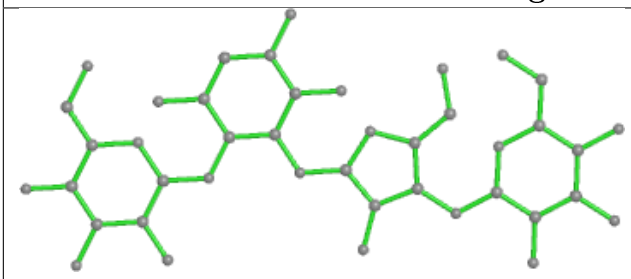


Torsions

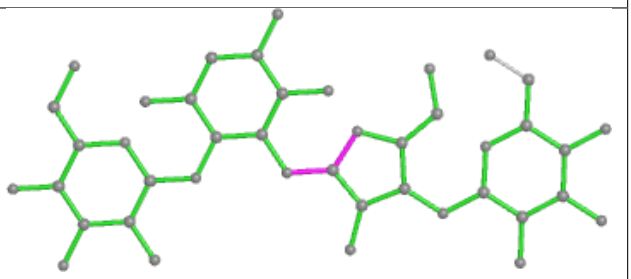


Rings

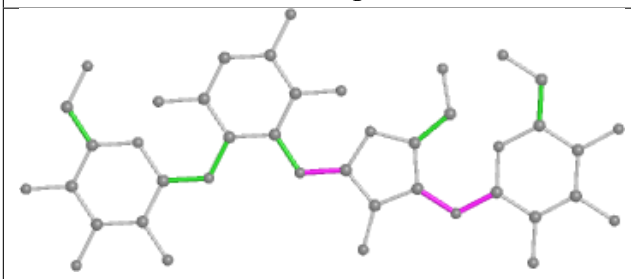
**Ligand PAR 8 202**



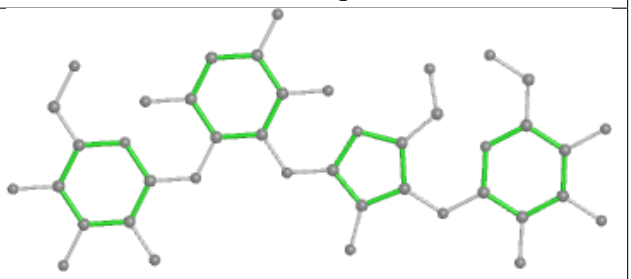
Bond lengths



Bond angles

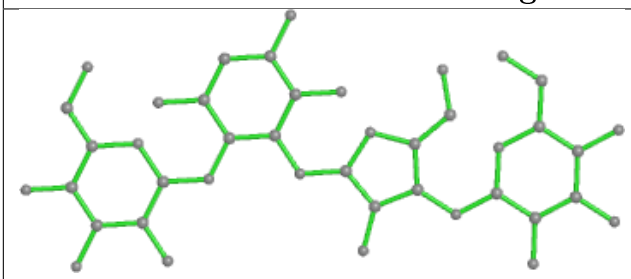


Torsions

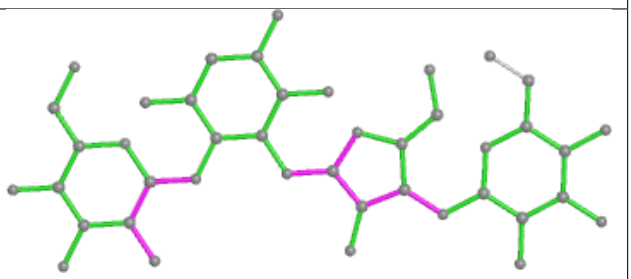


Rings

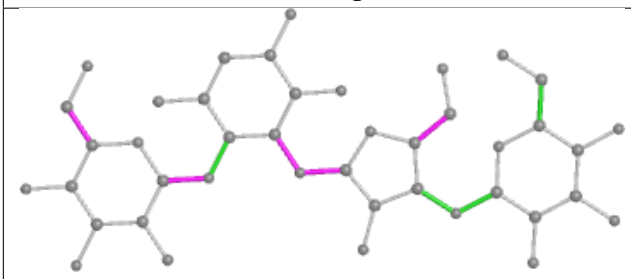
**Ligand PAR 5 3428**



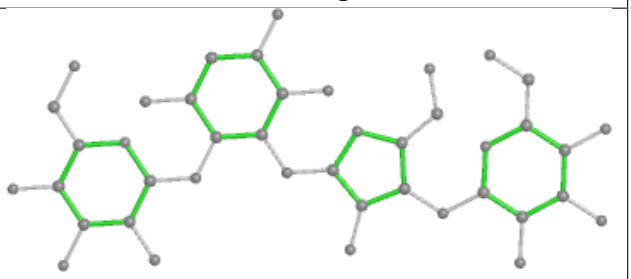
Bond lengths



Bond angles

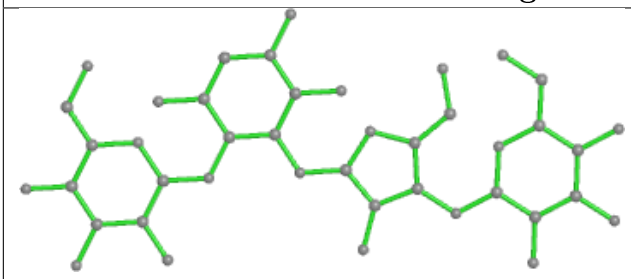


Torsions

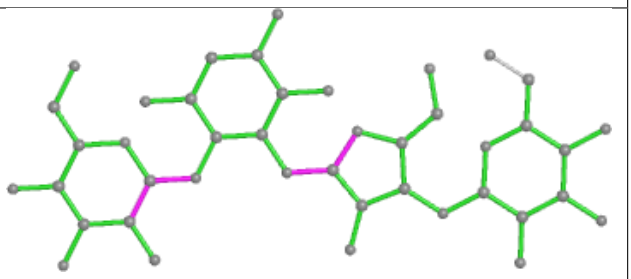


Rings

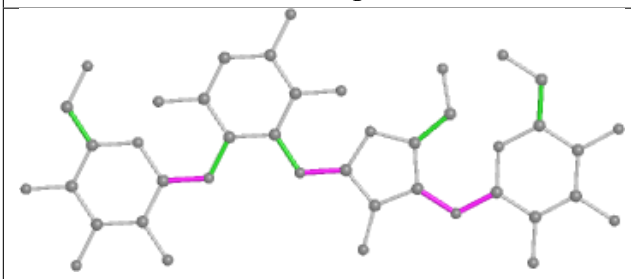
**Ligand PAR 1 3417**



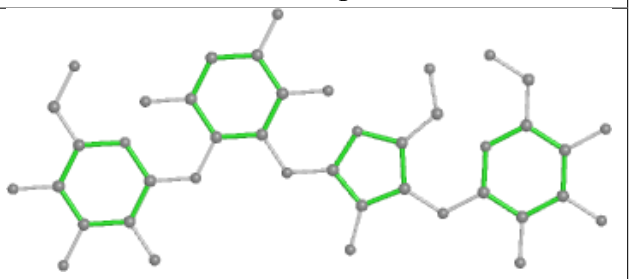
Bond lengths



Bond angles

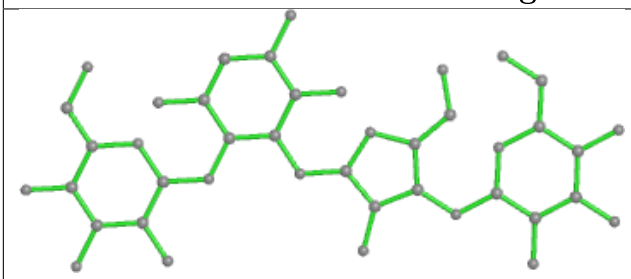


Torsions

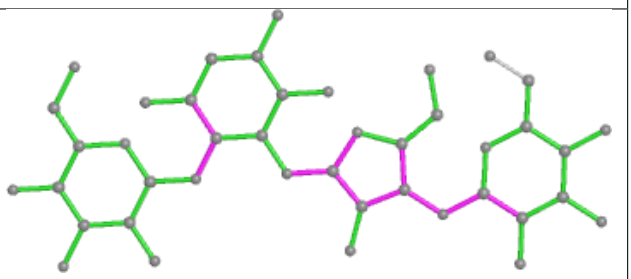


Rings

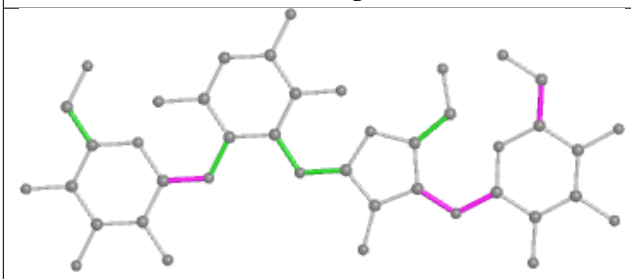
**Ligand PAR 1 3412**



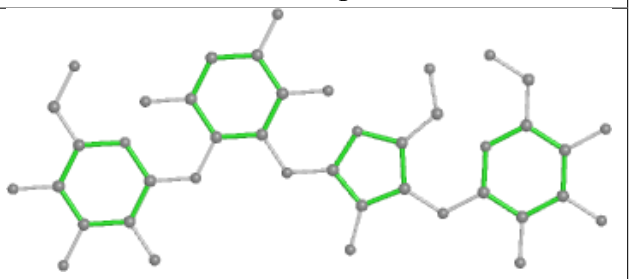
Bond lengths



Bond angles

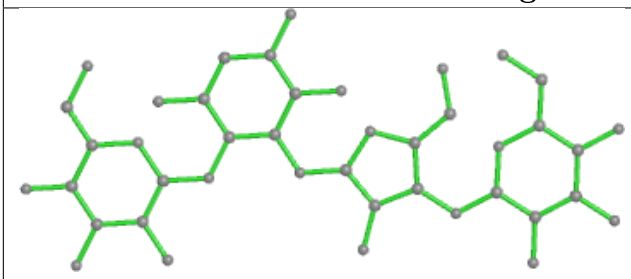


Torsions

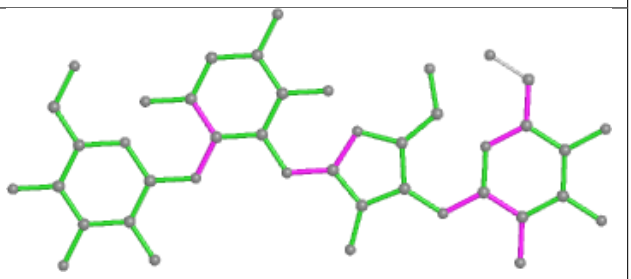


Rings

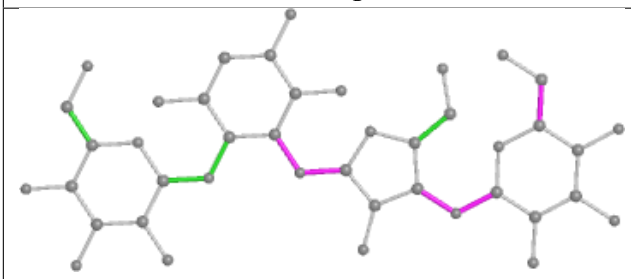
**Ligand PAR 1 3411**



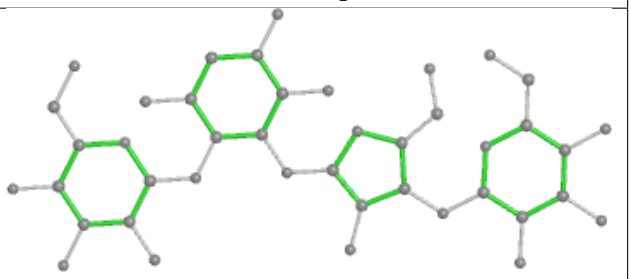
Bond lengths



Bond angles

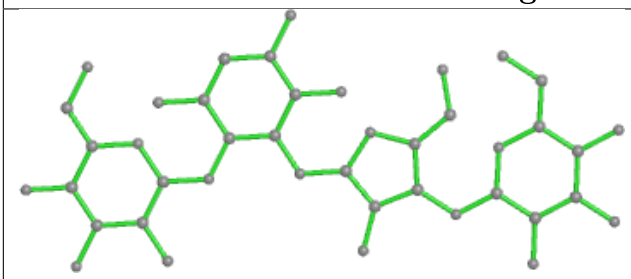


Torsions

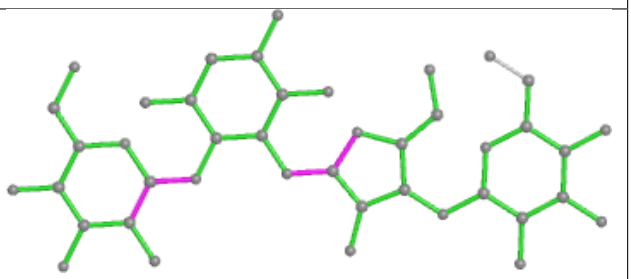


Rings

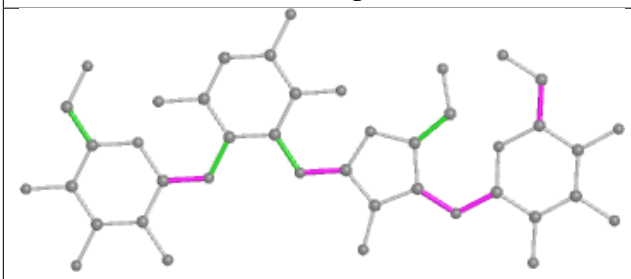
**Ligand PAR 5 3421**



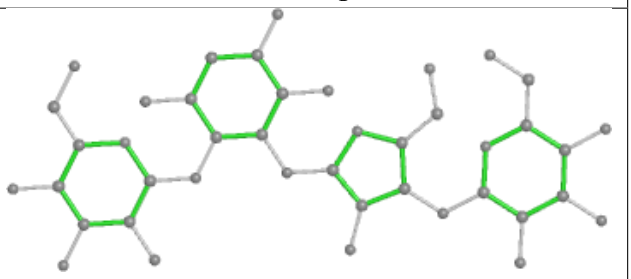
Bond lengths



Bond angles

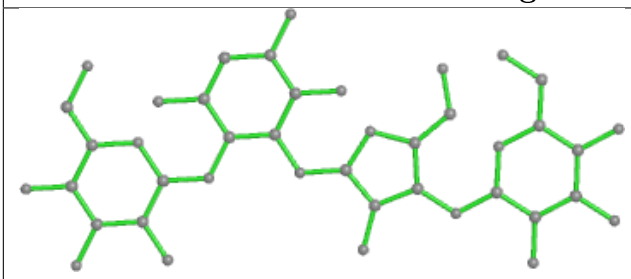


Torsions

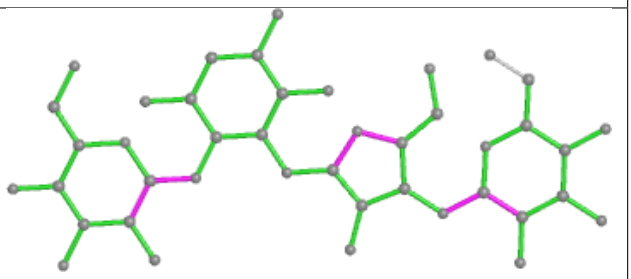


Rings

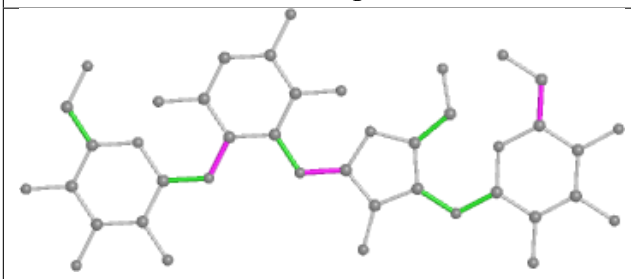
### Ligand PAR 2 1903



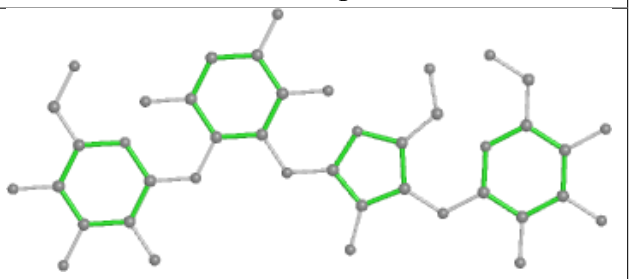
Bond lengths



Bond angles

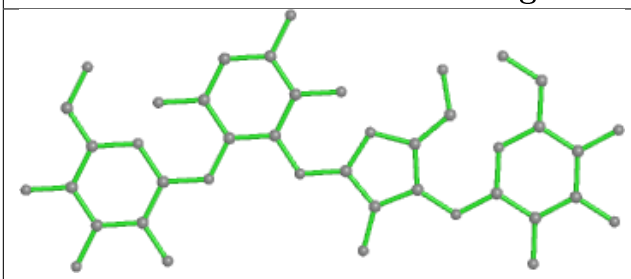


Torsions

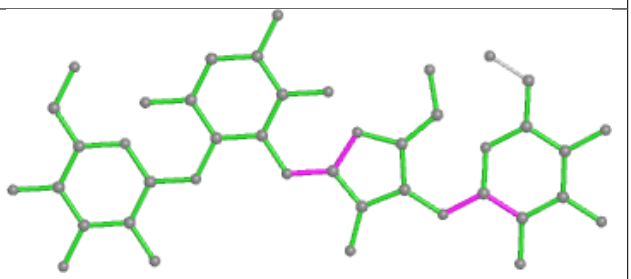


Rings

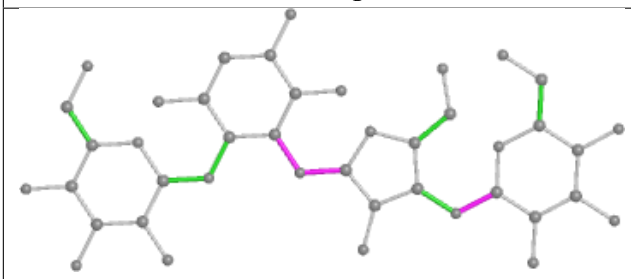
### Ligand PAR 1 3401



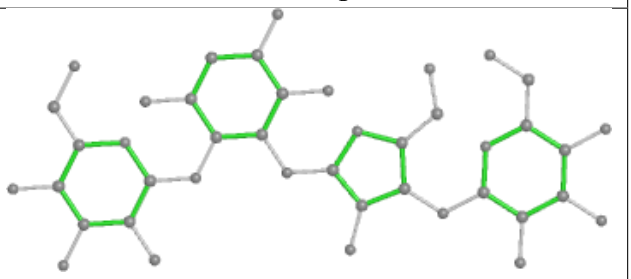
Bond lengths



Bond angles

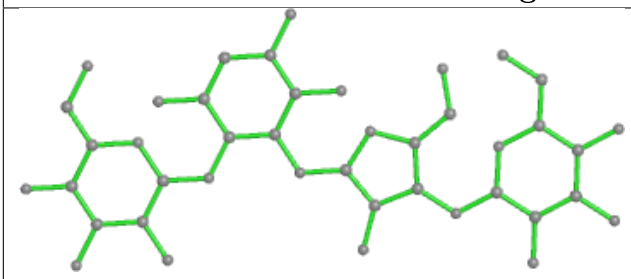


Torsions

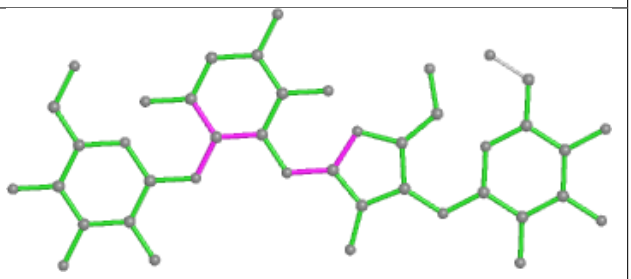


Rings

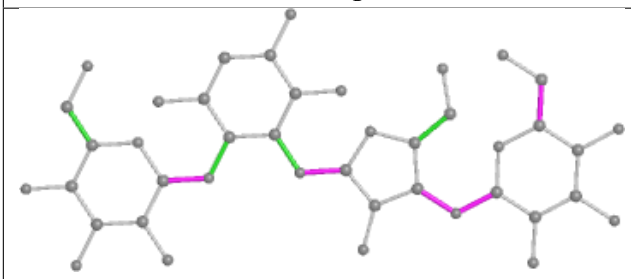
**Ligand PAR 6 1904**



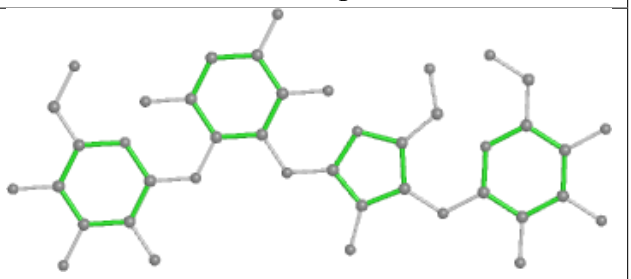
Bond lengths



Bond angles

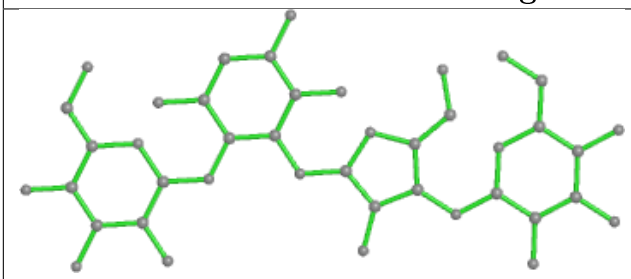


Torsions

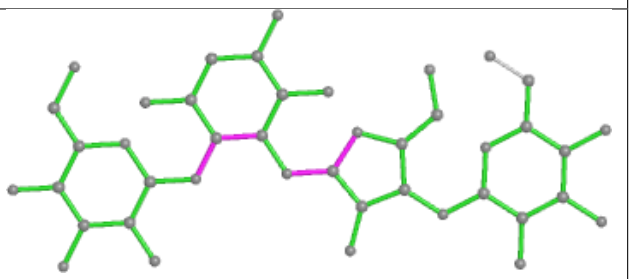


Rings

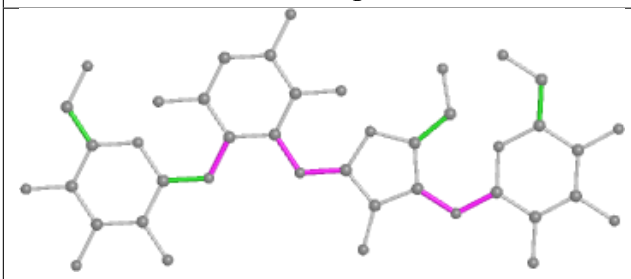
**Ligand PAR 5 3415**



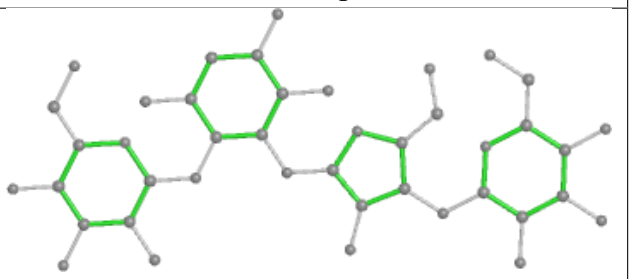
Bond lengths



Bond angles

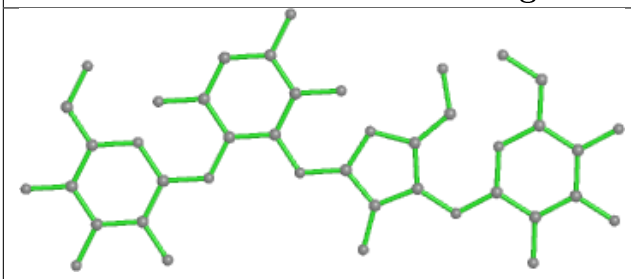


Torsions

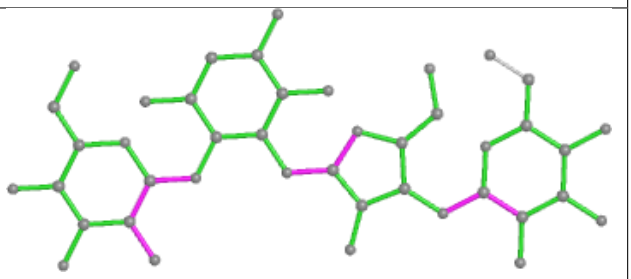


Rings

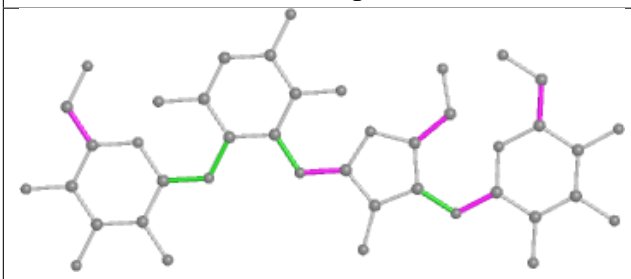
**Ligand PAR 5 3409**



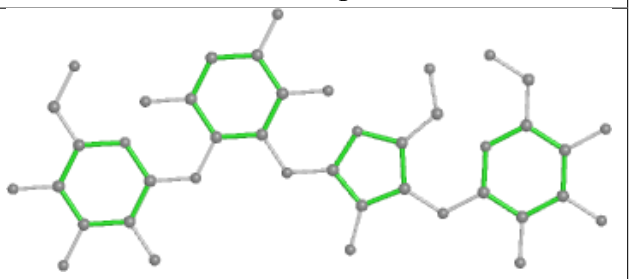
Bond lengths



Bond angles

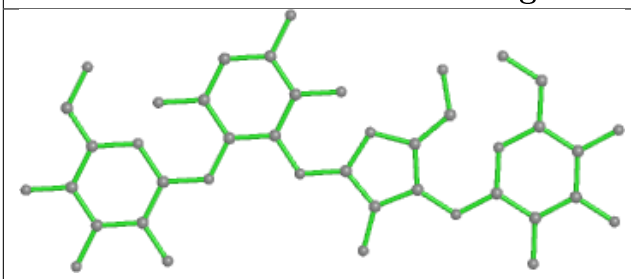


Torsions

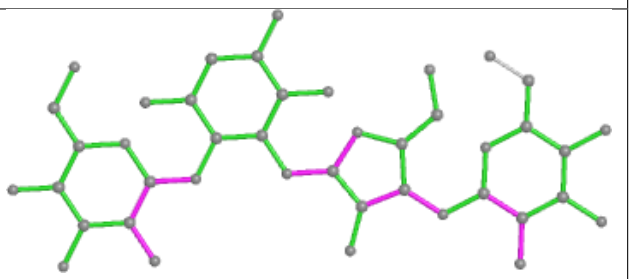


Rings

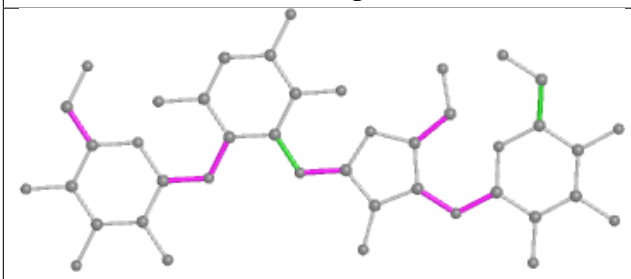
**Ligand PAR 1 3425**



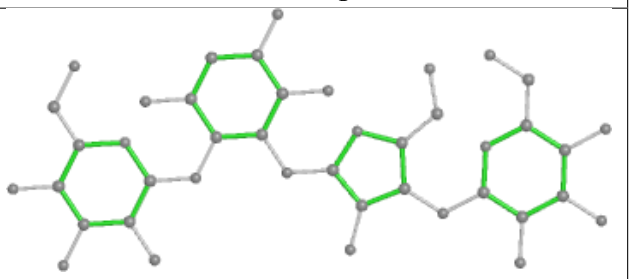
Bond lengths



Bond angles

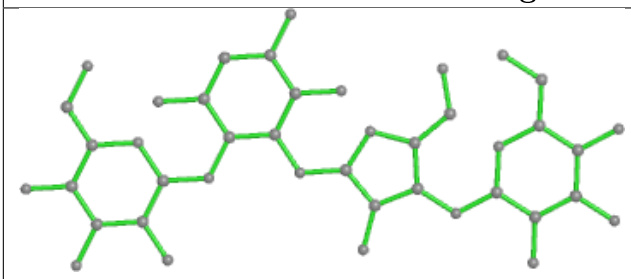


Torsions

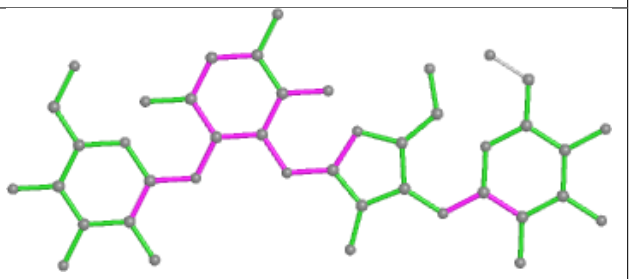


Rings

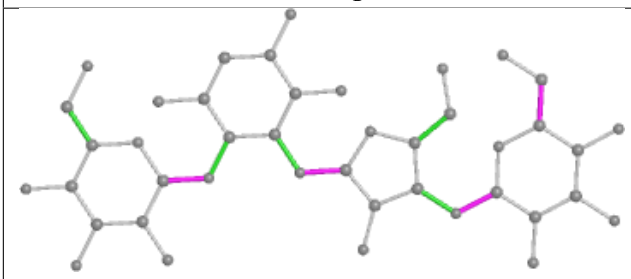
**Ligand PAR 1 3410**



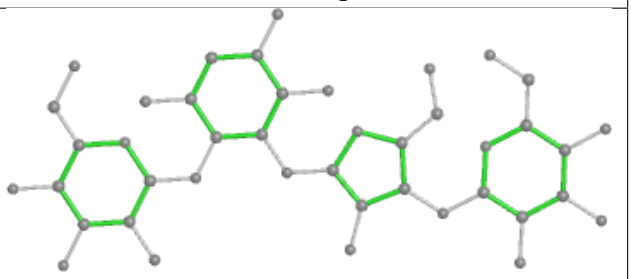
Bond lengths



Bond angles

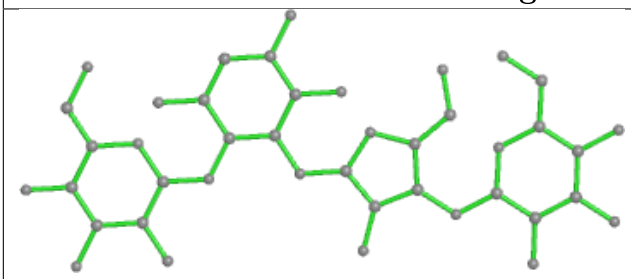


Torsions

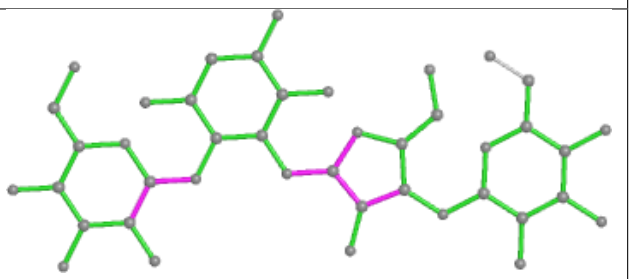


Rings

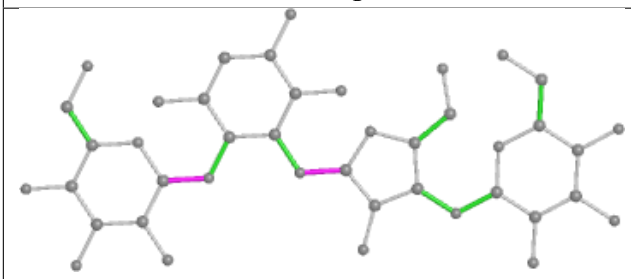
**Ligand PAR 5 3427**



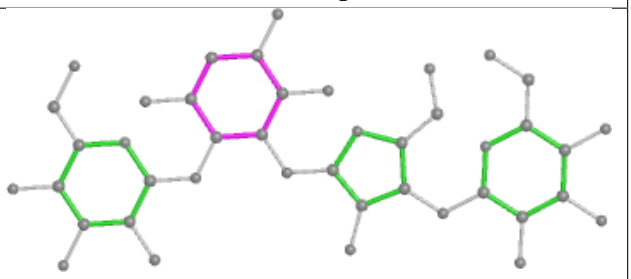
Bond lengths



Bond angles

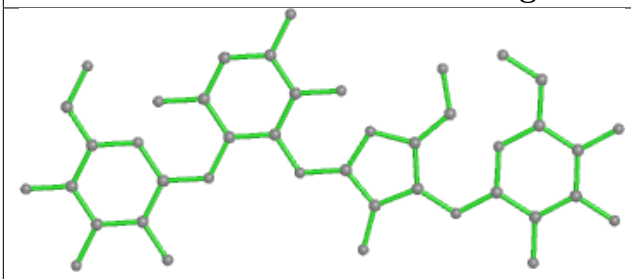


Torsions

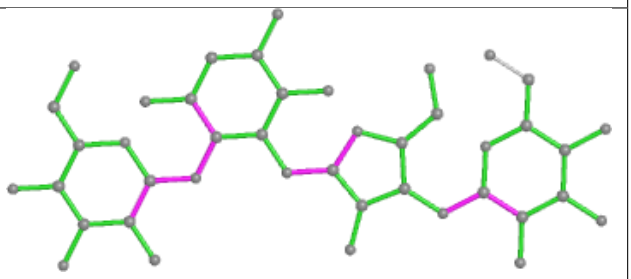


Rings

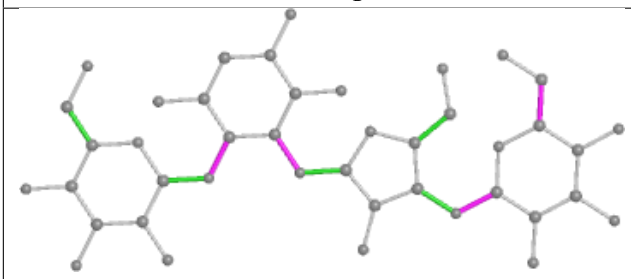
**Ligand PAR 2 1905**



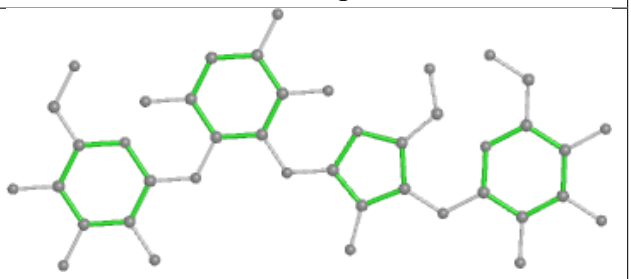
Bond lengths



Bond angles

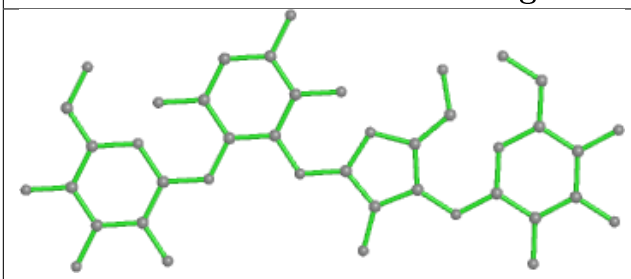


Torsions

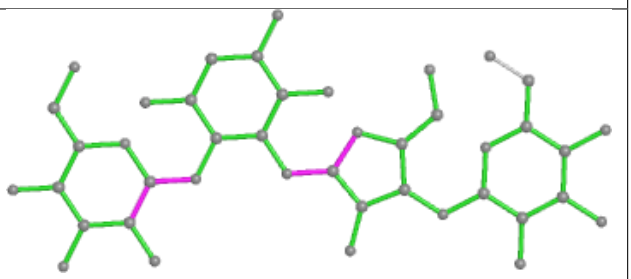


Rings

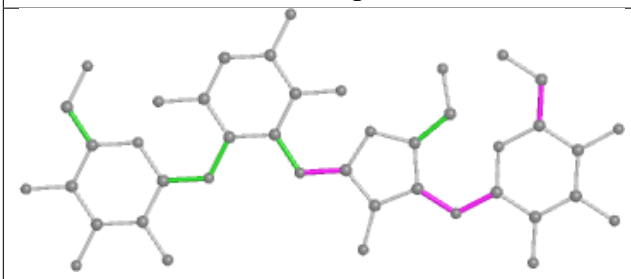
**Ligand PAR 5 3417**



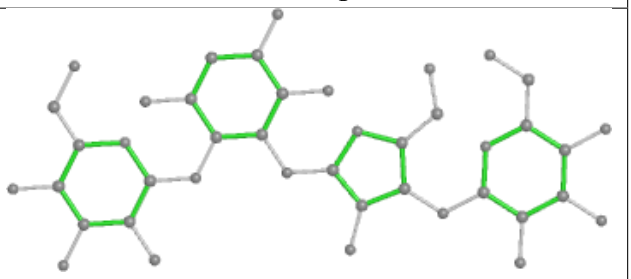
Bond lengths



Bond angles

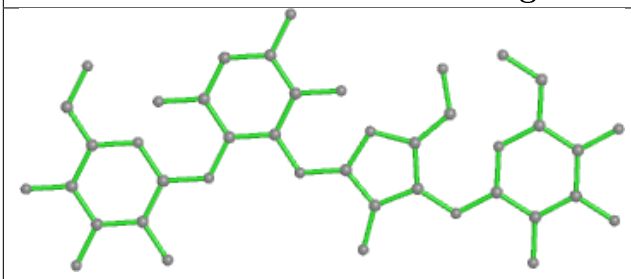


Torsions

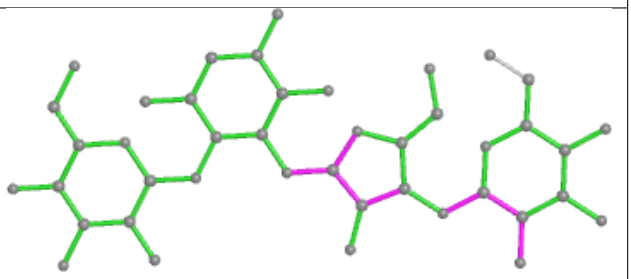


Rings

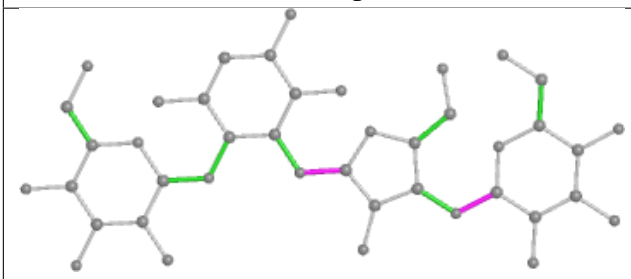
**Ligand PAR 1 3429**



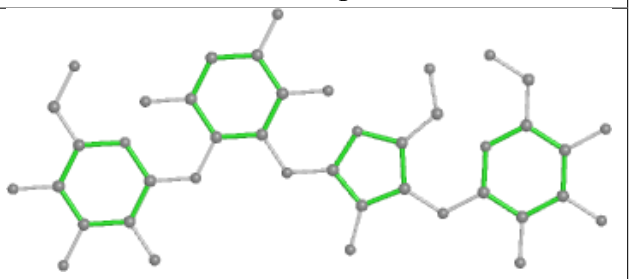
Bond lengths



Bond angles

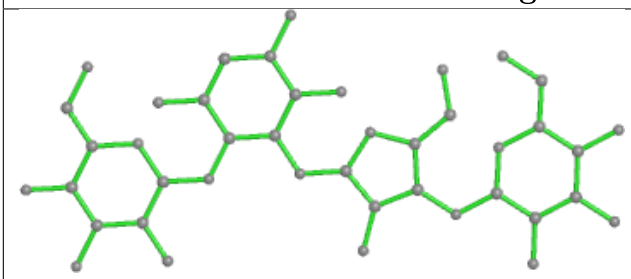


Torsions

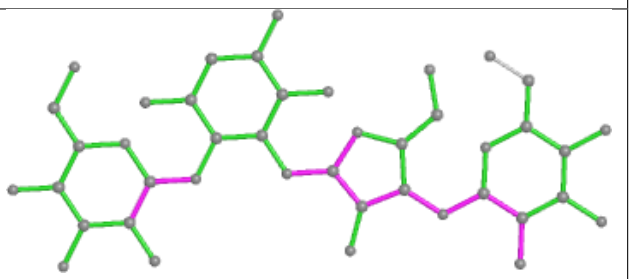


Rings

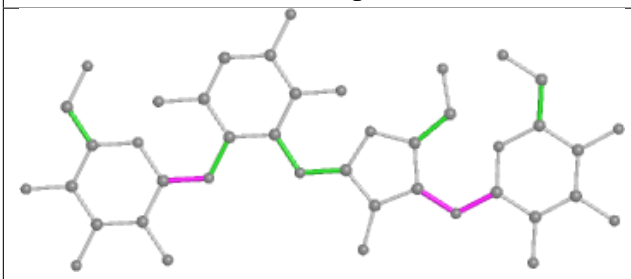
**Ligand PAR 5 3420**



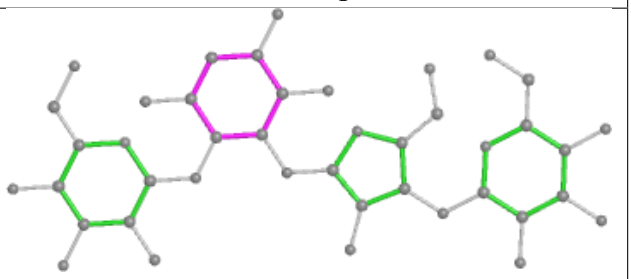
Bond lengths



Bond angles

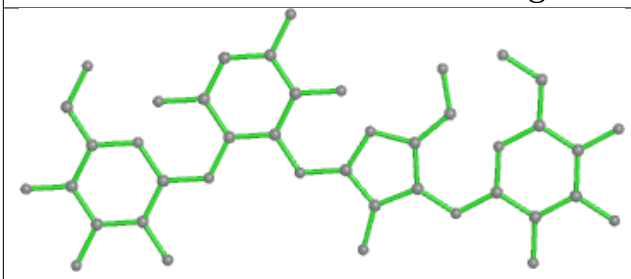


Torsions

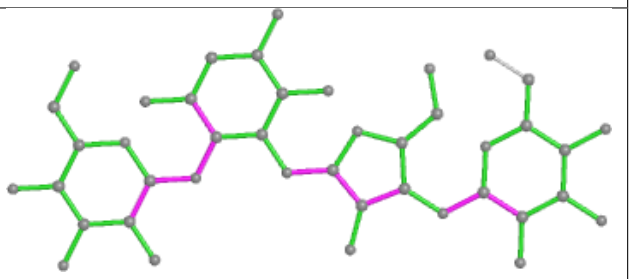


Rings

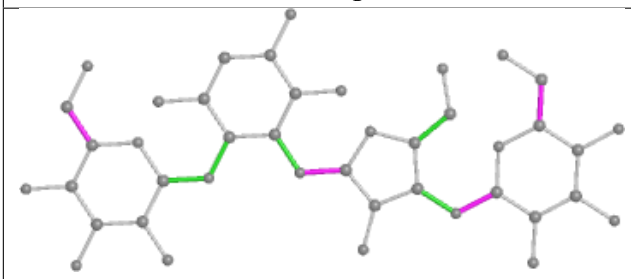
**Ligand PAR 4 201**



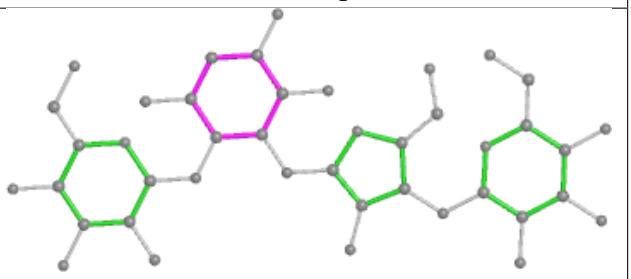
Bond lengths



Bond angles

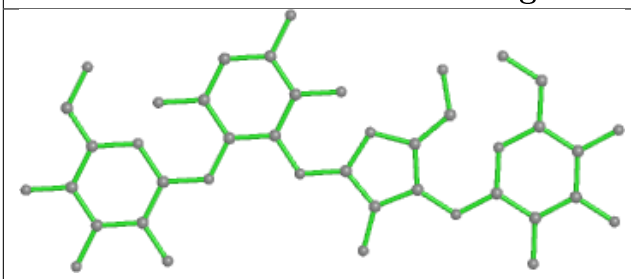


Torsions

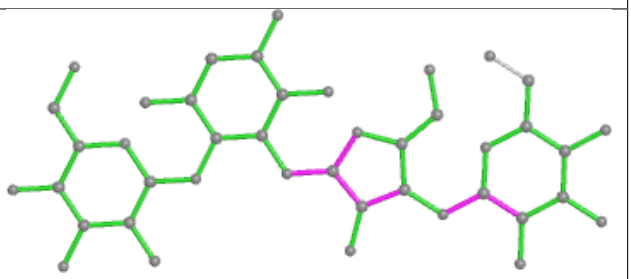


Rings

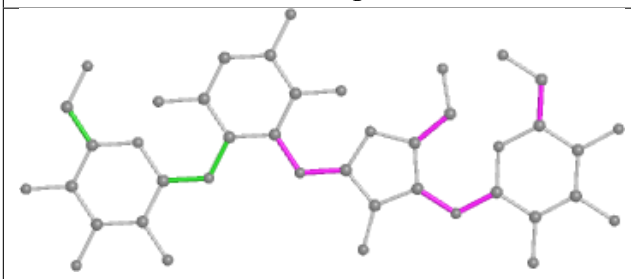
**Ligand PAR 5 3407**



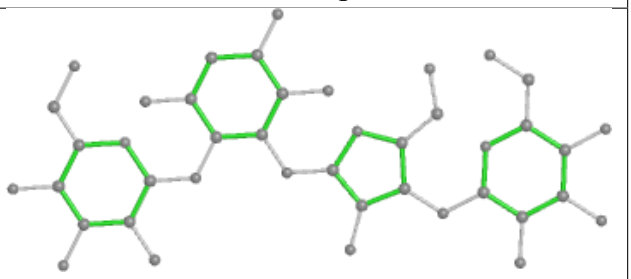
Bond lengths



Bond angles

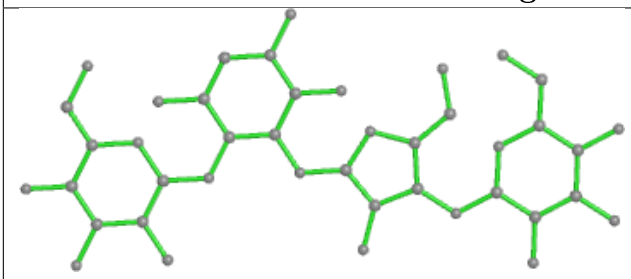


Torsions

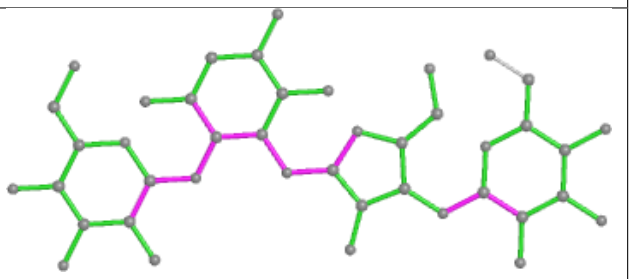


Rings

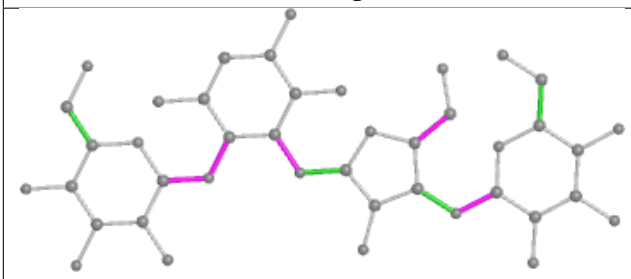
**Ligand PAR 1 3419**



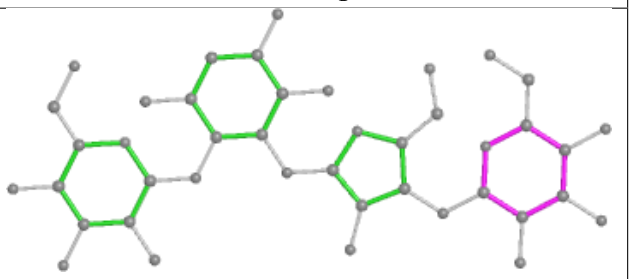
Bond lengths



Bond angles

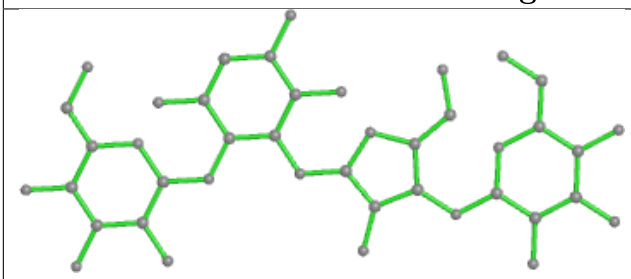


Torsions

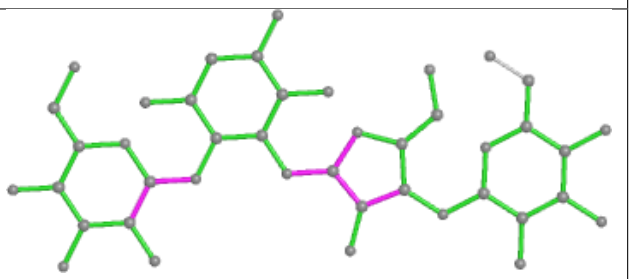


Rings

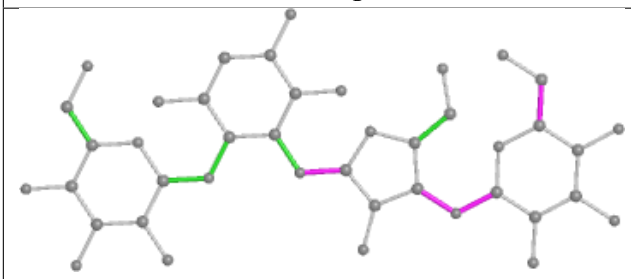
**Ligand PAR 5 3418**



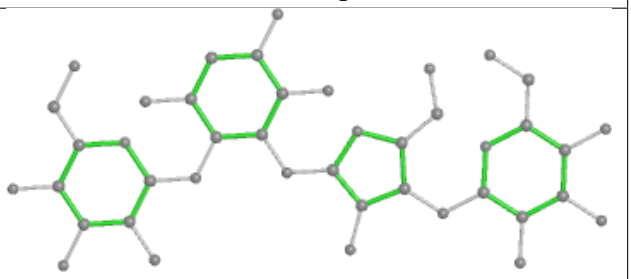
Bond lengths



Bond angles

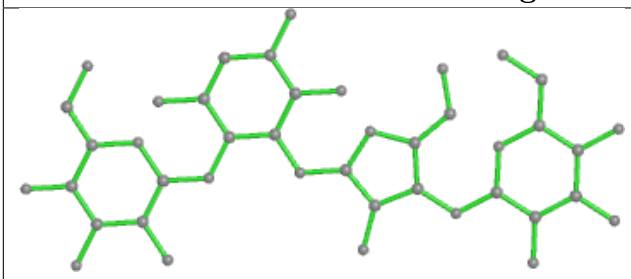


Torsions

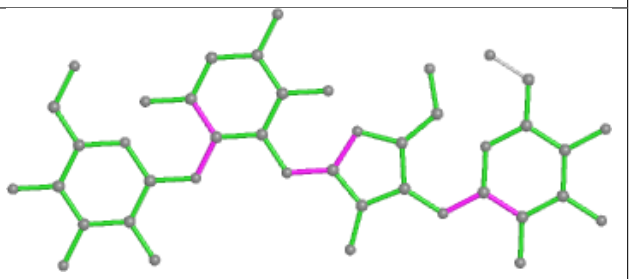


Rings

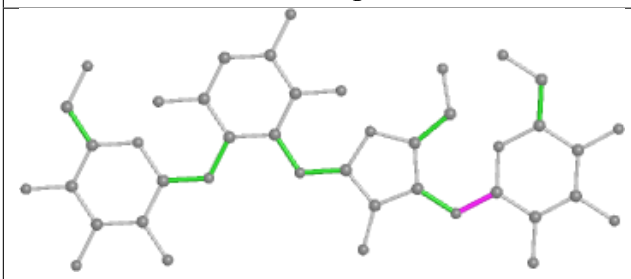
**Ligand PAR 1 3420**



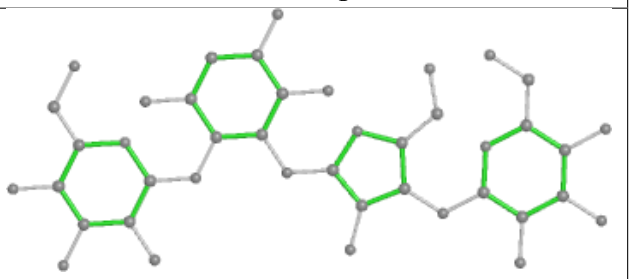
Bond lengths



Bond angles

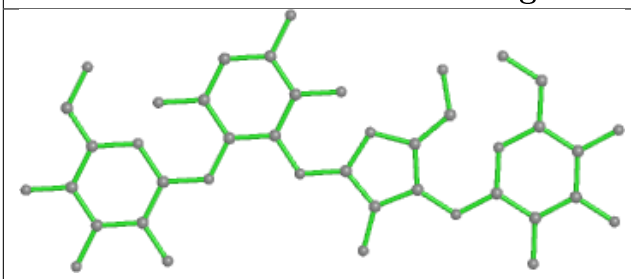


Torsions

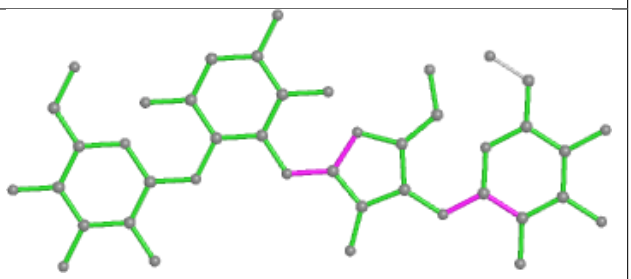


Rings

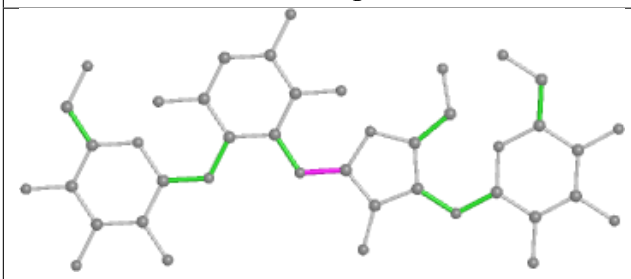
**Ligand PAR 6 1901**



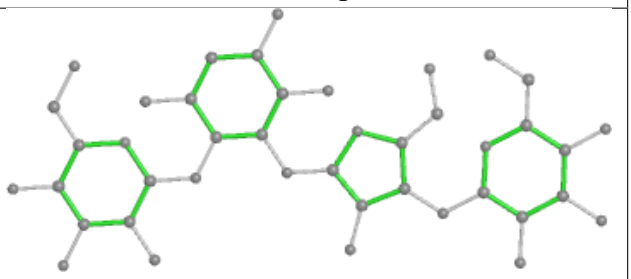
Bond lengths



Bond angles

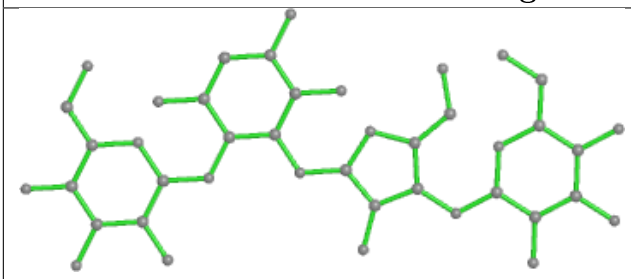


Torsions

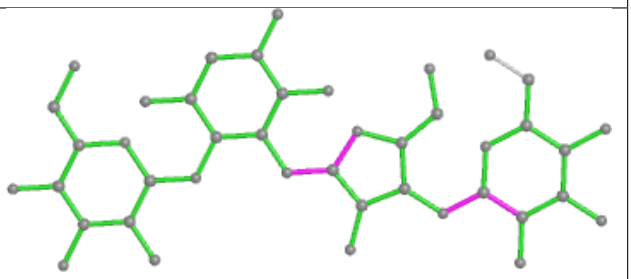


Rings

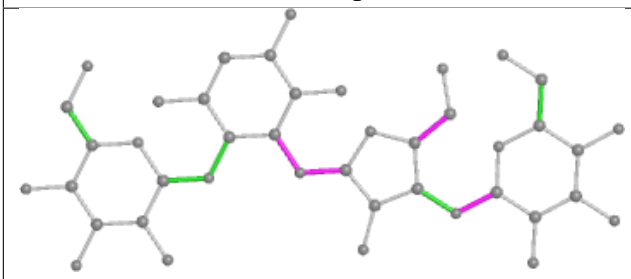
**Ligand PAR 5 3401**



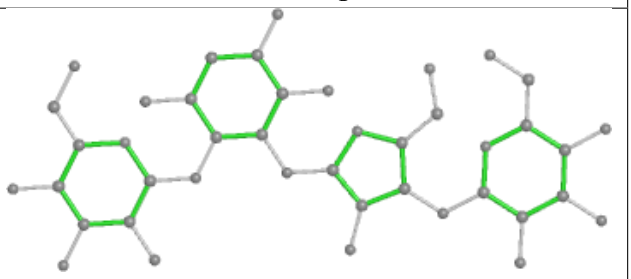
Bond lengths



Bond angles

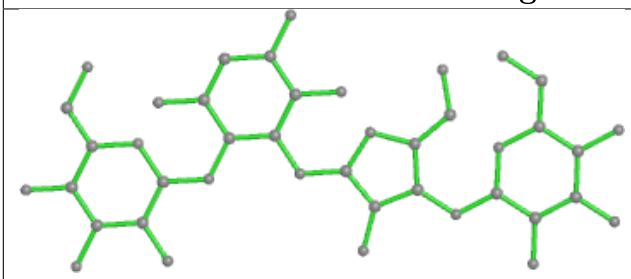


Torsions

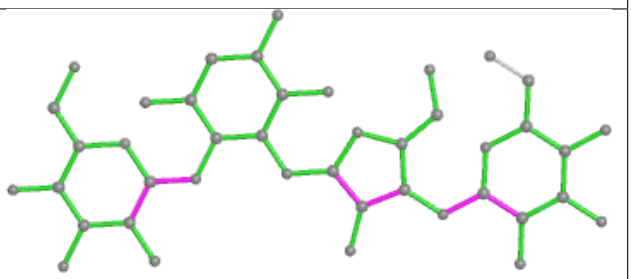


Rings

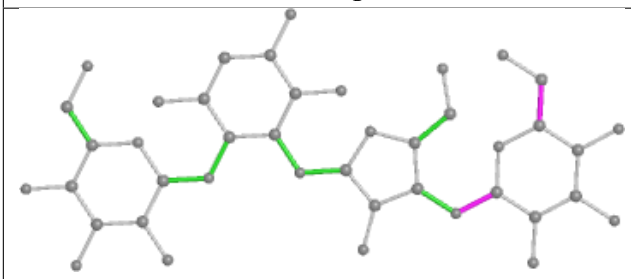
**Ligand PAR 1 3415**



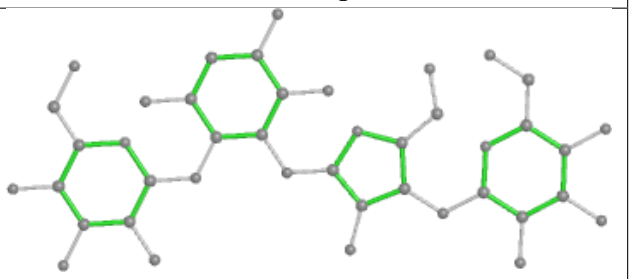
Bond lengths



Bond angles

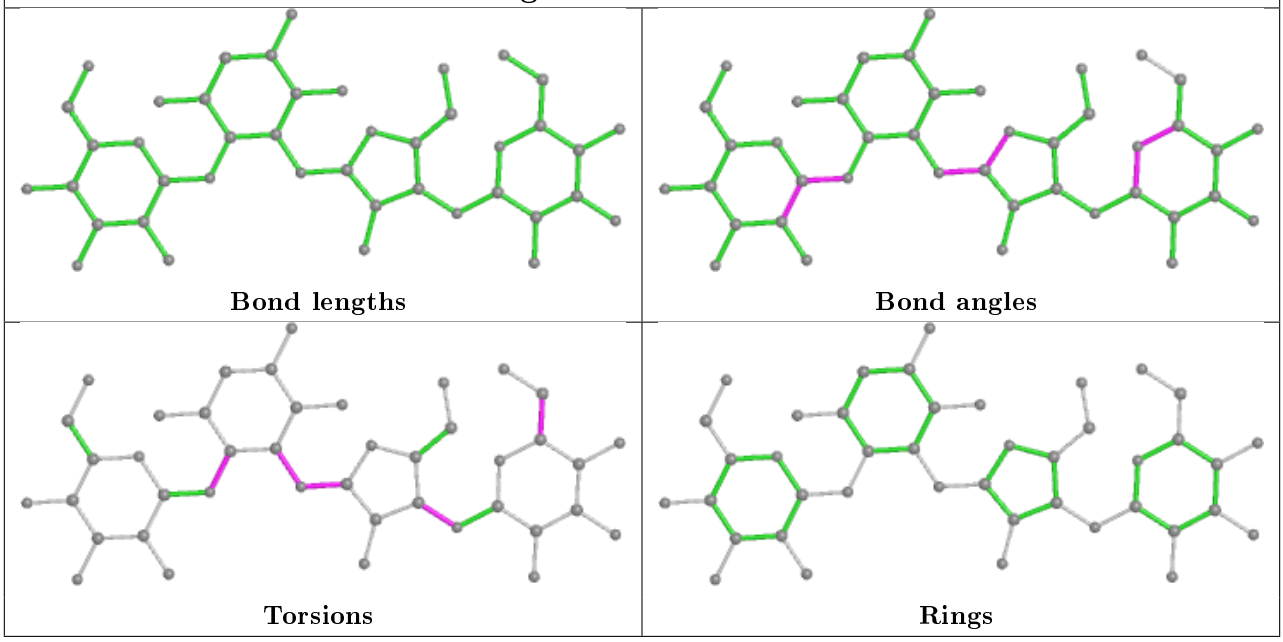


Torsions

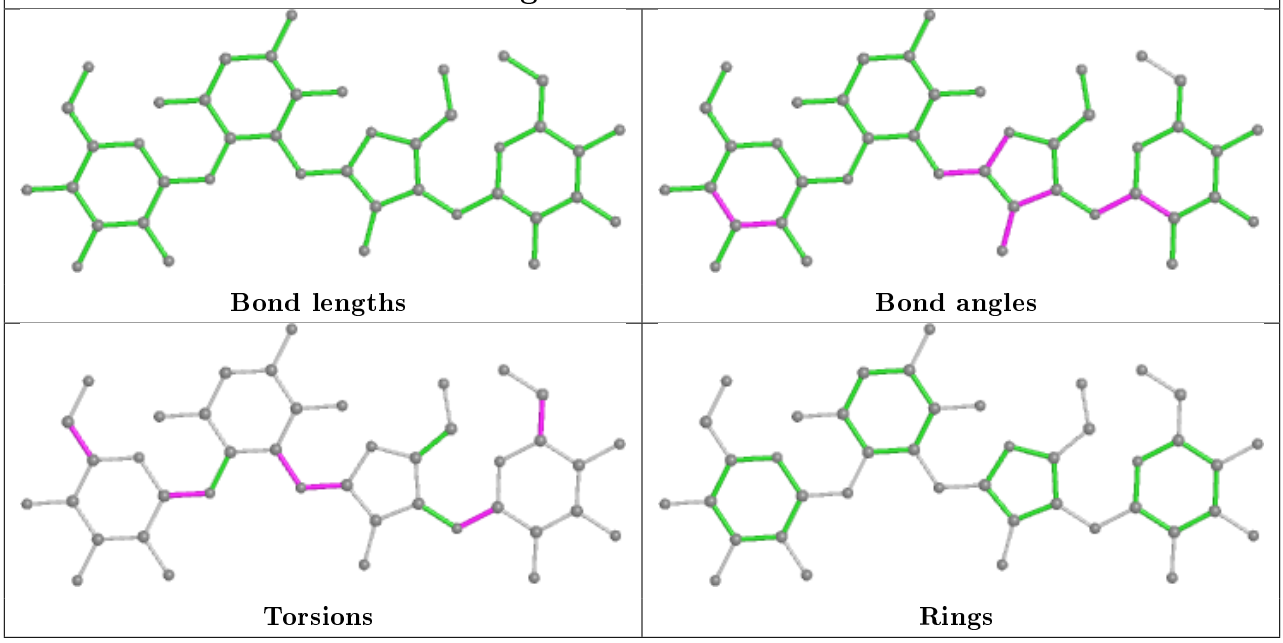


Rings

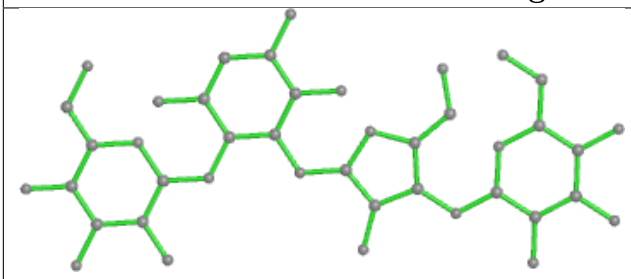
**Ligand PAR 1 3407**



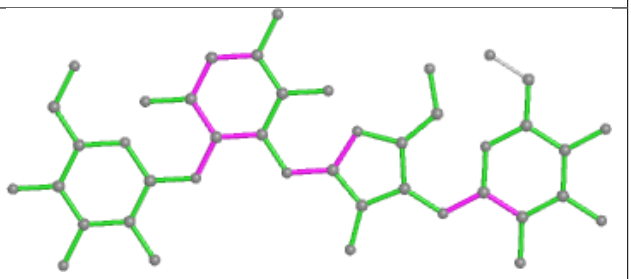

**Ligand PAR 1 3435**



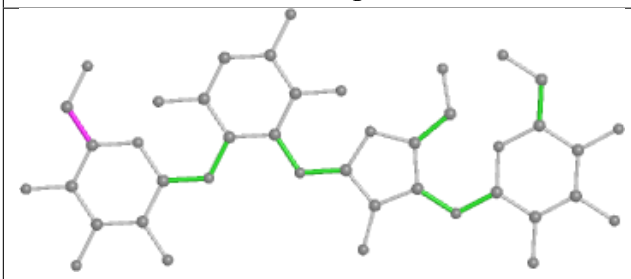
**Ligand PAR 8 201**



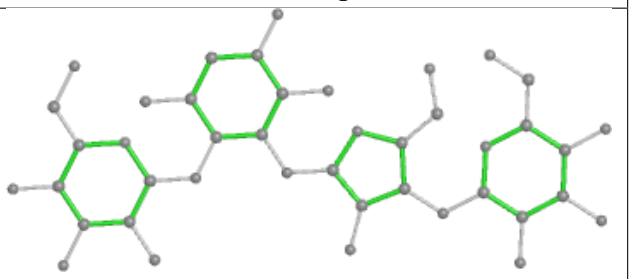
Bond lengths



Bond angles

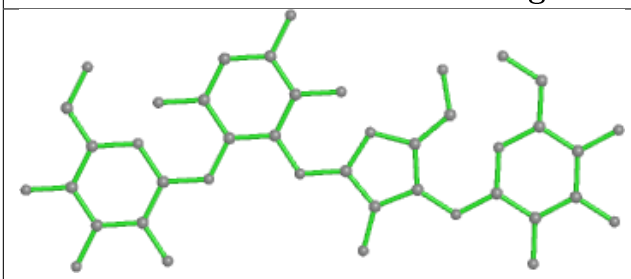


Torsions

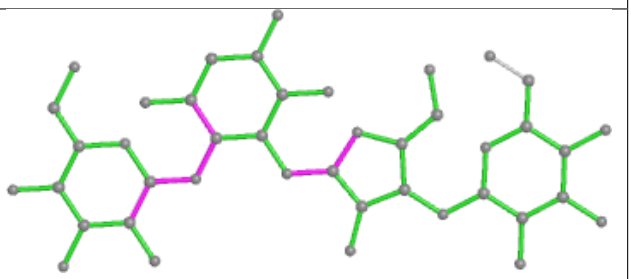


Rings

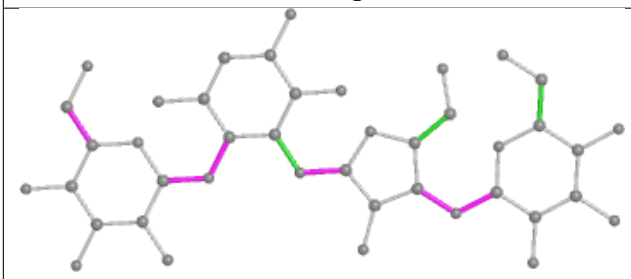
**Ligand PAR 7 202**



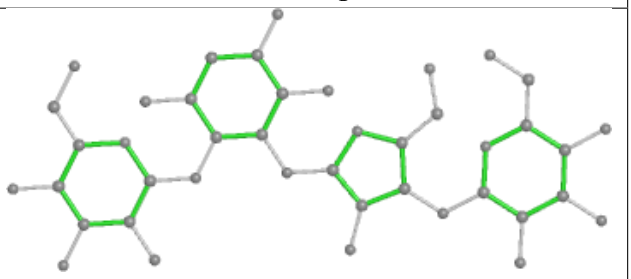
Bond lengths



Bond angles

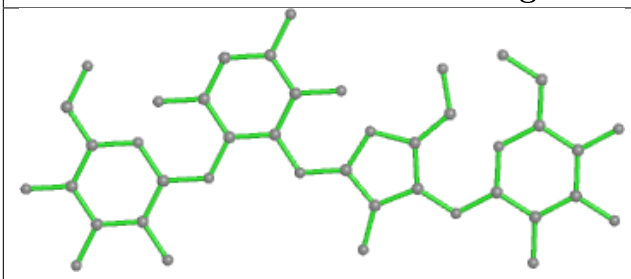


Torsions

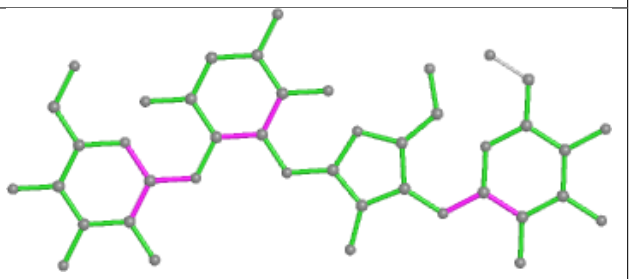


Rings

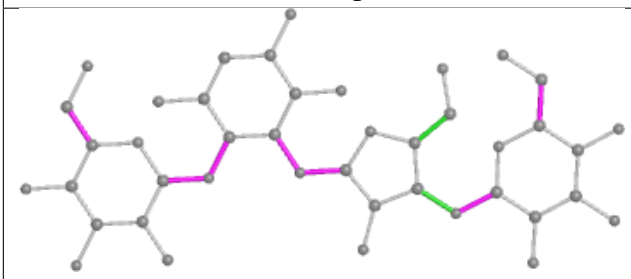
**Ligand PAR 1 3409**



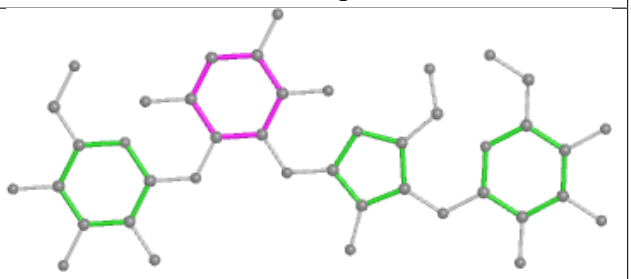
Bond lengths



Bond angles

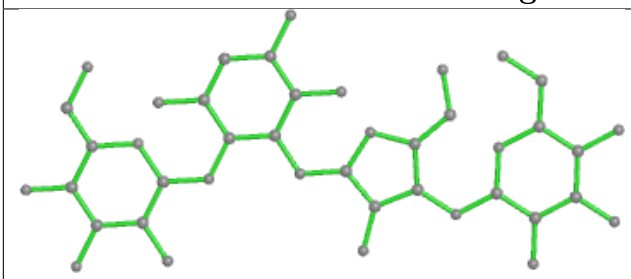


Torsions

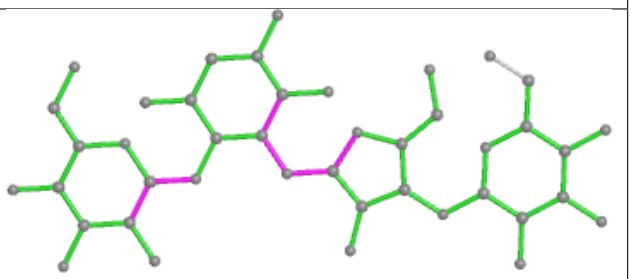


Rings

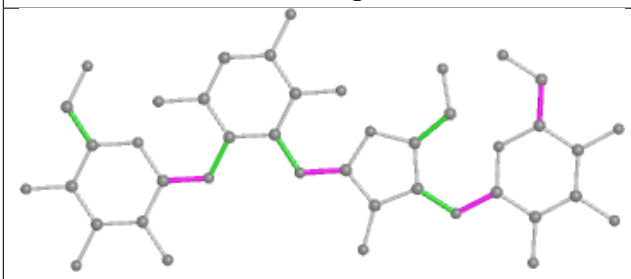
**Ligand PAR 5 3403**



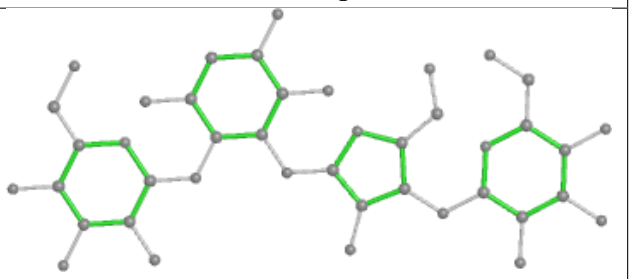
Bond lengths



Bond angles

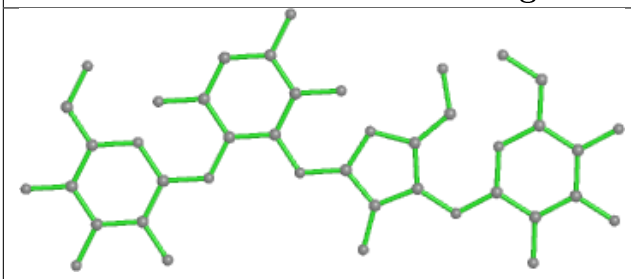


Torsions

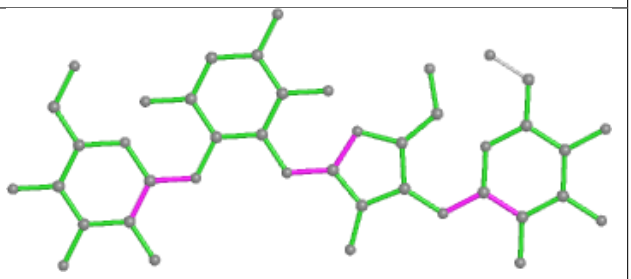


Rings

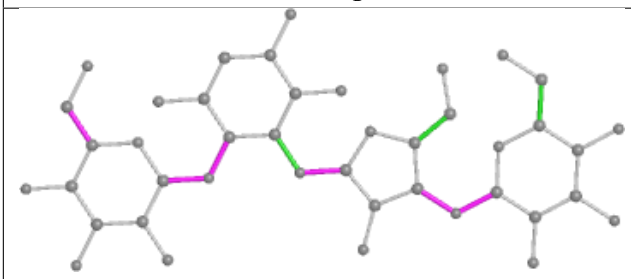
**Ligand PAR 1 3430**



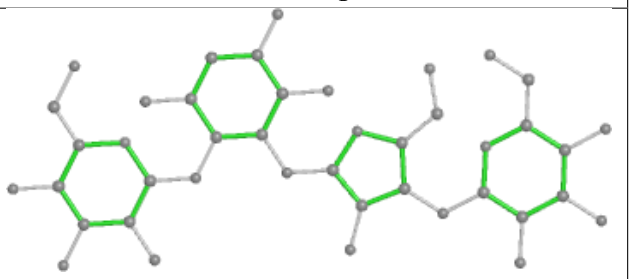
Bond lengths



Bond angles

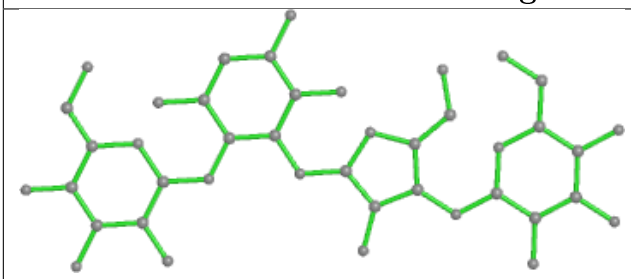


Torsions

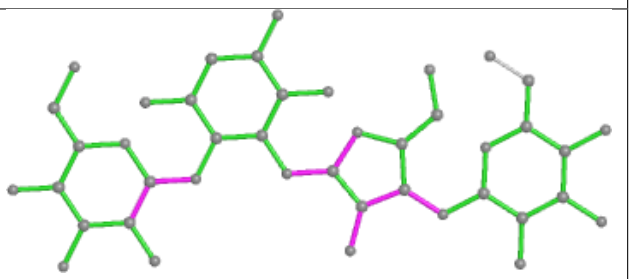


Rings

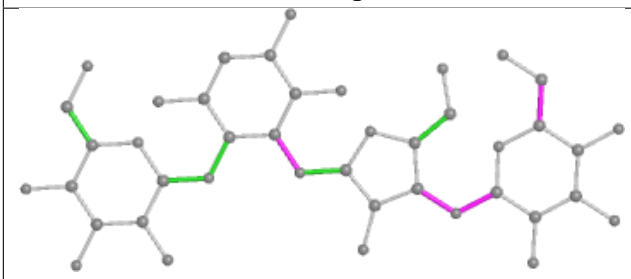
**Ligand PAR 5 3422**



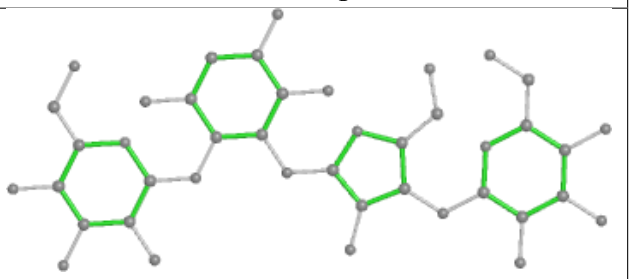
Bond lengths



Bond angles

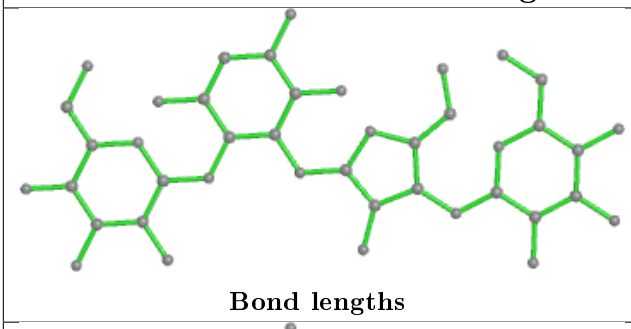


Torsions

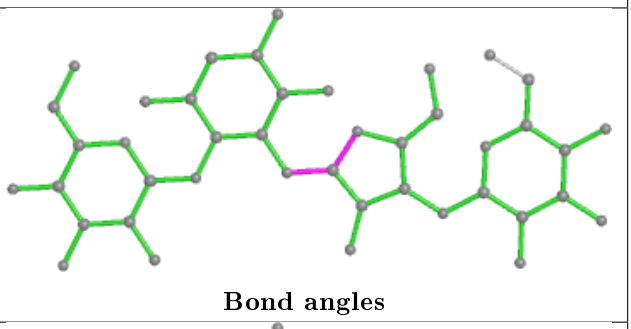


Rings

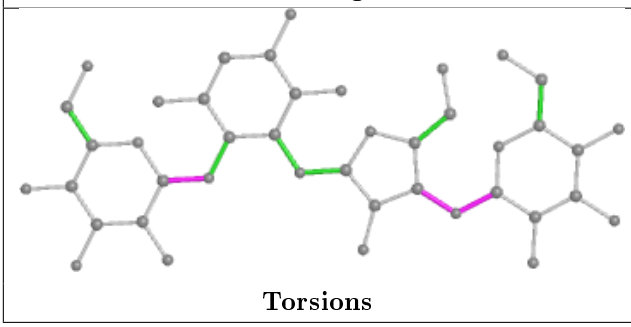
**Ligand PAR 1 3413**



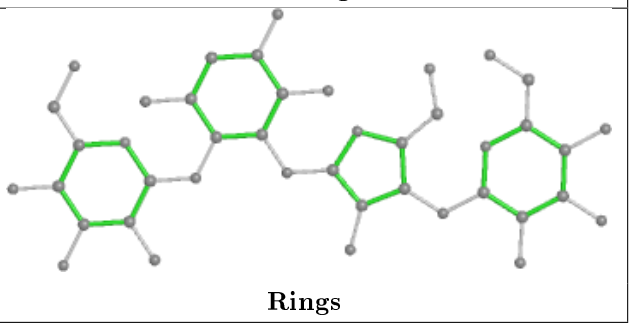
Bond lengths



Bond angles

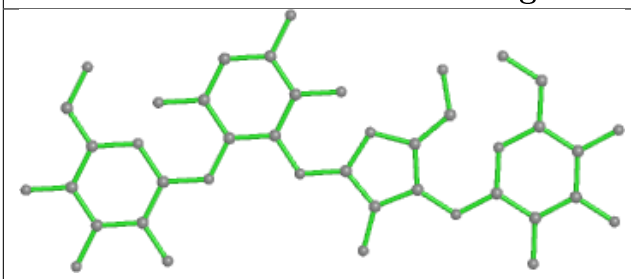


Torsions

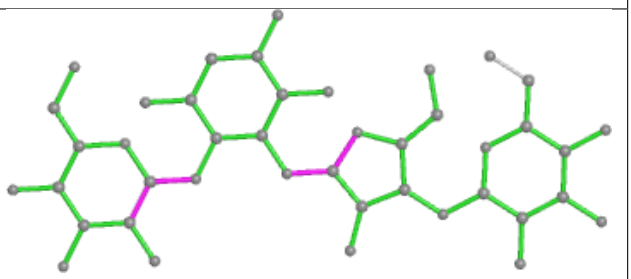


Rings

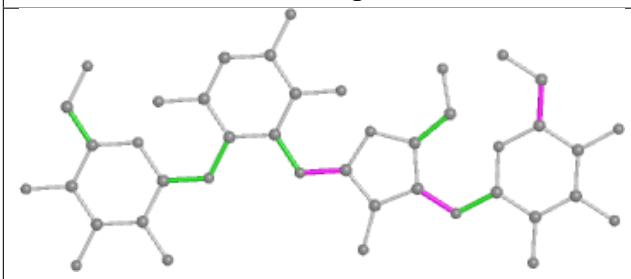
**Ligand PAR 1 3437**



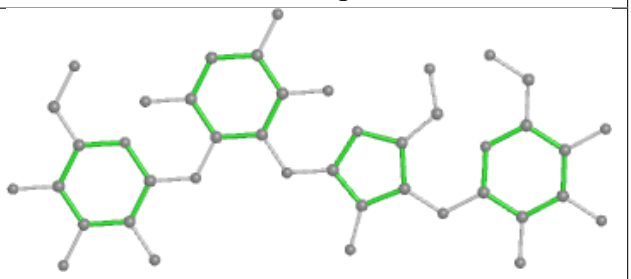
Bond lengths



Bond angles

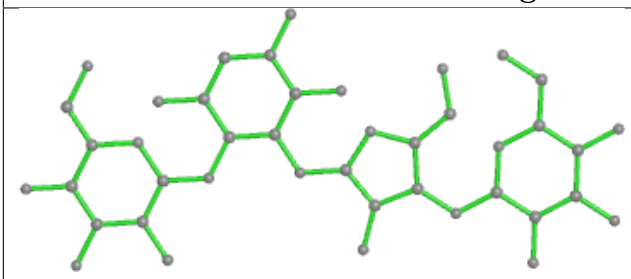


Torsions

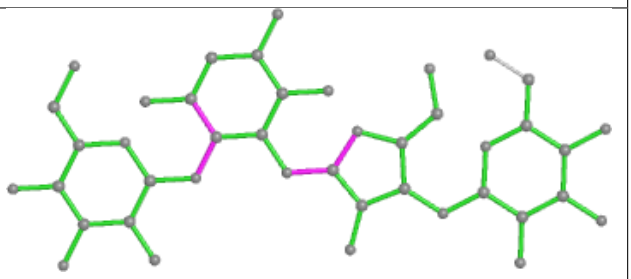


Rings

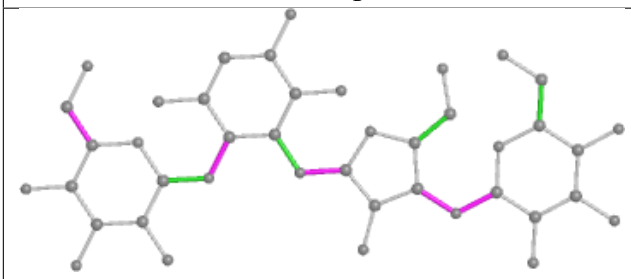
**Ligand PAR 1 3402**



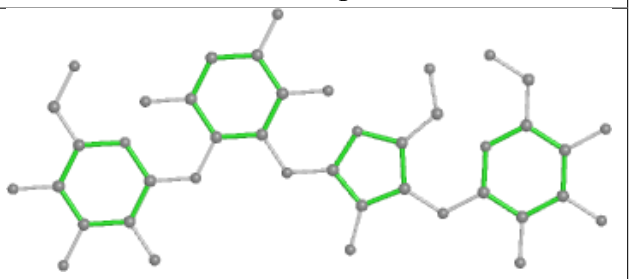
Bond lengths



Bond angles

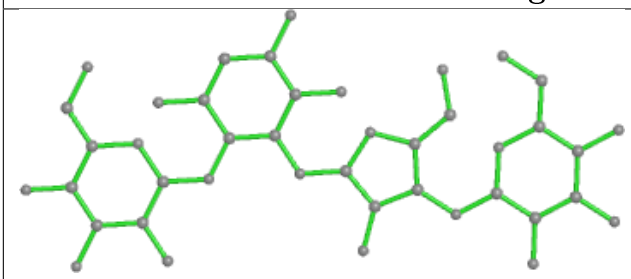


Torsions

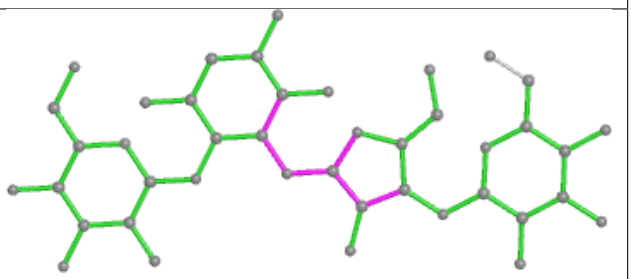


Rings

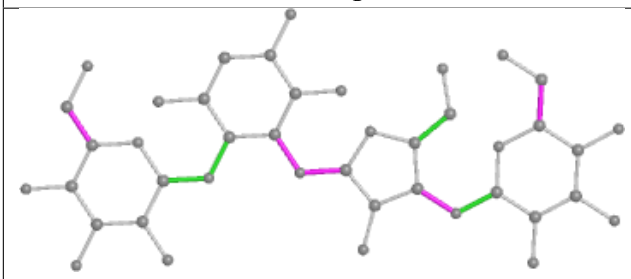
**Ligand PAR 3 202**



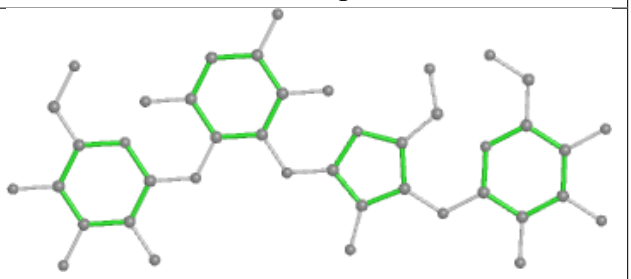
Bond lengths



Bond angles

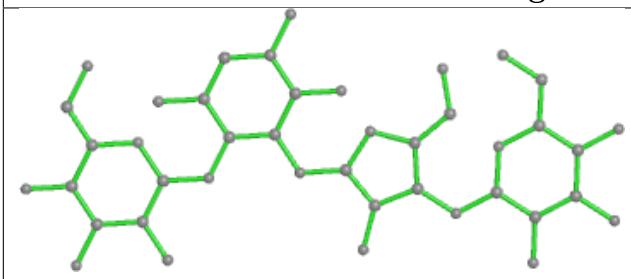


Torsions

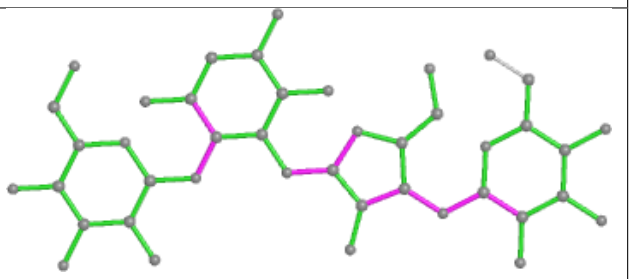


Rings

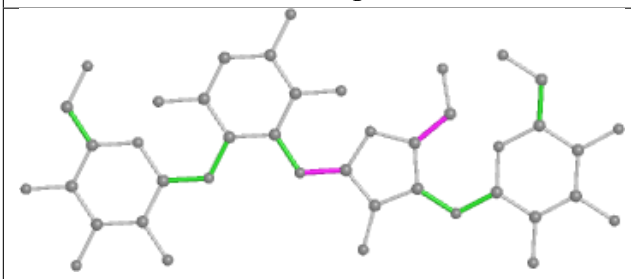
**Ligand PAR 4 202**



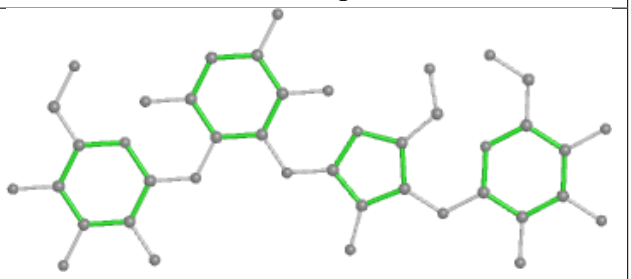
Bond lengths



Bond angles

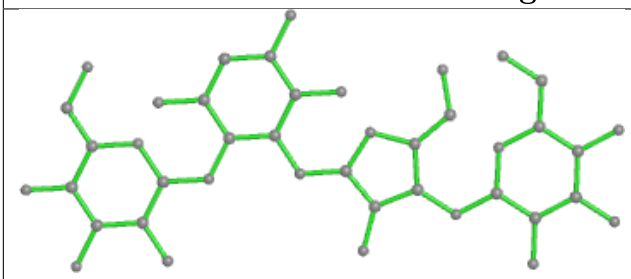


Torsions

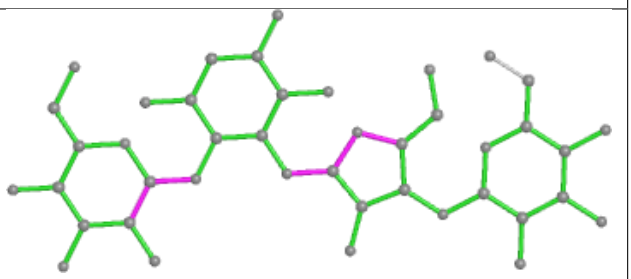


Rings

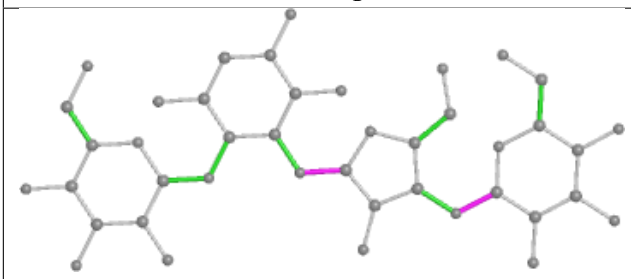
**Ligand PAR 5 3424**



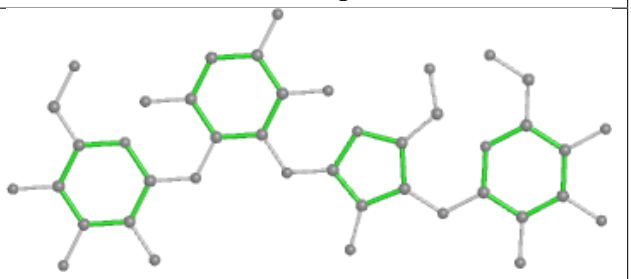
Bond lengths



Bond angles

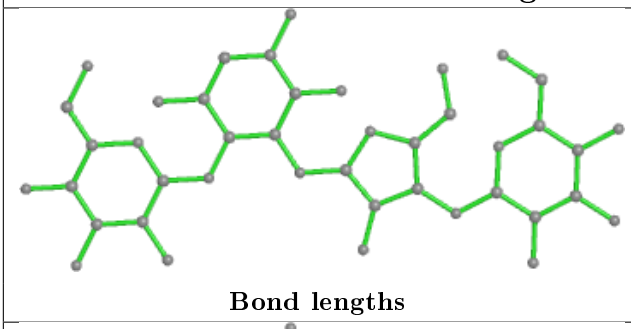


Torsions

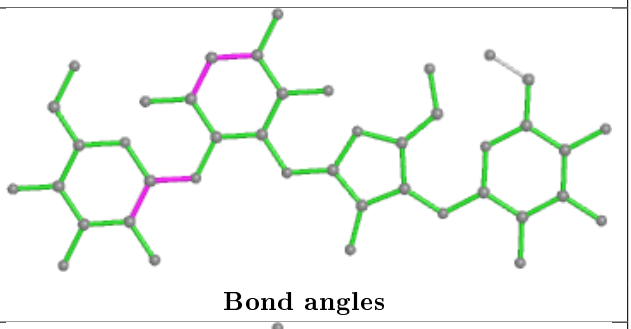


Rings

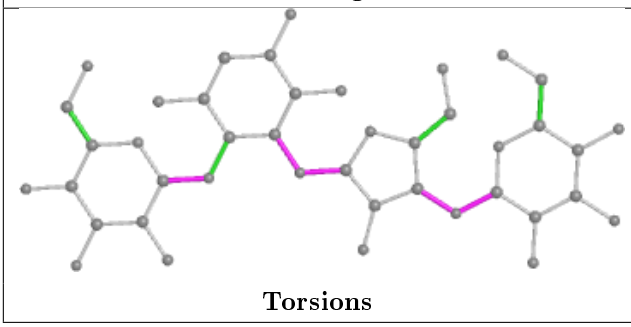
## Ligand PAR 5 3405



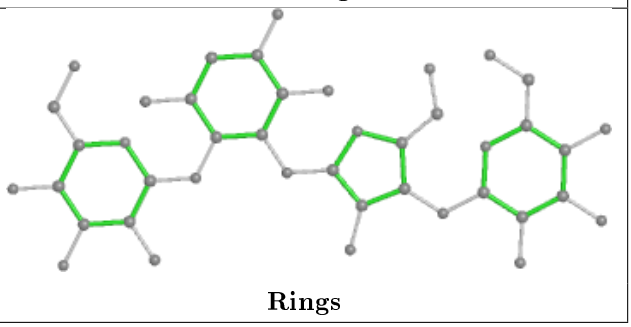
Bond lengths



Bond angles

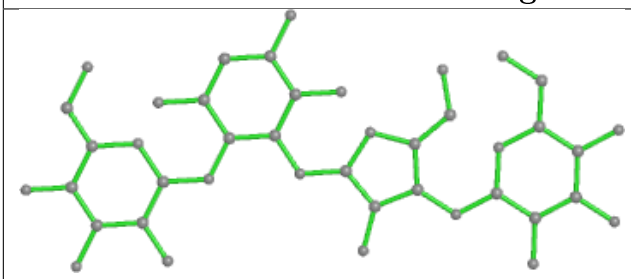


Torsions

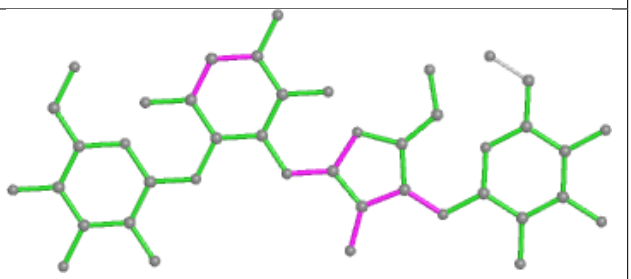


Rings

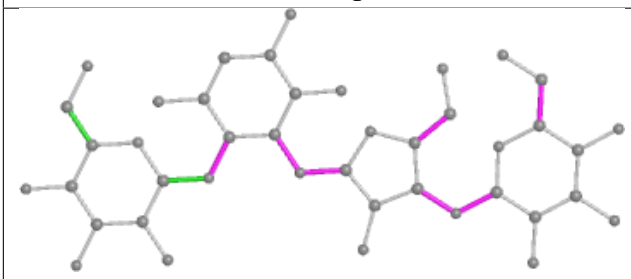
## Ligand PAR o2 201



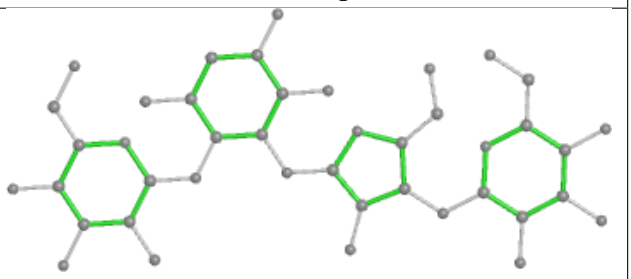
Bond lengths



Bond angles

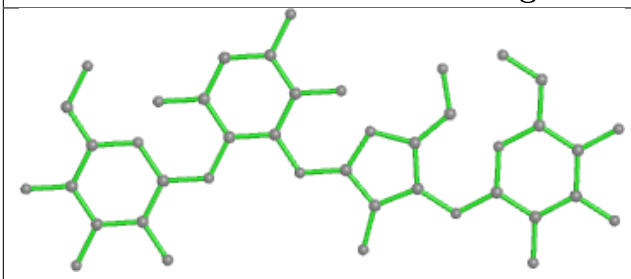


Torsions

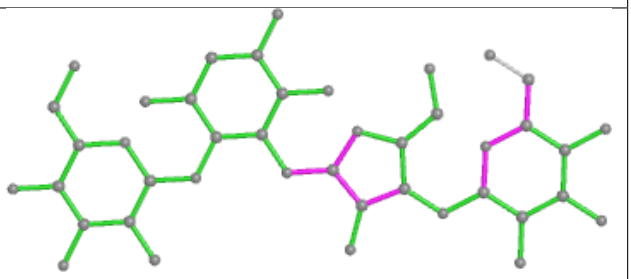


Rings

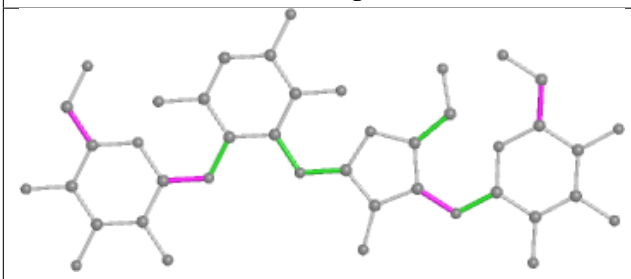
**Ligand PAR 5 3406**



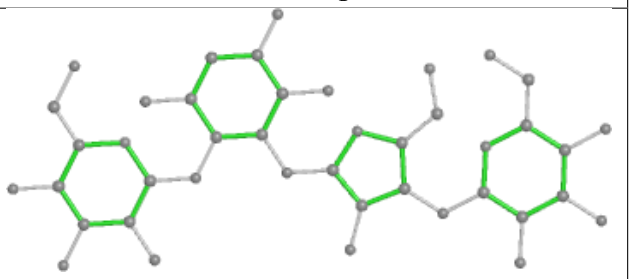
Bond lengths



Bond angles

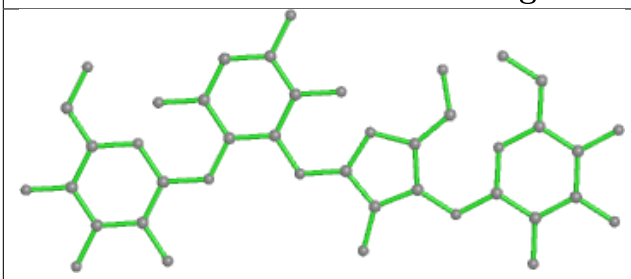


Torsions

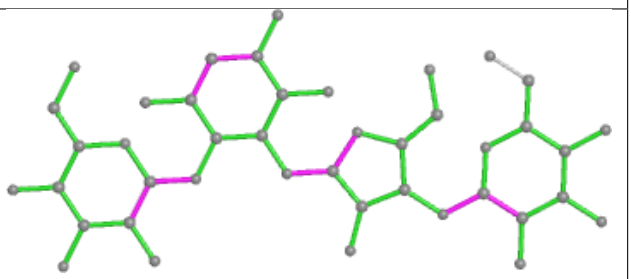


Rings

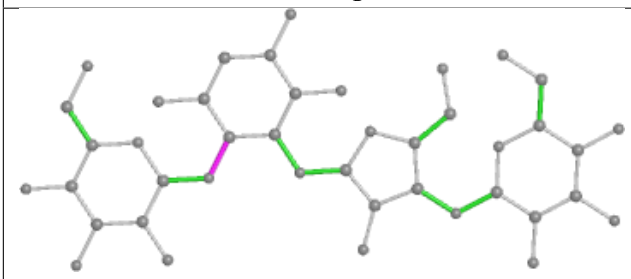
**Ligand PAR 5 3414**



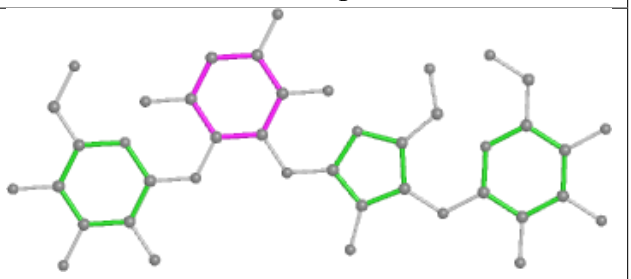
Bond lengths



Bond angles

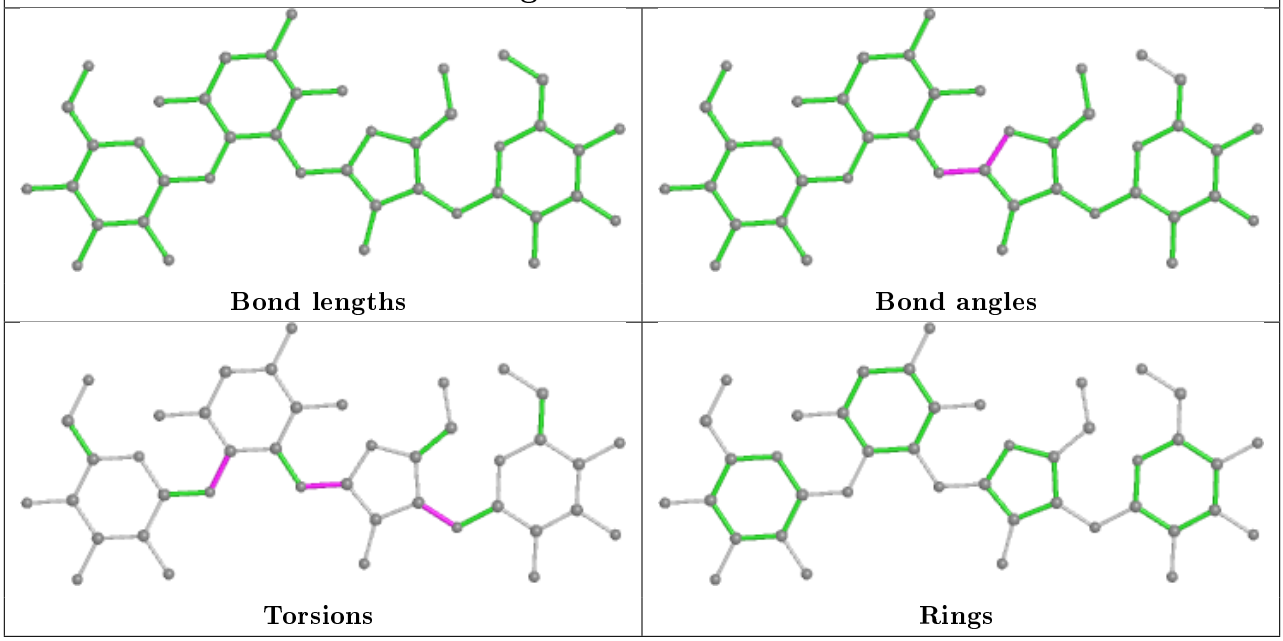


Torsions

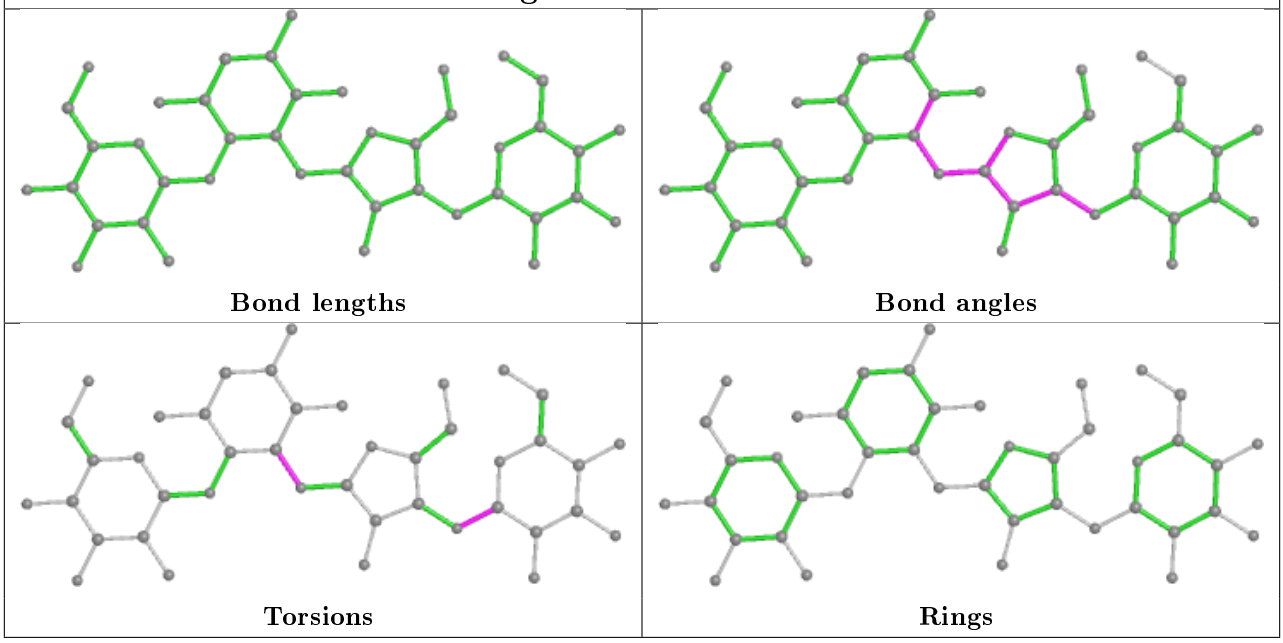


Rings

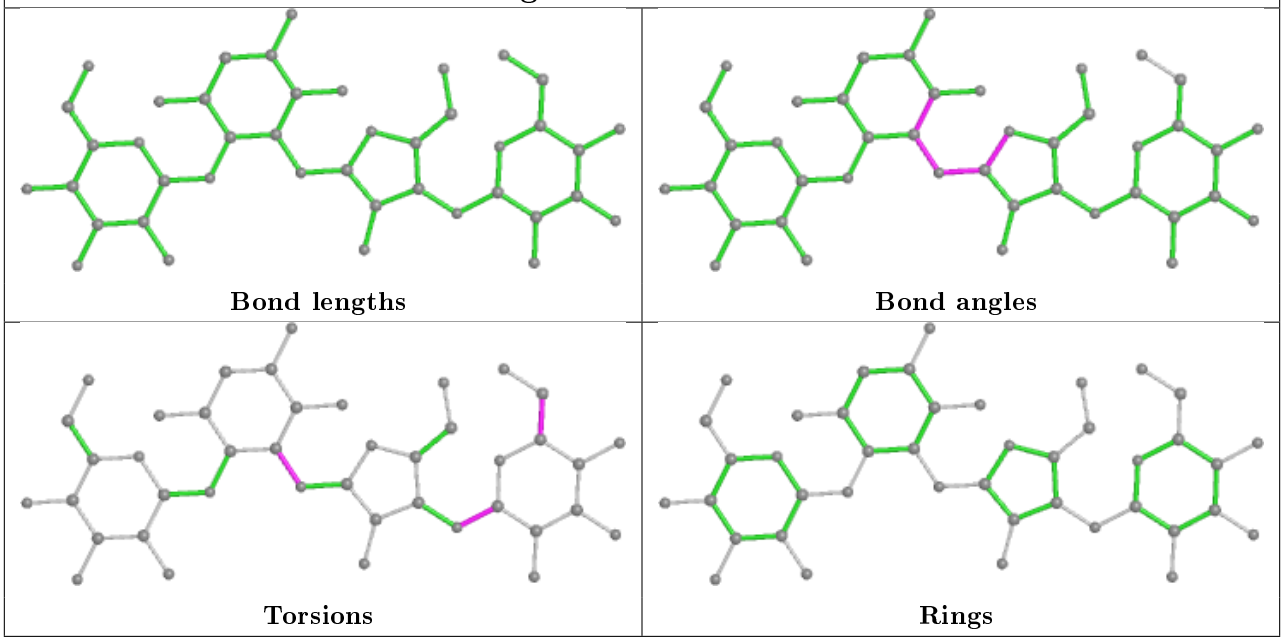
**Ligand PAR 1 3423**



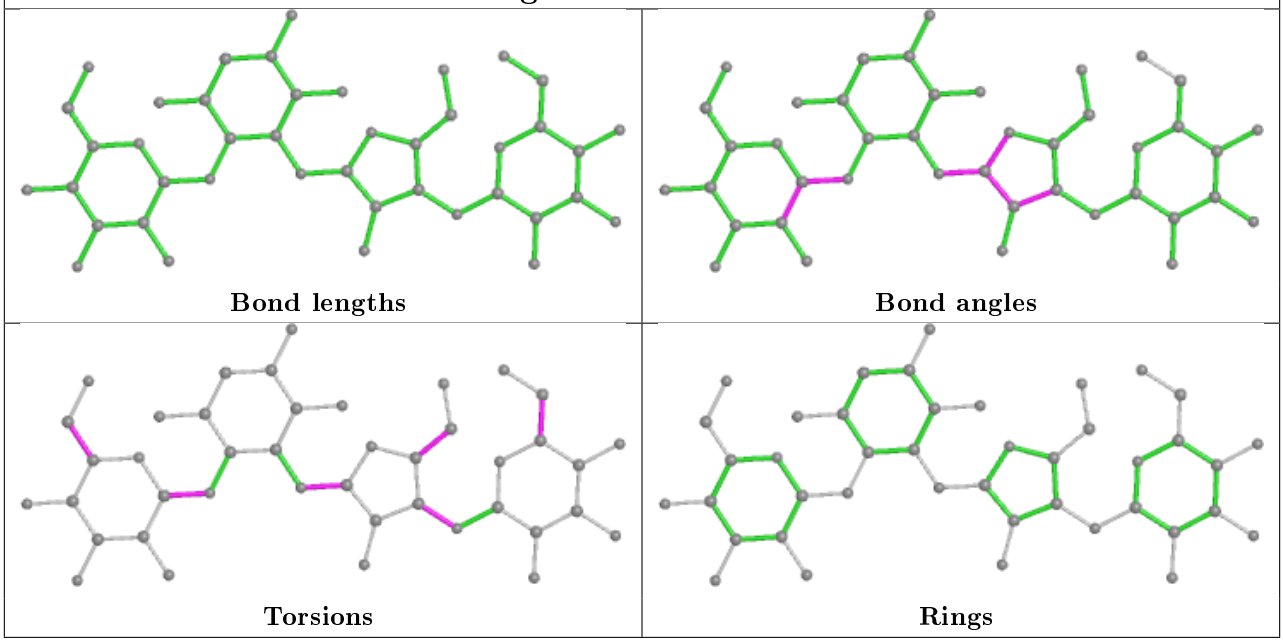

**Ligand PAR 1 3416**



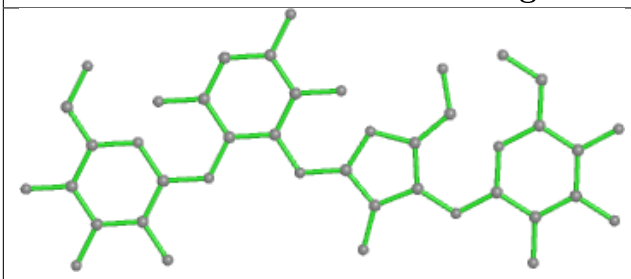
**Ligand PAR 1 3404**



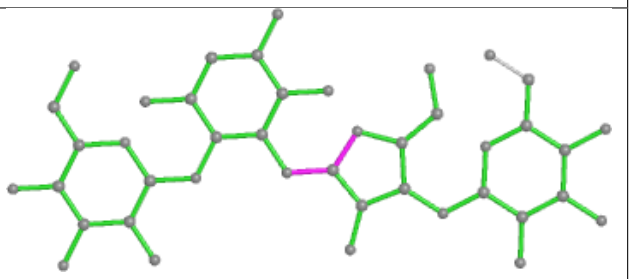

**Ligand PAR 1 3436**



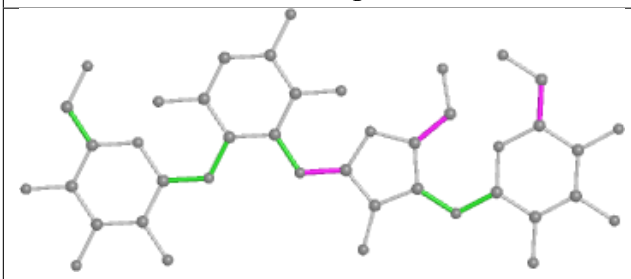
**Ligand PAR 6 1903**



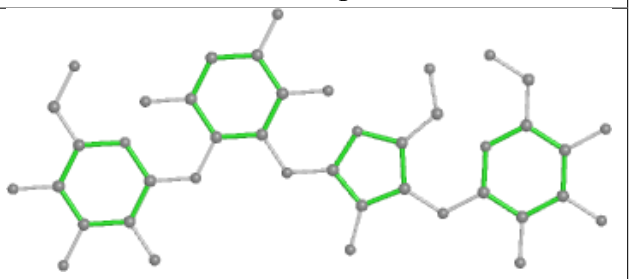
Bond lengths



Bond angles

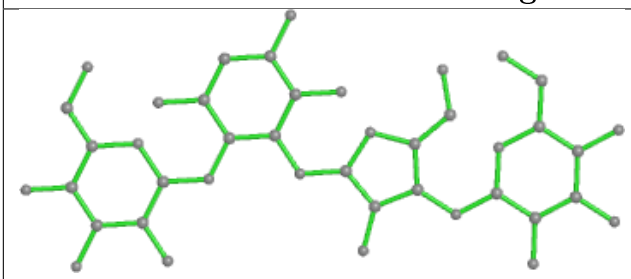


Torsions

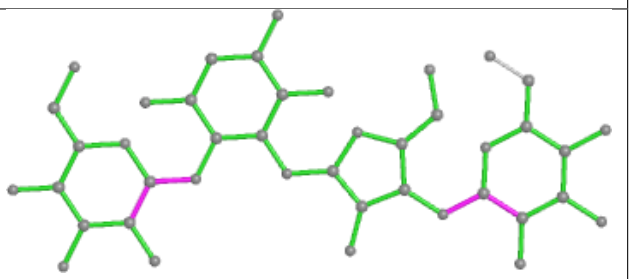


Rings

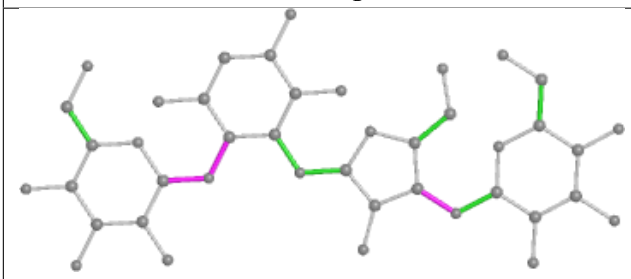
**Ligand PAR 1 3428**



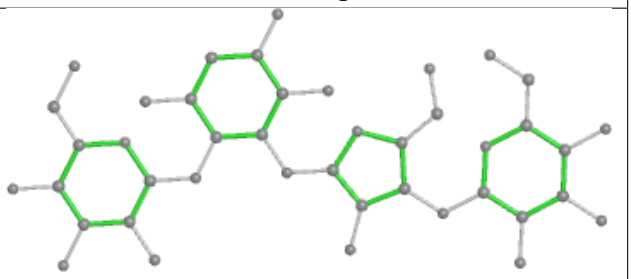
Bond lengths



Bond angles

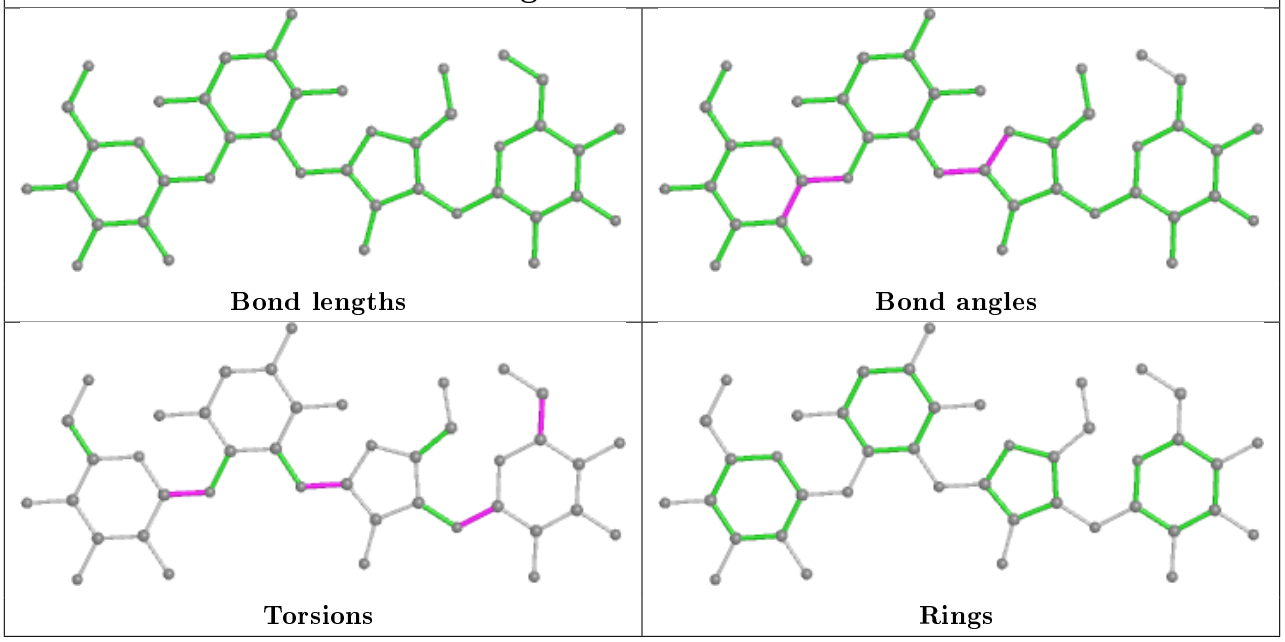


Torsions

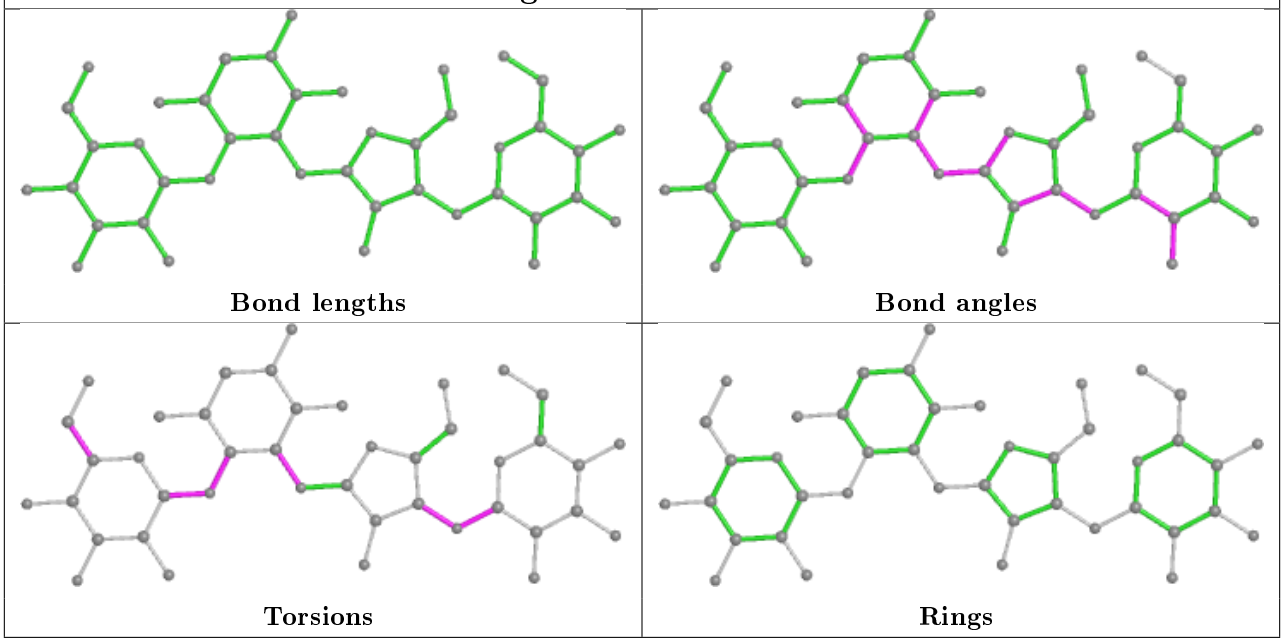


Rings

**Ligand PAR 5 3412**




**Ligand PAR 5 3411**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 78 | sM | 1 |
| 64 | C8 | 1 |
| 5 | l3 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | sM | 51:ARG | C | 52:PRO | N | 1.62 |
| 1 | C8 | 81:ILE | C | 82:PRO | N | 1.16 |
| 1 | l3 | 168:LYS | C | 169:THR | N | 1.16 |

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | 1 | 3078/3396 (90%) | 0.18 | 9 (0%) 94 94 | 29, 61, 151, 275 | 0 |
| 1 | 5 | 3087/3396 (90%) | 0.20 | 17 (0%) 89 90 | 36, 77, 179, 287 | 0 |
| 2 | 3 | 121/121 (100%) | 0.00 | 0 100 100 | 49, 98, 117, 142 | 0 |
| 2 | 7 | 121/121 (100%) | -0.12 | 0 100 100 | 51, 115, 151, 169 | 0 |
| 3 | 4 | 157/158 (99%) | 0.19 | 1 (0%) 89 90 | 36, 58, 138, 255 | 0 |
| 3 | 8 | 158/158 (100%) | 0.17 | 2 (1%) 77 77 | 48, 90, 161, 264 | 0 |
| 4 | L2 | 248/248 (100%) | 0.33 | 2 (0%) 86 86 | 22, 47, 66, 101 | 0 |
| 4 | l2 | 248/248 (100%) | 0.76 | 20 (8%) 12 11 | 49, 86, 120, 160 | 0 |
| 5 | L3 | 386/386 (100%) | 0.18 | 0 100 100 | 28, 69, 100, 156 | 0 |
| 5 | l3 | 386/386 (100%) | 0.02 | 1 (0%) 94 94 | 26, 64, 92, 160 | 0 |
| 6 | L4 | 361/361 (100%) | 0.12 | 0 100 100 | 23, 65, 101, 156 | 0 |
| 6 | l4 | 361/361 (100%) | 0.21 | 5 (1%) 75 75 | 32, 84, 121, 155 | 0 |
| 7 | L5 | 293/296 (98%) | 0.75 | 26 (8%) 9 10 | 72, 111, 149, 179 | 0 |
| 7 | l5 | 294/296 (99%) | 0.89 | 38 (12%) 3 3 | 81, 139, 182, 214 | 0 |
| 8 | L6 | 156/176 (88%) | 0.05 | 1 (0%) 89 90 | 47, 76, 109, 146 | 0 |
| 8 | l6 | 157/176 (89%) | 0.35 | 5 (3%) 47 46 | 55, 81, 127, 162 | 0 |
| 9 | L7 | 226/226 (100%) | 0.07 | 0 100 100 | 37, 63, 117, 200 | 0 |
| 9 | l7 | 223/226 (98%) | 0.11 | 0 100 100 | 43, 70, 123, 195 | 0 |
| 10 | L8 | 231/231 (100%) | 0.60 | 5 (2%) 62 60 | 48, 83, 139, 171 | 0 |
| 10 | l8 | 231/231 (100%) | 0.92 | 41 (17%) 1 1 | 93, 143, 197, 244 | 0 |
| 11 | L9 | 189/191 (98%) | 0.80 | 19 (10%) 7 6 | 56, 87, 120, 156 | 0 |
| 11 | l9 | 191/191 (100%) | 0.38 | 3 (1%) 72 70 | 52, 77, 100, 189 | 0 |
| 12 | M0 | 217/221 (98%) | 0.67 | 19 (8%) 10 10 | 47, 83, 141, 196 | 0 |
| 12 | m0 | 219/221 (99%) | 0.67 | 14 (6%) 19 19 | 49, 76, 148, 220 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | M1 | 169/169 (100%) | 1.02 | 29 (17%) 1 1 | 86, 113, 147, 170 | 0 |
| 13 | m1 | 169/169 (100%) | 1.01 | 28 (16%) 1 2 | 101, 142, 176, 196 | 0 |
| 14 | M3 | 193/194 (99%) | 0.38 | 7 (3%) 42 40 | 33, 75, 134, 214 | 0 |
| 14 | m3 | 194/194 (100%) | 0.44 | 8 (4%) 37 35 | 61, 120, 172, 211 | 0 |
| 15 | M4 | 136/137 (99%) | 0.33 | 4 (2%) 51 50 | 52, 78, 107, 152 | 0 |
| 15 | m4 | 137/137 (100%) | 0.14 | 1 (0%) 87 88 | 51, 77, 124, 152 | 0 |
| 16 | M5 | 203/203 (100%) | 0.37 | 3 (1%) 73 72 | 26, 50, 67, 80 | 0 |
| 16 | m5 | 203/203 (100%) | 0.85 | 14 (6%) 16 16 | 62, 96, 123, 139 | 0 |
| 17 | M6 | 197/197 (100%) | 0.33 | 1 (0%) 91 91 | 36, 57, 97, 118 | 0 |
| 17 | m6 | 197/197 (100%) | -0.01 | 0 100 100 | 35, 54, 107, 138 | 0 |
| 18 | M7 | 175/184 (95%) | 0.43 | 12 (6%) 16 16 | 30, 52, 139, 184 | 0 |
| 18 | m7 | 155/184 (84%) | 0.12 | 0 100 100 | 39, 55, 86, 143 | 0 |
| 19 | M8 | 185/185 (100%) | 0.26 | 2 (1%) 80 81 | 43, 65, 91, 111 | 0 |
| 19 | m8 | 185/185 (100%) | 0.48 | 10 (5%) 25 24 | 53, 93, 121, 143 | 0 |
| 20 | M9 | 185/188 (98%) | 0.26 | 0 100 100 | 45, 72, 158, 199 | 0 |
| 20 | m9 | 188/188 (100%) | 0.54 | 15 (7%) 12 11 | 50, 83, 212, 255 | 0 |
| 21 | N0 | 172/172 (100%) | 0.68 | 7 (4%) 37 35 | 51, 72, 105, 144 | 0 |
| 21 | n0 | 172/172 (100%) | 0.40 | 0 100 100 | 45, 71, 101, 139 | 0 |
| 22 | N1 | 159/159 (100%) | 0.54 | 4 (2%) 57 54 | 45, 74, 130, 198 | 0 |
| 22 | n1 | 159/159 (100%) | 1.10 | 32 (20%) 1 1 | 62, 90, 155, 204 | 0 |
| 23 | N2 | 99/99 (100%) | 0.32 | 3 (3%) 50 49 | 77, 110, 147, 168 | 0 |
| 23 | n2 | 98/99 (98%) | 0.76 | 8 (8%) 11 11 | 85, 120, 146, 169 | 0 |
| 24 | N3 | 132/136 (97%) | 0.20 | 0 100 100 | 38, 66, 93, 155 | 0 |
| 24 | n3 | 136/136 (100%) | 0.28 | 2 (1%) 73 72 | 33, 58, 98, 150 | 0 |
| 25 | N4 | 63/155 (40%) | 0.55 | 1 (1%) 72 70 | 52, 74, 98, 121 | 0 |
| 25 | n4 | 135/155 (87%) | 1.53 | 44 (32%) 0 0 | 44, 140, 224, 256 | 0 |
| 26 | N5 | 118/120 (98%) | 0.40 | 1 (0%) 86 86 | 42, 62, 91, 116 | 0 |
| 26 | n5 | 120/120 (100%) | 1.01 | 16 (13%) 3 3 | 59, 95, 135, 176 | 0 |
| 27 | N6 | 125/125 (100%) | 0.73 | 12 (9%) 8 8 | 34, 71, 101, 131 | 0 |
| 27 | n6 | 123/125 (98%) | 0.50 | 7 (5%) 23 23 | 55, 85, 123, 139 | 0 |
| 28 | N7 | 135/135 (100%) | 0.82 | 9 (6%) 17 17 | 57, 84, 115, 149 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | n7 | 135/135 (100%) | 1.80 | 50 (37%) 0 0 | 99, 133, 175, 194 | 0 |
| 29 | N8 | 148/148 (100%) | 0.64 | 12 (8%) 12 11 | 27, 63, 117, 156 | 0 |
| 29 | n8 | 148/148 (100%) | 0.83 | 21 (14%) 2 2 | 34, 104, 145, 167 | 0 |
| 30 | N9 | 56/58 (96%) | 0.57 | 3 (5%) 25 24 | 34, 81, 137, 171 | 0 |
| 30 | n9 | 58/58 (100%) | 0.75 | 6 (10%) 6 6 | 53, 112, 157, 189 | 0 |
| 31 | O0 | 97/100 (97%) | 0.70 | 3 (3%) 49 48 | 51, 76, 110, 145 | 0 |
| 31 | o0 | 100/100 (100%) | 0.16 | 3 (3%) 50 49 | 82, 117, 167, 201 | 0 |
| 32 | O1 | 106/112 (94%) | 1.14 | 16 (15%) 2 2 | 50, 77, 130, 149 | 0 |
| 32 | o1 | 109/112 (97%) | 0.53 | 2 (1%) 68 67 | 43, 75, 137, 178 | 0 |
| 33 | O2 | 125/127 (98%) | 0.23 | 1 (0%) 86 86 | 29, 55, 78, 114 | 0 |
| 33 | o2 | 127/127 (100%) | 0.32 | 3 (2%) 59 56 | 35, 65, 92, 147 | 0 |
| 34 | O3 | 106/106 (100%) | 0.18 | 1 (0%) 84 84 | 37, 55, 95, 133 | 0 |
| 34 | o3 | 106/106 (100%) | 0.31 | 2 (1%) 66 65 | 37, 59, 106, 127 | 0 |
| 35 | O4 | 112/112 (100%) | 0.66 | 5 (4%) 33 32 | 41, 61, 123, 175 | 0 |
| 35 | o4 | 112/112 (100%) | 0.97 | 16 (14%) 2 2 | 60, 96, 167, 193 | 0 |
| 36 | O5 | 119/119 (100%) | 0.41 | 2 (1%) 70 68 | 42, 75, 107, 130 | 0 |
| 36 | o5 | 119/119 (100%) | 0.81 | 15 (12%) 3 3 | 78, 108, 138, 167 | 0 |
| 37 | O6 | 97/99 (97%) | 0.26 | 0 100 100 | 51, 75, 108, 125 | 0 |
| 37 | o6 | 99/99 (100%) | 1.37 | 25 (25%) 0 0 | 95, 131, 170, 205 | 0 |
| 38 | O7 | 84/87 (96%) | 0.10 | 0 100 100 | 29, 43, 76, 102 | 0 |
| 38 | o7 | 87/87 (100%) | 0.54 | 4 (4%) 32 30 | 37, 71, 122, 180 | 0 |
| 39 | O8 | 77/77 (100%) | 0.55 | 5 (6%) 18 18 | 63, 94, 148, 185 | 0 |
| 39 | o8 | 77/77 (100%) | 1.09 | 12 (15%) 2 2 | 87, 121, 154, 182 | 0 |
| 40 | O9 | 50/50 (100%) | 0.41 | 0 100 100 | 37, 54, 77, 83 | 0 |
| 40 | o9 | 50/50 (100%) | 0.40 | 2 (4%) 38 36 | 57, 72, 95, 108 | 0 |
| 41 | Q0 | 52/52 (100%) | 1.14 | 8 (15%) 2 2 | 57, 76, 122, 133 | 0 |
| 41 | q0 | 52/52 (100%) | 0.46 | 2 (3%) 40 37 | 48, 62, 91, 122 | 0 |
| 42 | Q1 | 25/25 (100%) | 0.30 | 0 100 100 | 52, 66, 82, 94 | 0 |
| 42 | q1 | 25/25 (100%) | 0.19 | 0 100 100 | 61, 74, 90, 92 | 0 |
| 43 | Q2 | 105/105 (100%) | 0.90 | 17 (16%) 1 2 | 31, 66, 119, 192 | 0 |
| 43 | q2 | 105/105 (100%) | 0.73 | 9 (8%) 10 10 | 59, 102, 140, 185 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | Q3 | 91/91 (100%) | 0.09 | 0 100 100 | 33, 53, 85, 98 | 0 |
| 44 | q3 | 91/91 (100%) | 0.14 | 0 100 100 | 44, 83, 118, 135 | 0 |
| 45 | 2 | 1712/1800 (95%) | 0.24 | 27 (1%) 72 70 | 55, 121, 223, 318 | 0 |
| 45 | 6 | 1683/1800 (93%) | 0.20 | 23 (1%) 75 75 | 57, 119, 222, 300 | 0 |
| 46 | S0 | 206/206 (100%) | 1.14 | 44 (21%) 0 1 | 92, 133, 170, 223 | 0 |
| 46 | s0 | 206/206 (100%) | 1.00 | 35 (16%) 1 1 | 98, 140, 187, 229 | 0 |
| 47 | S1 | 211/216 (97%) | 1.47 | 64 (30%) 0 0 | 89, 142, 196, 244 | 0 |
| 47 | s1 | 216/216 (100%) | 1.55 | 65 (30%) 0 0 | 94, 145, 190, 236 | 0 |
| 48 | S2 | 217/217 (100%) | 0.72 | 25 (11%) 4 4 | 76, 119, 159, 170 | 0 |
| 48 | s2 | 217/217 (100%) | 1.31 | 53 (24%) 0 0 | 74, 120, 156, 179 | 0 |
| 49 | S3 | 209/223 (93%) | 1.00 | 34 (16%) 1 2 | 87, 131, 176, 214 | 0 |
| 49 | s3 | 223/223 (100%) | 1.67 | 75 (33%) 0 0 | 97, 140, 196, 224 | 0 |
| 50 | S4 | 256/260 (98%) | 1.67 | 89 (34%) 0 0 | 92, 137, 169, 240 | 0 |
| 50 | s4 | 260/260 (100%) | 0.99 | 38 (14%) 2 2 | 80, 125, 157, 209 | 0 |
| 51 | S5 | 206/206 (100%) | 2.79 | 127 (61%) 0 0 | 107, 158, 207, 239 | 0 |
| 51 | s5 | 206/206 (100%) | 1.56 | 66 (32%) 0 0 | 108, 156, 202, 234 | 0 |
| 52 | S6 | 200/236 (84%) | 1.03 | 42 (21%) 1 1 | 77, 138, 206, 301 | 0 |
| 53 | S7 | 179/186 (96%) | 0.86 | 27 (15%) 2 2 | 97, 147, 192, 216 | 0 |
| 53 | s7 | 186/186 (100%) | 1.00 | 34 (18%) 1 1 | 101, 162, 213, 267 | 0 |
| 54 | S8 | 185/200 (92%) | 1.03 | 28 (15%) 2 2 | 63, 106, 162, 218 | 0 |
| 54 | s8 | 188/200 (94%) | 0.85 | 20 (10%) 6 6 | 65, 104, 156, 206 | 0 |
| 55 | S9 | 174/185 (94%) | 1.31 | 38 (21%) 0 1 | 98, 145, 187, 217 | 0 |
| 55 | s9 | 185/185 (100%) | 1.23 | 45 (24%) 0 0 | 93, 130, 177, 209 | 0 |
| 56 | C0 | 90/105 (85%) | 0.64 | 10 (11%) 5 5 | 120, 153, 193, 210 | 0 |
| 56 | c0 | 96/105 (91%) | 1.33 | 31 (32%) 0 0 | 119, 171, 207, 261 | 0 |
| 57 | C1 | 139/146 (95%) | 1.01 | 14 (10%) 7 6 | 68, 98, 146, 171 | 0 |
| 57 | c1 | 146/146 (100%) | 0.88 | 17 (11%) 4 4 | 70, 96, 165, 231 | 0 |
| 58 | C2 | 102/143 (71%) | 1.90 | 33 (32%) 0 0 | 147, 210, 256, 296 | 0 |
| 58 | c2 | 124/143 (86%) | 1.85 | 54 (43%) 0 0 | 170, 230, 275, 291 | 0 |
| 59 | C3 | 150/150 (100%) | 0.77 | 16 (10%) 6 5 | 65, 107, 140, 180 | 0 |
| 59 | c3 | 150/150 (100%) | 0.32 | 9 (6%) 21 21 | 78, 127, 170, 199 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 60 | C4 | 127/128 (99%) | 0.34 | 7 (5%) 25 23 | 71, 133, 184, 207 | 0 |
| 60 | c4 | 128/128 (100%) | 1.19 | 31 (24%) 0 0 | 77, 138, 177, 239 | 0 |
| 61 | C5 | 116/141 (82%) | 1.15 | 24 (20%) 1 1 | 97, 149, 199, 225 | 0 |
| 61 | c5 | 135/141 (95%) | 2.29 | 65 (48%) 0 0 | 111, 152, 206, 244 | 0 |
| 62 | C6 | 136/142 (95%) | 2.90 | 92 (67%) 0 0 | 88, 160, 201, 253 | 0 |
| 62 | c6 | 142/142 (100%) | 2.64 | 88 (61%) 0 0 | 98, 160, 210, 264 | 0 |
| 63 | C7 | 115/136 (84%) | 1.68 | 41 (35%) 0 0 | 109, 149, 191, 223 | 0 |
| 63 | c7 | 117/136 (86%) | 1.02 | 18 (15%) 2 2 | 104, 152, 200, 226 | 0 |
| 64 | C8 | 143/145 (98%) | 1.40 | 39 (27%) 0 0 | 104, 163, 211, 244 | 0 |
| 64 | c8 | 145/145 (100%) | 1.48 | 47 (32%) 0 0 | 103, 149, 197, 217 | 0 |
| 65 | C9 | 137/143 (95%) | 1.76 | 47 (34%) 0 0 | 104, 168, 206, 231 | 0 |
| 65 | c9 | 143/143 (100%) | 1.48 | 41 (28%) 0 0 | 117, 170, 215, 240 | 0 |
| 66 | D0 | 102/109 (93%) | 1.57 | 35 (34%) 0 0 | 92, 163, 218, 276 | 0 |
| 66 | d0 | 109/109 (100%) | 1.20 | 26 (23%) 0 0 | 91, 159, 218, 265 | 0 |
| 67 | D1 | 87/87 (100%) | 0.99 | 16 (18%) 1 1 | 101, 130, 167, 213 | 0 |
| 67 | d1 | 87/87 (100%) | 0.88 | 12 (13%) 2 2 | 101, 131, 176, 206 | 0 |
| 68 | D2 | 129/129 (100%) | 1.47 | 42 (32%) 0 0 | 73, 110, 134, 165 | 0 |
| 68 | d2 | 129/129 (100%) | 0.92 | 18 (13%) 2 2 | 85, 111, 133, 175 | 0 |
| 69 | D3 | 144/144 (100%) | 0.52 | 1 (0%) 87 88 | 63, 86, 109, 154 | 0 |
| 69 | d3 | 144/144 (100%) | 0.53 | 7 (4%) 29 27 | 61, 86, 107, 141 | 0 |
| 70 | D4 | 134/134 (100%) | 1.06 | 29 (21%) 0 1 | 106, 155, 191, 221 | 0 |
| 70 | d4 | 134/134 (100%) | 1.05 | 23 (17%) 1 1 | 100, 140, 175, 195 | 0 |
| 71 | D5 | 70/70 (100%) | 2.78 | 43 (61%) 0 0 | 137, 193, 229, 237 | 0 |
| 71 | d5 | 69/70 (98%) | 1.95 | 30 (43%) 0 0 | 131, 174, 211, 238 | 0 |
| 72 | D6 | 97/97 (100%) | 0.48 | 3 (3%) 49 48 | 67, 105, 176, 218 | 0 |
| 72 | d6 | 97/97 (100%) | 1.05 | 13 (13%) 3 3 | 79, 111, 173, 203 | 0 |
| 73 | D7 | 81/81 (100%) | 1.08 | 14 (17%) 1 1 | 84, 127, 181, 205 | 0 |
| 73 | d7 | 81/81 (100%) | 0.69 | 12 (14%) 2 2 | 96, 147, 202, 227 | 0 |
| 74 | D8 | 63/63 (100%) | 1.76 | 25 (39%) 0 0 | 114, 146, 173, 198 | 0 |
| 74 | d8 | 63/63 (100%) | 2.64 | 36 (57%) 0 0 | 110, 163, 192, 218 | 0 |
| 75 | D9 | 53/53 (100%) | 1.41 | 16 (30%) 0 0 | 101, 121, 151, 224 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 75 | d9 | 53/53 (100%) | 0.68 | 6 (11%) 5 5 | 106, 127, 150, 180 | 0 |
| 76 | E0 | 60/62 (96%) | 1.47 | 18 (30%) 0 0 | 76, 140, 183, 197 | 0 |
| 76 | e0 | 62/62 (100%) | 1.52 | 15 (24%) 0 0 | 74, 133, 181, 208 | 0 |
| 77 | SR | 317/318 (99%) | 2.50 | 184 (58%) 0 0 | 137, 198, 248, 295 | 0 |
| 77 | sR | 318/318 (100%) | 2.42 | 171 (53%) 0 0 | 136, 194, 243, 296 | 0 |
| 78 | SM | 147/272 (54%) | 1.18 | 30 (20%) 1 1 | 74, 137, 205, 240 | 0 |
| 78 | sM | 95/272 (34%) | 1.29 | 24 (25%) 0 0 | 99, 146, 191, 217 | 0 |
| 79 | s6 | 218/218 (100%) | 1.82 | 84 (38%) 0 0 | 75, 136, 176, 211 | 0 |
| All | All | 32255/33922 (95%) | 0.67 | 3409 (10%) 6 6 | 22, 100, 194, 318 | 0 |

All (3409) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 76 | e0 | 63 | GLN | 14.3 |
| 51 | S5 | 152 | GLY | 13.9 |
| 51 | S5 | 71 | ALA | 13.9 |
| 51 | S5 | 151 | GLY | 12.3 |
| 51 | S5 | 70 | VAL | 11.1 |
| 77 | SR | 79 | TYR | 10.9 |
| 78 | SM | 141 | ALA | 10.8 |
| 77 | SR | 244 | ALA | 10.2 |
| 12 | m0 | 104 | SER | 9.9 |
| 62 | c6 | 6 | SER | 9.9 |
| 62 | c6 | 60 | PHE | 9.7 |
| 53 | s7 | 3 | ALA | 9.6 |
| 77 | sR | 50 | ASP | 9.3 |
| 78 | SM | 16 | ASP | 9.3 |
| 77 | SR | 121 | MET | 9.2 |
| 61 | c5 | 134 | THR | 9.1 |
| 12 | m0 | 105 | CYS | 9.1 |
| 48 | s2 | 93 | GLY | 9.1 |
| 77 | SR | 81 | LEU | 8.7 |
| 48 | s2 | 92 | ALA | 8.7 |
| 58 | c2 | 110 | GLY | 8.6 |
| 58 | c2 | 111 | ASN | 8.5 |
| 58 | C2 | 63 | VAL | 8.4 |
| 25 | n4 | 131 | ALA | 8.4 |
| 65 | c9 | 3 | GLY | 8.4 |
| 37 | o6 | 98 | ARG | 8.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 58 | C2 | 82 | PRO | 8.3 |
| 45 | 2 | 134 | U | 8.2 |
| 77 | sR | 158 | PRO | 8.2 |
| 45 | 2 | 135 | A | 8.1 |
| 77 | sR | 51 | ASP | 8.1 |
| 57 | c1 | 2 | SER | 8.0 |
| 77 | SR | 80 | ALA | 8.0 |
| 76 | E0 | 61 | SER | 7.9 |
| 47 | s1 | 92 | GLN | 7.9 |
| 77 | sR | 214 | ALA | 7.9 |
| 47 | S1 | 91 | VAL | 7.8 |
| 65 | c9 | 2 | PRO | 7.7 |
| 47 | s1 | 100 | PHE | 7.7 |
| 47 | s1 | 84 | ILE | 7.6 |
| 77 | sR | 16 | HIS | 7.6 |
| 77 | sR | 157 | VAL | 7.6 |
| 77 | sR | 311 | ARG | 7.6 |
| 77 | SR | 253 | ALA | 7.6 |
| 61 | c5 | 135 | THR | 7.5 |
| 77 | SR | 211 | ILE | 7.4 |
| 50 | S4 | 47 | PHE | 7.4 |
| 25 | n4 | 132 | GLY | 7.3 |
| 77 | SR | 73 | LEU | 7.2 |
| 61 | c5 | 136 | SER | 7.2 |
| 53 | s7 | 2 | SER | 7.1 |
| 62 | c6 | 51 | PRO | 7.1 |
| 38 | o7 | 87 | SER | 7.1 |
| 77 | sR | 5 | GLU | 7.0 |
| 79 | s6 | 158 | ILE | 7.0 |
| 51 | S5 | 20 | PHE | 7.0 |
| 60 | c4 | 14 | PHE | 6.9 |
| 55 | S9 | 147 | MET | 6.9 |
| 74 | d8 | 54 | LEU | 6.9 |
| 62 | C6 | 41 | PRO | 6.9 |
| 51 | S5 | 119 | ASP | 6.9 |
| 77 | sR | 55 | GLY | 6.9 |
| 76 | e0 | 62 | VAL | 6.8 |
| 61 | c5 | 119 | PHE | 6.8 |
| 50 | s4 | 261 | LEU | 6.8 |
| 70 | D4 | 7 | ILE | 6.8 |
| 74 | d8 | 55 | VAL | 6.8 |
| 25 | n4 | 135 | SER | 6.8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 61 | c5 | 138 | PHE | 6.8 |
| 65 | c9 | 4 | VAL | 6.8 |
| 58 | C2 | 61 | VAL | 6.7 |
| 77 | sR | 253 | ALA | 6.7 |
| 76 | E0 | 48 | THR | 6.7 |
| 62 | c6 | 83 | GLN | 6.7 |
| 47 | S1 | 92 | GLN | 6.7 |
| 58 | c2 | 112 | ALA | 6.6 |
| 62 | c6 | 7 | VAL | 6.6 |
| 70 | D4 | 2 | SER | 6.5 |
| 77 | SR | 122 | ILE | 6.5 |
| 62 | C6 | 65 | ILE | 6.5 |
| 74 | d8 | 65 | ARG | 6.5 |
| 77 | SR | 115 | ILE | 6.4 |
| 62 | C6 | 66 | ARG | 6.4 |
| 53 | s7 | 7 | LYS | 6.4 |
| 77 | sR | 34 | LEU | 6.4 |
| 51 | S5 | 54 | LYS | 6.4 |
| 18 | M7 | 177 | ALA | 6.4 |
| 51 | S5 | 32 | GLU | 6.4 |
| 62 | C6 | 52 | LEU | 6.3 |
| 77 | SR | 72 | THR | 6.3 |
| 62 | c6 | 12 | LYS | 6.3 |
| 61 | c5 | 133 | ALA | 6.3 |
| 66 | d0 | 84 | MET | 6.3 |
| 79 | s6 | 156 | PHE | 6.3 |
| 47 | S1 | 217 | LEU | 6.3 |
| 77 | SR | 225 | LEU | 6.2 |
| 61 | c5 | 112 | LEU | 6.2 |
| 47 | s1 | 139 | ALA | 6.2 |
| 77 | sR | 15 | GLY | 6.2 |
| 41 | Q0 | 77 | ILE | 6.2 |
| 56 | c0 | 96 | ASN | 6.2 |
| 77 | SR | 210 | LEU | 6.2 |
| 62 | C6 | 29 | ILE | 6.2 |
| 51 | S5 | 170 | GLN | 6.2 |
| 58 | C2 | 62 | LEU | 6.2 |
| 79 | s6 | 157 | VAL | 6.2 |
| 49 | s3 | 184 | ILE | 6.1 |
| 76 | e0 | 2 | ALA | 6.1 |
| 53 | s7 | 5 | GLN | 6.1 |
| 74 | d8 | 53 | ILE | 6.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | s1 | 235 | GLY | 6.1 |
| 25 | n4 | 64 | THR | 6.1 |
| 65 | c9 | 18 | TYR | 6.1 |
| 78 | SM | 17 | VAL | 6.1 |
| 53 | s7 | 63 | PRO | 6.1 |
| 21 | N0 | 1 | MET | 6.1 |
| 58 | C2 | 60 | VAL | 6.0 |
| 77 | SR | 119 | ALA | 6.0 |
| 77 | sR | 167 | VAL | 6.0 |
| 77 | sR | 204 | ALA | 6.0 |
| 62 | C6 | 40 | GLU | 6.0 |
| 77 | sR | 244 | ALA | 6.0 |
| 77 | sR | 252 | LEU | 6.0 |
| 77 | sR | 168 | THR | 6.0 |
| 77 | sR | 295 | SER | 6.0 |
| 62 | c6 | 66 | ARG | 6.0 |
| 77 | sR | 293 | ALA | 5.9 |
| 77 | sR | 300 | THR | 5.9 |
| 64 | C8 | 47 | CYS | 5.9 |
| 7 | l5 | 185 | PHE | 5.9 |
| 78 | sM | 53 | ARG | 5.9 |
| 51 | S5 | 184 | PHE | 5.9 |
| 50 | s4 | 229 | GLY | 5.9 |
| 61 | c5 | 105 | VAL | 5.9 |
| 78 | sM | 52 | PRO | 5.9 |
| 78 | SM | 18 | VAL | 5.8 |
| 77 | sR | 24 | ALA | 5.8 |
| 70 | d4 | 135 | ASP | 5.8 |
| 71 | D5 | 91 | PRO | 5.8 |
| 18 | M7 | 169 | THR | 5.8 |
| 72 | d6 | 40 | ALA | 5.8 |
| 77 | SR | 284 | ALA | 5.8 |
| 78 | SM | 88 | ARG | 5.8 |
| 61 | c5 | 137 | ARG | 5.8 |
| 7 | L5 | 154 | THR | 5.7 |
| 55 | s9 | 2 | PRO | 5.7 |
| 29 | n8 | 79 | TRP | 5.7 |
| 51 | S5 | 78 | ALA | 5.7 |
| 61 | c5 | 104 | GLN | 5.7 |
| 46 | s0 | 36 | TYR | 5.7 |
| 77 | SR | 74 | THR | 5.6 |
| 7 | L5 | 4 | GLN | 5.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 62 | C6 | 117 | LEU | 5.6 |
| 77 | sR | 301 | LEU | 5.6 |
| 74 | d8 | 48 | VAL | 5.6 |
| 47 | s1 | 102 | GLY | 5.6 |
| 51 | S5 | 72 | HIS | 5.6 |
| 77 | sR | 299 | GLN | 5.6 |
| 77 | SR | 134 | TRP | 5.6 |
| 71 | D5 | 60 | VAL | 5.6 |
| 50 | S4 | 103 | TYR | 5.6 |
| 45 | 2 | 194 | U | 5.6 |
| 52 | S6 | 80 | ASN | 5.6 |
| 51 | S5 | 51 | VAL | 5.6 |
| 74 | d8 | 28 | VAL | 5.6 |
| 71 | D5 | 36 | ALA | 5.6 |
| 62 | C6 | 28 | LEU | 5.6 |
| 50 | S4 | 54 | TYR | 5.5 |
| 74 | d8 | 27 | GLN | 5.5 |
| 56 | c0 | 97 | PRO | 5.5 |
| 62 | C6 | 10 | PHE | 5.5 |
| 65 | C9 | 143 | ASP | 5.5 |
| 70 | D4 | 72 | PHE | 5.5 |
| 77 | sR | 3 | SER | 5.5 |
| 62 | C6 | 21 | HIS | 5.5 |
| 78 | sM | 61 | ILE | 5.5 |
| 56 | c0 | 98 | THR | 5.5 |
| 61 | c5 | 75 | PRO | 5.5 |
| 10 | l8 | 49 | TYR | 5.5 |
| 46 | S0 | 201 | LEU | 5.5 |
| 51 | S5 | 90 | ILE | 5.5 |
| 71 | D5 | 41 | ILE | 5.5 |
| 71 | D5 | 80 | LEU | 5.5 |
| 77 | sR | 183 | LEU | 5.5 |
| 78 | sM | 60 | ALA | 5.5 |
| 62 | c6 | 22 | VAL | 5.4 |
| 62 | c6 | 29 | ILE | 5.4 |
| 64 | c8 | 22 | VAL | 5.4 |
| 28 | n7 | 136 | PHE | 5.4 |
| 51 | s5 | 71 | ALA | 5.4 |
| 45 | 2 | 1361 | U | 5.4 |
| 58 | c2 | 102 | GLY | 5.4 |
| 51 | s5 | 31 | GLU | 5.4 |
| 77 | sR | 319 | ASN | 5.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | sR | 33 | LEU | 5.4 |
| 25 | n4 | 97 | LYS | 5.4 |
| 50 | S4 | 190 | GLY | 5.4 |
| 64 | C8 | 53 | ASP | 5.4 |
| 74 | d8 | 67 | ARG | 5.4 |
| 56 | c0 | 20 | VAL | 5.4 |
| 79 | s6 | 169 | TYR | 5.4 |
| 48 | s2 | 95 | ARG | 5.4 |
| 71 | D5 | 102 | THR | 5.4 |
| 55 | S9 | 148 | VAL | 5.3 |
| 77 | SR | 120 | SER | 5.3 |
| 58 | c2 | 31 | VAL | 5.3 |
| 48 | s2 | 89 | GLN | 5.3 |
| 49 | s3 | 48 | VAL | 5.3 |
| 64 | c8 | 146 | ALA | 5.3 |
| 61 | c5 | 93 | VAL | 5.3 |
| 77 | SR | 181 | TRP | 5.3 |
| 77 | sR | 159 | ASN | 5.3 |
| 25 | n4 | 134 | GLN | 5.3 |
| 77 | sR | 6 | VAL | 5.3 |
| 79 | s6 | 147 | LEU | 5.3 |
| 79 | s6 | 145 | PHE | 5.2 |
| 38 | o7 | 88 | ALA | 5.2 |
| 49 | s3 | 186 | VAL | 5.2 |
| 77 | sR | 315 | VAL | 5.2 |
| 51 | S5 | 21 | THR | 5.2 |
| 71 | D5 | 59 | TYR | 5.2 |
| 49 | s3 | 188 | ILE | 5.2 |
| 65 | c9 | 10 | ALA | 5.2 |
| 62 | C6 | 12 | LYS | 5.2 |
| 31 | o0 | 7 | GLN | 5.2 |
| 47 | s1 | 223 | PHE | 5.2 |
| 71 | D5 | 71 | ILE | 5.2 |
| 62 | c6 | 89 | LEU | 5.2 |
| 58 | C2 | 59 | LEU | 5.2 |
| 51 | S5 | 190 | ILE | 5.2 |
| 4 | l2 | 249 | SER | 5.2 |
| 64 | c8 | 73 | MET | 5.2 |
| 55 | S9 | 6 | ARG | 5.2 |
| 74 | d8 | 26 | THR | 5.2 |
| 77 | SR | 252 | LEU | 5.2 |
| 47 | s1 | 90 | GLU | 5.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | S5 | 153 | GLY | 5.2 |
| 77 | SR | 26 | SER | 5.1 |
| 62 | C6 | 22 | VAL | 5.1 |
| 61 | C5 | 87 | PRO | 5.1 |
| 62 | C6 | 26 | LYS | 5.1 |
| 64 | c8 | 131 | LEU | 5.1 |
| 11 | l9 | 190 | ASP | 5.1 |
| 77 | sR | 245 | PHE | 5.1 |
| 47 | s1 | 103 | MET | 5.1 |
| 49 | s3 | 150 | MET | 5.1 |
| 77 | SR | 168 | THR | 5.1 |
| 60 | c4 | 15 | GLY | 5.1 |
| 62 | C6 | 7 | VAL | 5.1 |
| 53 | s7 | 6 | ALA | 5.1 |
| 71 | d5 | 101 | TYR | 5.1 |
| 10 | l8 | 200 | LEU | 5.1 |
| 49 | s3 | 30 | ALA | 5.1 |
| 62 | C6 | 138 | PHE | 5.1 |
| 51 | S5 | 25 | LEU | 5.1 |
| 53 | s7 | 70 | PHE | 5.1 |
| 74 | d8 | 29 | ARG | 5.1 |
| 51 | S5 | 93 | LEU | 5.1 |
| 36 | O5 | 120 | ALA | 5.1 |
| 62 | C6 | 11 | GLY | 5.1 |
| 58 | C2 | 93 | ASP | 5.0 |
| 77 | SR | 83 | ALA | 5.0 |
| 49 | S3 | 170 | THR | 5.0 |
| 62 | C6 | 42 | GLU | 5.0 |
| 71 | D5 | 97 | LYS | 5.0 |
| 43 | Q2 | 104 | LEU | 5.0 |
| 51 | s5 | 152 | GLY | 5.0 |
| 77 | sR | 7 | LEU | 5.0 |
| 77 | sR | 211 | ILE | 5.0 |
| 78 | SM | 19 | VAL | 5.0 |
| 20 | m9 | 185 | LEU | 5.0 |
| 77 | SR | 116 | ASP | 5.0 |
| 53 | s7 | 8 | ILE | 5.0 |
| 61 | c5 | 78 | THR | 5.0 |
| 79 | s6 | 22 | HIS | 5.0 |
| 61 | c5 | 121 | ILE | 5.0 |
| 50 | S4 | 123 | LEU | 5.0 |
| 47 | s1 | 101 | HIS | 5.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 65 | C9 | 108 | LEU | 5.0 |
| 46 | S0 | 20 | ALA | 5.0 |
| 64 | c8 | 21 | ASN | 5.0 |
| 79 | s6 | 141 | ILE | 5.0 |
| 63 | C7 | 70 | SER | 5.0 |
| 63 | C7 | 71 | PHE | 5.0 |
| 70 | d4 | 25 | VAL | 5.0 |
| 60 | c4 | 98 | GLY | 5.0 |
| 51 | S5 | 62 | VAL | 5.0 |
| 51 | s5 | 70 | VAL | 5.0 |
| 62 | C6 | 36 | ILE | 5.0 |
| 47 | s1 | 227 | ALA | 4.9 |
| 55 | s9 | 80 | LEU | 4.9 |
| 62 | c6 | 127 | LYS | 4.9 |
| 62 | C6 | 20 | ALA | 4.9 |
| 58 | c2 | 32 | LEU | 4.9 |
| 1 | 5 | 1350 | A | 4.9 |
| 63 | C7 | 21 | TYR | 4.9 |
| 58 | C2 | 28 | LEU | 4.9 |
| 37 | o6 | 97 | SER | 4.9 |
| 51 | S5 | 24 | VAL | 4.9 |
| 66 | D0 | 21 | LYS | 4.9 |
| 66 | D0 | 91 | ILE | 4.9 |
| 79 | s6 | 1 | MET | 4.9 |
| 62 | c6 | 27 | GLY | 4.9 |
| 47 | s1 | 48 | VAL | 4.9 |
| 70 | d4 | 119 | PHE | 4.9 |
| 77 | SR | 302 | PHE | 4.9 |
| 53 | S7 | 47 | ARG | 4.9 |
| 77 | SR | 141 | LEU | 4.9 |
| 78 | sM | 57 | ASN | 4.9 |
| 37 | o6 | 79 | SER | 4.9 |
| 71 | D5 | 104 | ALA | 4.9 |
| 72 | d6 | 39 | MET | 4.9 |
| 48 | s2 | 90 | THR | 4.9 |
| 77 | SR | 183 | LEU | 4.9 |
| 58 | C2 | 42 | ALA | 4.9 |
| 77 | sR | 4 | ASN | 4.9 |
| 65 | c9 | 55 | TYR | 4.9 |
| 77 | SR | 32 | LEU | 4.8 |
| 70 | d4 | 74 | LEU | 4.8 |
| 77 | SR | 314 | GLN | 4.8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 13 | m1 | 104 | PHE | 4.8 |
| 61 | c5 | 103 | ASN | 4.8 |
| 77 | sR | 294 | TRP | 4.8 |
| 68 | D2 | 108 | ALA | 4.8 |
| 64 | c8 | 15 | LEU | 4.8 |
| 61 | c5 | 132 | GLY | 4.8 |
| 47 | S1 | 87 | ARG | 4.8 |
| 58 | c2 | 33 | ARG | 4.8 |
| 77 | sR | 62 | LYS | 4.8 |
| 12 | m0 | 106 | ALA | 4.8 |
| 14 | M3 | 135 | ALA | 4.8 |
| 50 | S4 | 188 | ASN | 4.8 |
| 77 | SR | 227 | ALA | 4.8 |
| 74 | d8 | 66 | LEU | 4.8 |
| 47 | S1 | 101 | HIS | 4.8 |
| 51 | s5 | 100 | ASN | 4.8 |
| 51 | S5 | 77 | TYR | 4.8 |
| 47 | S1 | 61 | LEU | 4.8 |
| 74 | D8 | 67 | ARG | 4.7 |
| 77 | SR | 124 | SER | 4.7 |
| 50 | S4 | 100 | ARG | 4.7 |
| 51 | S5 | 33 | VAL | 4.7 |
| 77 | sR | 121 | MET | 4.7 |
| 78 | SM | 84 | LYS | 4.7 |
| 71 | D5 | 101 | TYR | 4.7 |
| 61 | c5 | 102 | PHE | 4.7 |
| 45 | 2 | 1360 | A | 4.7 |
| 71 | D5 | 103 | ARG | 4.7 |
| 57 | c1 | 3 | THR | 4.7 |
| 47 | S1 | 96 | LEU | 4.7 |
| 77 | sR | 52 | GLN | 4.7 |
| 78 | SM | 86 | ASN | 4.7 |
| 79 | s6 | 131 | LYS | 4.7 |
| 77 | sR | 144 | LEU | 4.7 |
| 62 | c6 | 141 | SER | 4.7 |
| 28 | n7 | 92 | PHE | 4.7 |
| 47 | s1 | 91 | VAL | 4.7 |
| 49 | S3 | 184 | ILE | 4.7 |
| 65 | c9 | 9 | VAL | 4.7 |
| 20 | m9 | 187 | GLU | 4.7 |
| 55 | s9 | 134 | ILE | 4.7 |
| 65 | c9 | 14 | PHE | 4.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 75 | D9 | 54 | LYS | 4.7 |
| 46 | S0 | 28 | ASN | 4.7 |
| 58 | c2 | 84 | ASN | 4.7 |
| 64 | C8 | 32 | LEU | 4.7 |
| 25 | n4 | 98 | PRO | 4.7 |
| 62 | C6 | 87 | LYS | 4.7 |
| 1 | 5 | 1349 | G | 4.7 |
| 62 | C6 | 57 | LEU | 4.7 |
| 56 | c0 | 25 | LYS | 4.7 |
| 65 | C9 | 124 | ILE | 4.6 |
| 61 | c5 | 116 | LEU | 4.6 |
| 52 | S6 | 36 | VAL | 4.6 |
| 71 | d5 | 54 | VAL | 4.6 |
| 29 | n8 | 102 | ILE | 4.6 |
| 25 | n4 | 67 | VAL | 4.6 |
| 63 | c7 | 2 | GLY | 4.6 |
| 51 | S5 | 48 | PHE | 4.6 |
| 77 | sR | 220 | ILE | 4.6 |
| 49 | s3 | 178 | ARG | 4.6 |
| 71 | D5 | 69 | LEU | 4.6 |
| 71 | D5 | 100 | ILE | 4.6 |
| 51 | S5 | 37 | GLN | 4.6 |
| 77 | sR | 302 | PHE | 4.6 |
| 77 | sR | 292 | LEU | 4.6 |
| 45 | 6 | 226 | A | 4.6 |
| 77 | SR | 185 | GLN | 4.6 |
| 47 | s1 | 73 | LEU | 4.6 |
| 49 | s3 | 53 | THR | 4.6 |
| 62 | c6 | 9 | THR | 4.6 |
| 74 | D8 | 24 | GLY | 4.6 |
| 51 | S5 | 199 | ILE | 4.6 |
| 62 | C6 | 24 | ALA | 4.6 |
| 47 | S1 | 97 | LEU | 4.6 |
| 25 | n4 | 100 | VAL | 4.6 |
| 77 | SR | 123 | ILE | 4.5 |
| 77 | sR | 71 | CYS | 4.5 |
| 25 | n4 | 65 | GLU | 4.5 |
| 64 | c8 | 129 | TRP | 4.5 |
| 77 | sR | 56 | VAL | 4.5 |
| 37 | o6 | 2 | THR | 4.5 |
| 62 | c6 | 28 | LEU | 4.5 |
| 68 | D2 | 69 | LEU | 4.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | SR | 172 | ALA | 4.5 |
| 77 | SR | 254 | ALA | 4.5 |
| 79 | s6 | 155 | ASP | 4.5 |
| 58 | c2 | 88 | LEU | 4.5 |
| 71 | D5 | 93 | SER | 4.5 |
| 51 | S5 | 69 | PHE | 4.5 |
| 77 | sR | 191 | ASP | 4.5 |
| 62 | c6 | 116 | LEU | 4.5 |
| 79 | s6 | 108 | VAL | 4.5 |
| 78 | SM | 15 | ALA | 4.5 |
| 63 | C7 | 55 | THR | 4.5 |
| 1 | 5 | 1353 | U | 4.5 |
| 45 | 6 | 238 | U | 4.5 |
| 79 | s6 | 142 | ARG | 4.5 |
| 77 | SR | 25 | THR | 4.5 |
| 76 | E0 | 45 | VAL | 4.5 |
| 77 | sR | 257 | ALA | 4.5 |
| 53 | S7 | 48 | GLU | 4.5 |
| 46 | s0 | 33 | GLN | 4.5 |
| 61 | c5 | 111 | MET | 4.5 |
| 62 | c6 | 114 | ARG | 4.4 |
| 64 | c8 | 16 | ARG | 4.4 |
| 70 | d4 | 26 | ASP | 4.4 |
| 62 | C6 | 85 | ILE | 4.4 |
| 77 | sR | 63 | GLY | 4.4 |
| 50 | S4 | 219 | VAL | 4.4 |
| 77 | SR | 62 | LYS | 4.4 |
| 77 | SR | 118 | LYS | 4.4 |
| 58 | c2 | 37 | VAL | 4.4 |
| 74 | d8 | 14 | LYS | 4.4 |
| 51 | S5 | 47 | SER | 4.4 |
| 51 | S5 | 118 | LEU | 4.4 |
| 46 | S0 | 107 | PHE | 4.4 |
| 56 | c0 | 65 | TYR | 4.4 |
| 71 | d5 | 41 | ILE | 4.4 |
| 55 | S9 | 133 | HIS | 4.4 |
| 53 | s7 | 43 | PHE | 4.4 |
| 64 | C8 | 98 | TYR | 4.4 |
| 78 | sM | 62 | ARG | 4.4 |
| 77 | SR | 91 | LEU | 4.4 |
| 77 | SR | 226 | ALA | 4.4 |
| 79 | s6 | 143 | LYS | 4.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 58 | C2 | 91 | VAL | 4.4 |
| 51 | S5 | 50 | GLU | 4.4 |
| 51 | S5 | 100 | ASN | 4.4 |
| 55 | s9 | 156 | ILE | 4.4 |
| 7 | L5 | 5 | LYS | 4.4 |
| 71 | D5 | 42 | LEU | 4.3 |
| 50 | S4 | 191 | ARG | 4.3 |
| 79 | s6 | 144 | PHE | 4.3 |
| 25 | n4 | 81 | PRO | 4.3 |
| 49 | s3 | 183 | GLY | 4.3 |
| 46 | s0 | 107 | PHE | 4.3 |
| 54 | S8 | 179 | CYS | 4.3 |
| 72 | d6 | 41 | ILE | 4.3 |
| 78 | sM | 69 | ARG | 4.3 |
| 61 | c5 | 79 | HIS | 4.3 |
| 49 | s3 | 35 | SER | 4.3 |
| 77 | SR | 3 | SER | 4.3 |
| 65 | C9 | 71 | VAL | 4.3 |
| 70 | d4 | 18 | LEU | 4.3 |
| 49 | s3 | 218 | LEU | 4.3 |
| 51 | S5 | 108 | LEU | 4.3 |
| 70 | d4 | 69 | SER | 4.3 |
| 7 | L5 | 3 | PHE | 4.3 |
| 62 | c6 | 93 | HIS | 4.3 |
| 20 | m9 | 186 | LYS | 4.3 |
| 43 | Q2 | 2 | VAL | 4.3 |
| 61 | c5 | 95 | GLY | 4.3 |
| 62 | C6 | 55 | VAL | 4.3 |
| 31 | O0 | 105 | ALA | 4.3 |
| 77 | SR | 13 | LEU | 4.3 |
| 55 | s9 | 148 | VAL | 4.3 |
| 49 | s3 | 34 | TYR | 4.3 |
| 77 | SR | 313 | TRP | 4.3 |
| 29 | N8 | 92 | LYS | 4.3 |
| 76 | E0 | 36 | LYS | 4.3 |
| 70 | d4 | 2 | SER | 4.3 |
| 71 | d5 | 57 | TYR | 4.3 |
| 51 | S5 | 175 | LEU | 4.3 |
| 47 | S1 | 213 | ARG | 4.3 |
| 62 | c6 | 86 | ALA | 4.3 |
| 65 | C9 | 59 | ALA | 4.3 |
| 62 | C6 | 79 | TYR | 4.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | sR | 313 | TRP | 4.3 |
| 47 | S1 | 60 | ALA | 4.3 |
| 52 | S6 | 78 | THR | 4.2 |
| 62 | c6 | 92 | TYR | 4.2 |
| 46 | S0 | 57 | LEU | 4.2 |
| 62 | C6 | 116 | LEU | 4.2 |
| 22 | n1 | 67 | VAL | 4.2 |
| 71 | d5 | 60 | VAL | 4.2 |
| 74 | d8 | 44 | VAL | 4.2 |
| 62 | c6 | 54 | LEU | 4.2 |
| 70 | D4 | 22 | GLN | 4.2 |
| 62 | c6 | 36 | ILE | 4.2 |
| 70 | d4 | 27 | VAL | 4.2 |
| 28 | n7 | 10 | VAL | 4.2 |
| 65 | C9 | 88 | VAL | 4.2 |
| 77 | sR | 316 | MET | 4.2 |
| 48 | s2 | 88 | LYS | 4.2 |
| 51 | S5 | 155 | ALA | 4.2 |
| 48 | s2 | 150 | GLN | 4.2 |
| 51 | S5 | 130 | ILE | 4.2 |
| 51 | S5 | 147 | THR | 4.2 |
| 77 | sR | 20 | VAL | 4.2 |
| 77 | sR | 251 | TRP | 4.2 |
| 48 | s2 | 82 | ASN | 4.2 |
| 61 | c5 | 77 | ARG | 4.2 |
| 79 | s6 | 153 | VAL | 4.2 |
| 62 | c6 | 85 | ILE | 4.2 |
| 77 | SR | 136 | ILE | 4.2 |
| 56 | c0 | 57 | THR | 4.2 |
| 53 | S7 | 142 | TYR | 4.2 |
| 49 | s3 | 52 | ALA | 4.2 |
| 58 | c2 | 41 | LEU | 4.2 |
| 61 | c5 | 56 | PHE | 4.2 |
| 62 | C6 | 39 | VAL | 4.2 |
| 58 | c2 | 136 | ILE | 4.2 |
| 61 | C5 | 85 | ILE | 4.2 |
| 56 | c0 | 75 | TYR | 4.2 |
| 78 | sM | 55 | SER | 4.2 |
| 62 | C6 | 81 | ILE | 4.2 |
| 71 | D5 | 88 | ILE | 4.2 |
| 77 | sR | 262 | VAL | 4.2 |
| 62 | C6 | 51 | PRO | 4.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | n4 | 75 | THR | 4.2 |
| 48 | s2 | 94 | GLN | 4.1 |
| 70 | d4 | 98 | GLU | 4.1 |
| 68 | d2 | 101 | TYR | 4.1 |
| 66 | D0 | 52 | LYS | 4.1 |
| 47 | S1 | 98 | THR | 4.1 |
| 77 | SR | 7 | LEU | 4.1 |
| 50 | s4 | 260 | GLY | 4.1 |
| 62 | C6 | 49 | TYR | 4.1 |
| 62 | C6 | 43 | ILE | 4.1 |
| 77 | sR | 263 | PHE | 4.1 |
| 46 | s0 | 158 | VAL | 4.1 |
| 56 | c0 | 21 | VAL | 4.1 |
| 77 | SR | 63 | GLY | 4.1 |
| 51 | s5 | 68 | ILE | 4.1 |
| 10 | l8 | 34 | PHE | 4.1 |
| 51 | S5 | 179 | ALA | 4.1 |
| 77 | SR | 212 | ALA | 4.1 |
| 10 | l8 | 118 | GLU | 4.1 |
| 56 | c0 | 95 | ARG | 4.1 |
| 62 | C6 | 60 | PHE | 4.1 |
| 79 | s6 | 27 | PHE | 4.1 |
| 71 | D5 | 40 | VAL | 4.1 |
| 13 | m1 | 65 | ILE | 4.1 |
| 77 | SR | 82 | SER | 4.1 |
| 50 | S4 | 65 | LEU | 4.1 |
| 61 | c5 | 86 | VAL | 4.1 |
| 79 | s6 | 91 | GLU | 4.1 |
| 45 | 2 | 136 | C | 4.1 |
| 46 | S0 | 177 | LEU | 4.1 |
| 62 | c6 | 35 | PRO | 4.1 |
| 60 | c4 | 21 | ALA | 4.1 |
| 71 | D5 | 99 | ALA | 4.1 |
| 61 | c5 | 5 | VAL | 4.1 |
| 78 | SM | 61 | ILE | 4.1 |
| 49 | s3 | 142 | LEU | 4.1 |
| 50 | S4 | 101 | LEU | 4.1 |
| 51 | S5 | 174 | LEU | 4.1 |
| 79 | s6 | 178 | LEU | 4.1 |
| 68 | d2 | 85 | ASP | 4.1 |
| 61 | C5 | 61 | ARG | 4.1 |
| 47 | s1 | 38 | PHE | 4.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | S1 | 211 | HIS | 4.1 |
| 25 | n4 | 78 | ALA | 4.0 |
| 62 | c6 | 132 | LYS | 4.0 |
| 66 | D0 | 80 | GLU | 4.0 |
| 74 | D8 | 19 | THR | 4.0 |
| 79 | s6 | 34 | GLN | 4.0 |
| 65 | C9 | 76 | LEU | 4.0 |
| 25 | n4 | 133 | THR | 4.0 |
| 45 | 2 | 1362 | U | 4.0 |
| 77 | sR | 156 | VAL | 4.0 |
| 77 | SR | 165 | ASP | 4.0 |
| 77 | SR | 251 | TRP | 4.0 |
| 64 | C8 | 6 | GLN | 4.0 |
| 77 | SR | 235 | SER | 4.0 |
| 49 | s3 | 148 | LYS | 4.0 |
| 51 | s5 | 20 | PHE | 4.0 |
| 50 | S4 | 181 | VAL | 4.0 |
| 51 | S5 | 181 | GLU | 4.0 |
| 62 | C6 | 50 | GLU | 4.0 |
| 51 | s5 | 150 | GLY | 4.0 |
| 65 | c9 | 132 | LEU | 4.0 |
| 66 | D0 | 64 | LYS | 4.0 |
| 47 | S1 | 135 | LEU | 4.0 |
| 47 | s1 | 55 | LYS | 4.0 |
| 73 | d7 | 33 | LEU | 4.0 |
| 62 | C6 | 92 | TYR | 4.0 |
| 66 | d0 | 82 | TYR | 4.0 |
| 77 | SR | 186 | PHE | 4.0 |
| 49 | S3 | 206 | VAL | 4.0 |
| 79 | s6 | 90 | GLY | 4.0 |
| 1 | 5 | 1565 | G | 4.0 |
| 46 | S0 | 50 | VAL | 4.0 |
| 60 | c4 | 13 | VAL | 4.0 |
| 77 | sR | 280 | GLY | 4.0 |
| 51 | s5 | 58 | LEU | 4.0 |
| 29 | n8 | 124 | ILE | 4.0 |
| 62 | C6 | 23 | LYS | 4.0 |
| 10 | l8 | 117 | ALA | 4.0 |
| 64 | c8 | 17 | LEU | 4.0 |
| 53 | s7 | 92 | PHE | 4.0 |
| 25 | n4 | 130 | SER | 4.0 |
| 18 | M7 | 167 | ARG | 4.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | S5 | 156 | ARG | 4.0 |
| 48 | s2 | 87 | GLN | 4.0 |
| 46 | S0 | 54 | TRP | 4.0 |
| 51 | S5 | 133 | VAL | 4.0 |
| 65 | c9 | 58 | ALA | 4.0 |
| 64 | C8 | 46 | VAL | 3.9 |
| 50 | S4 | 124 | GLY | 3.9 |
| 66 | d0 | 63 | LEU | 3.9 |
| 47 | s1 | 229 | MET | 3.9 |
| 70 | D4 | 68 | LYS | 3.9 |
| 47 | s1 | 123 | ALA | 3.9 |
| 61 | c5 | 54 | ALA | 3.9 |
| 74 | d8 | 13 | ILE | 3.9 |
| 77 | sR | 291 | SER | 3.9 |
| 45 | 2 | 132 | U | 3.9 |
| 70 | D4 | 70 | VAL | 3.9 |
| 73 | D7 | 68 | GLY | 3.9 |
| 53 | s7 | 11 | GLN | 3.9 |
| 55 | S9 | 128 | LEU | 3.9 |
| 7 | L5 | 231 | ILE | 3.9 |
| 13 | m1 | 106 | ILE | 3.9 |
| 55 | S9 | 134 | ILE | 3.9 |
| 61 | c5 | 125 | PRO | 3.9 |
| 65 | C9 | 135 | ILE | 3.9 |
| 66 | D0 | 65 | ILE | 3.9 |
| 77 | sR | 279 | ALA | 3.9 |
| 51 | S5 | 145 | ASP | 3.9 |
| 66 | D0 | 53 | LYS | 3.9 |
| 55 | S9 | 156 | ILE | 3.9 |
| 61 | C5 | 130 | ARG | 3.9 |
| 62 | C6 | 54 | LEU | 3.9 |
| 48 | S2 | 97 | ARG | 3.9 |
| 55 | S9 | 85 | VAL | 3.9 |
| 61 | C5 | 86 | VAL | 3.9 |
| 66 | d0 | 87 | HIS | 3.9 |
| 79 | s6 | 109 | LEU | 3.9 |
| 62 | C6 | 16 | ALA | 3.9 |
| 55 | S9 | 130 | THR | 3.9 |
| 62 | C6 | 132 | LYS | 3.9 |
| 68 | D2 | 110 | ILE | 3.9 |
| 77 | sR | 303 | ALA | 3.9 |
| 62 | C6 | 19 | VAL | 3.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 8 | 80 | A | 3.9 |
| 46 | S0 | 22 | THR | 3.9 |
| 62 | c6 | 37 | THR | 3.9 |
| 46 | s0 | 149 | LEU | 3.9 |
| 62 | c6 | 38 | LEU | 3.9 |
| 64 | C8 | 5 | VAL | 3.9 |
| 28 | n7 | 22 | LYS | 3.9 |
| 65 | c9 | 92 | LYS | 3.9 |
| 64 | c8 | 138 | THR | 3.9 |
| 39 | o8 | 14 | LEU | 3.9 |
| 50 | S4 | 25 | GLY | 3.9 |
| 46 | s0 | 48 | ILE | 3.9 |
| 28 | n7 | 23 | VAL | 3.9 |
| 53 | S7 | 93 | LEU | 3.9 |
| 60 | c4 | 102 | LEU | 3.9 |
| 62 | c6 | 87 | LYS | 3.9 |
| 74 | D8 | 66 | LEU | 3.9 |
| 46 | s0 | 161 | PRO | 3.9 |
| 63 | C7 | 35 | CYS | 3.9 |
| 56 | c0 | 66 | TYR | 3.8 |
| 61 | c5 | 97 | TYR | 3.8 |
| 10 | l8 | 254 | ASP | 3.8 |
| 77 | SR | 41 | THR | 3.8 |
| 77 | SR | 52 | GLN | 3.8 |
| 46 | s0 | 23 | HIS | 3.8 |
| 78 | SM | 87 | THR | 3.8 |
| 79 | s6 | 135 | PRO | 3.8 |
| 29 | N8 | 94 | ALA | 3.8 |
| 77 | sR | 73 | LEU | 3.8 |
| 49 | S3 | 208 | ILE | 3.8 |
| 51 | S5 | 138 | THR | 3.8 |
| 55 | S9 | 86 | LEU | 3.8 |
| 68 | D2 | 102 | VAL | 3.8 |
| 77 | sR | 162 | ALA | 3.8 |
| 62 | c6 | 104 | GLU | 3.8 |
| 62 | c6 | 61 | SER | 3.8 |
| 51 | s5 | 130 | ILE | 3.8 |
| 71 | D5 | 92 | ILE | 3.8 |
| 47 | S1 | 231 | LEU | 3.8 |
| 28 | n7 | 41 | ALA | 3.8 |
| 51 | s5 | 153 | GLY | 3.8 |
| 61 | c5 | 92 | SER | 3.8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 71 | d5 | 103 | ARG | 3.8 |
| 75 | D9 | 29 | GLY | 3.8 |
| 49 | s3 | 174 | HIS | 3.8 |
| 51 | S5 | 52 | GLU | 3.8 |
| 46 | S0 | 21 | ASN | 3.8 |
| 62 | C6 | 89 | LEU | 3.8 |
| 65 | C9 | 28 | LEU | 3.8 |
| 47 | S1 | 206 | PRO | 3.8 |
| 47 | s1 | 98 | THR | 3.8 |
| 63 | C7 | 8 | THR | 3.8 |
| 7 | l5 | 236 | LEU | 3.8 |
| 53 | s7 | 129 | LEU | 3.8 |
| 49 | S3 | 173 | ARG | 3.8 |
| 11 | L9 | 95 | ALA | 3.8 |
| 18 | M7 | 184 | ALA | 3.8 |
| 62 | c6 | 84 | ALA | 3.8 |
| 65 | c9 | 59 | ALA | 3.8 |
| 71 | d5 | 72 | GLY | 3.8 |
| 63 | C7 | 54 | THR | 3.8 |
| 71 | d5 | 102 | THR | 3.8 |
| 57 | c1 | 28 | SER | 3.8 |
| 27 | N6 | 126 | LEU | 3.8 |
| 47 | s1 | 137 | ILE | 3.8 |
| 61 | c5 | 107 | ILE | 3.8 |
| 50 | S4 | 183 | VAL | 3.8 |
| 1 | 5 | 1566 | A | 3.8 |
| 65 | c9 | 54 | PHE | 3.8 |
| 62 | C6 | 84 | ALA | 3.8 |
| 47 | s1 | 219 | LYS | 3.8 |
| 49 | s3 | 113 | LEU | 3.8 |
| 59 | C3 | 66 | ILE | 3.8 |
| 26 | n5 | 23 | ALA | 3.8 |
| 28 | n7 | 47 | GLU | 3.8 |
| 77 | SR | 106 | HIS | 3.8 |
| 77 | SR | 178 | VAL | 3.8 |
| 13 | M1 | 90 | GLN | 3.7 |
| 75 | d9 | 56 | ARG | 3.7 |
| 58 | C2 | 136 | ILE | 3.7 |
| 61 | c5 | 84 | ILE | 3.7 |
| 47 | S1 | 139 | ALA | 3.7 |
| 52 | S6 | 178 | LEU | 3.7 |
| 53 | s7 | 4 | PRO | 3.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 75 | D9 | 30 | LEU | 3.7 |
| 77 | SR | 54 | PHE | 3.7 |
| 24 | n3 | 2 | SER | 3.7 |
| 71 | d5 | 56 | THR | 3.7 |
| 77 | SR | 55 | GLY | 3.7 |
| 78 | SM | 69 | ARG | 3.7 |
| 48 | s2 | 199 | GLN | 3.7 |
| 50 | S4 | 182 | TYR | 3.7 |
| 57 | C1 | 35 | TYR | 3.7 |
| 58 | c2 | 28 | LEU | 3.7 |
| 64 | C8 | 17 | LEU | 3.7 |
| 79 | s6 | 77 | LEU | 3.7 |
| 50 | s4 | 109 | PHE | 3.7 |
| 76 | E0 | 47 | VAL | 3.7 |
| 20 | m9 | 181 | ARG | 3.7 |
| 25 | n4 | 93 | ARG | 3.7 |
| 57 | c1 | 145 | ALA | 3.7 |
| 48 | s2 | 229 | LEU | 3.7 |
| 59 | C3 | 62 | GLN | 3.7 |
| 49 | s3 | 115 | ILE | 3.7 |
| 77 | SR | 243 | LEU | 3.7 |
| 77 | SR | 292 | LEU | 3.7 |
| 46 | s0 | 156 | VAL | 3.7 |
| 51 | s5 | 62 | VAL | 3.7 |
| 10 | L8 | 252 | ASN | 3.7 |
| 25 | n4 | 99 | GLU | 3.7 |
| 77 | sR | 53 | LYS | 3.7 |
| 65 | C9 | 18 | TYR | 3.7 |
| 4 | l2 | 63 | PHE | 3.7 |
| 65 | C9 | 30 | VAL | 3.7 |
| 73 | d7 | 32 | PHE | 3.7 |
| 54 | s8 | 179 | CYS | 3.7 |
| 61 | c5 | 89 | MET | 3.7 |
| 47 | s1 | 97 | LEU | 3.7 |
| 77 | sR | 243 | LEU | 3.7 |
| 22 | n1 | 70 | SER | 3.7 |
| 61 | c5 | 96 | ILE | 3.7 |
| 49 | s3 | 91 | VAL | 3.7 |
| 61 | c5 | 76 | VAL | 3.7 |
| 54 | s8 | 200 | LYS | 3.7 |
| 78 | sM | 83 | LYS | 3.7 |
| 49 | s3 | 49 | ILE | 3.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 56 | C0 | 65 | TYR | 3.7 |
| 68 | d2 | 83 | ILE | 3.7 |
| 25 | n4 | 72 | SER | 3.7 |
| 49 | s3 | 139 | SER | 3.7 |
| 12 | m0 | 218 | ALA | 3.7 |
| 50 | s4 | 165 | ALA | 3.7 |
| 51 | S5 | 194 | LEU | 3.7 |
| 51 | s5 | 225 | ARG | 3.7 |
| 58 | C2 | 41 | LEU | 3.7 |
| 65 | C9 | 132 | LEU | 3.7 |
| 76 | E0 | 46 | ASN | 3.7 |
| 56 | c0 | 64 | TYR | 3.7 |
| 49 | s3 | 106 | LYS | 3.7 |
| 50 | s4 | 10 | LYS | 3.7 |
| 51 | S5 | 53 | VAL | 3.7 |
| 77 | sR | 186 | PHE | 3.7 |
| 62 | C6 | 35 | PRO | 3.7 |
| 64 | C8 | 7 | GLU | 3.7 |
| 78 | SM | 140 | ASP | 3.7 |
| 51 | S5 | 137 | ILE | 3.7 |
| 58 | C2 | 122 | VAL | 3.7 |
| 51 | S5 | 96 | SER | 3.7 |
| 70 | D4 | 61 | ARG | 3.7 |
| 32 | O1 | 71 | LEU | 3.7 |
| 28 | N7 | 92 | PHE | 3.7 |
| 63 | C7 | 69 | ILE | 3.7 |
| 28 | n7 | 43 | VAL | 3.7 |
| 47 | S1 | 95 | ASN | 3.7 |
| 77 | SR | 315 | VAL | 3.7 |
| 47 | s1 | 177 | GLN | 3.7 |
| 62 | C6 | 104 | GLU | 3.7 |
| 47 | S1 | 102 | GLY | 3.7 |
| 59 | c3 | 59 | GLY | 3.7 |
| 79 | s6 | 196 | ARG | 3.7 |
| 37 | o6 | 50 | LEU | 3.7 |
| 50 | S4 | 246 | LEU | 3.7 |
| 51 | s5 | 30 | PRO | 3.7 |
| 62 | C6 | 38 | LEU | 3.7 |
| 77 | SR | 267 | PRO | 3.7 |
| 77 | sR | 45 | TRP | 3.7 |
| 22 | n1 | 34 | TYR | 3.7 |
| 77 | sR | 304 | GLY | 3.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 18 | M7 | 168 | LEU | 3.6 |
| 53 | S7 | 99 | LEU | 3.6 |
| 62 | C6 | 18 | ALA | 3.6 |
| 79 | s6 | 148 | SER | 3.6 |
| 62 | C6 | 68 | ARG | 3.6 |
| 37 | o6 | 94 | ILE | 3.6 |
| 62 | C6 | 45 | ARG | 3.6 |
| 47 | S1 | 210 | ILE | 3.6 |
| 47 | s1 | 60 | ALA | 3.6 |
| 70 | d4 | 118 | ILE | 3.6 |
| 10 | l8 | 152 | LEU | 3.6 |
| 25 | n4 | 79 | GLN | 3.6 |
| 62 | c6 | 52 | LEU | 3.6 |
| 76 | E0 | 43 | ARG | 3.6 |
| 25 | n4 | 68 | ALA | 3.6 |
| 75 | D9 | 38 | ILE | 3.6 |
| 77 | sR | 296 | ALA | 3.6 |
| 61 | c5 | 87 | PRO | 3.6 |
| 10 | l8 | 150 | LEU | 3.6 |
| 28 | n7 | 60 | LYS | 3.6 |
| 49 | s3 | 27 | ARG | 3.6 |
| 51 | s5 | 28 | PRO | 3.6 |
| 49 | s3 | 185 | LYS | 3.6 |
| 62 | c6 | 13 | LYS | 3.6 |
| 26 | n5 | 30 | ALA | 3.6 |
| 12 | M0 | 109 | ASP | 3.6 |
| 62 | C6 | 139 | GLN | 3.6 |
| 71 | d5 | 37 | GLN | 3.6 |
| 77 | sR | 72 | THR | 3.6 |
| 37 | o6 | 68 | ARG | 3.6 |
| 51 | S5 | 134 | VAL | 3.6 |
| 63 | C7 | 78 | ARG | 3.6 |
| 64 | C8 | 52 | VAL | 3.6 |
| 43 | q2 | 13 | LYS | 3.6 |
| 47 | s1 | 184 | LEU | 3.6 |
| 55 | S9 | 80 | LEU | 3.6 |
| 77 | SR | 148 | ASN | 3.6 |
| 77 | sR | 192 | PHE | 3.6 |
| 49 | S3 | 207 | THR | 3.6 |
| 51 | S5 | 120 | ILE | 3.6 |
| 70 | D4 | 69 | SER | 3.6 |
| 60 | c4 | 72 | LYS | 3.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | SR | 236 | ALA | 3.6 |
| 62 | C6 | 77 | GLN | 3.6 |
| 78 | SM | 68 | ARG | 3.6 |
| 29 | n8 | 66 | ALA | 3.6 |
| 47 | s1 | 89 | ASP | 3.6 |
| 77 | sR | 203 | THR | 3.6 |
| 56 | c0 | 59 | PHE | 3.6 |
| 62 | c6 | 10 | PHE | 3.6 |
| 77 | sR | 57 | PRO | 3.6 |
| 66 | D0 | 83 | GLU | 3.6 |
| 77 | SR | 139 | GLN | 3.6 |
| 79 | s6 | 36 | VAL | 3.6 |
| 12 | m0 | 109 | ASP | 3.6 |
| 25 | n4 | 95 | SER | 3.6 |
| 36 | o5 | 18 | ALA | 3.6 |
| 47 | s1 | 46 | THR | 3.6 |
| 62 | c6 | 115 | THR | 3.6 |
| 13 | m1 | 127 | PHE | 3.5 |
| 77 | sR | 118 | LYS | 3.5 |
| 56 | c0 | 28 | ASN | 3.5 |
| 28 | n7 | 59 | ALA | 3.5 |
| 71 | d5 | 80 | LEU | 3.5 |
| 61 | c5 | 120 | SER | 3.5 |
| 22 | n1 | 72 | VAL | 3.5 |
| 48 | s2 | 151 | PRO | 3.5 |
| 49 | s3 | 138 | VAL | 3.5 |
| 53 | s7 | 13 | PRO | 3.5 |
| 64 | C8 | 70 | VAL | 3.5 |
| 69 | d3 | 60 | GLU | 3.5 |
| 65 | c9 | 15 | ILE | 3.5 |
| 71 | d5 | 92 | ILE | 3.5 |
| 47 | S1 | 26 | ARG | 3.5 |
| 77 | sR | 230 | ALA | 3.5 |
| 48 | s2 | 166 | THR | 3.5 |
| 58 | C2 | 75 | VAL | 3.5 |
| 77 | sR | 247 | PRO | 3.5 |
| 25 | n4 | 96 | LEU | 3.5 |
| 77 | sR | 206 | PRO | 3.5 |
| 12 | m0 | 103 | LEU | 3.5 |
| 51 | S5 | 75 | GLY | 3.5 |
| 58 | C2 | 55 | GLY | 3.5 |
| 61 | c5 | 55 | GLY | 3.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | SR | 40 | LYS | 3.5 |
| 62 | c6 | 63 | ILE | 3.5 |
| 65 | C9 | 85 | SER | 3.5 |
| 74 | D8 | 25 | VAL | 3.5 |
| 51 | s5 | 34 | GLN | 3.5 |
| 61 | c5 | 53 | PRO | 3.5 |
| 62 | c6 | 140 | LYS | 3.5 |
| 63 | C7 | 72 | LYS | 3.5 |
| 65 | C9 | 48 | GLN | 3.5 |
| 76 | E0 | 49 | LEU | 3.5 |
| 77 | SR | 223 | TRP | 3.5 |
| 47 | S1 | 205 | PHE | 3.5 |
| 57 | c1 | 105 | LYS | 3.5 |
| 76 | e0 | 53 | LYS | 3.5 |
| 77 | sR | 170 | ILE | 3.5 |
| 62 | c6 | 20 | ALA | 3.5 |
| 7 | l5 | 178 | ASN | 3.5 |
| 45 | 6 | 75 | U | 3.5 |
| 55 | s9 | 136 | VAL | 3.5 |
| 46 | s0 | 148 | ASP | 3.5 |
| 77 | SR | 220 | ILE | 3.5 |
| 62 | c6 | 117 | LEU | 3.5 |
| 71 | d5 | 51 | LEU | 3.5 |
| 77 | SR | 34 | LEU | 3.5 |
| 46 | s0 | 195 | TRP | 3.5 |
| 77 | sR | 212 | ALA | 3.5 |
| 63 | C7 | 53 | TYR | 3.5 |
| 52 | S6 | 143 | LYS | 3.5 |
| 20 | m9 | 182 | ASP | 3.5 |
| 25 | n4 | 101 | ARG | 3.5 |
| 37 | o6 | 80 | PHE | 3.5 |
| 57 | c1 | 20 | PHE | 3.5 |
| 65 | C9 | 84 | LYS | 3.5 |
| 66 | D0 | 94 | GLU | 3.5 |
| 19 | m8 | 81 | VAL | 3.5 |
| 58 | c2 | 121 | VAL | 3.5 |
| 62 | c6 | 65 | ILE | 3.5 |
| 64 | C8 | 66 | LEU | 3.5 |
| 67 | d1 | 11 | LEU | 3.5 |
| 51 | s5 | 139 | ASN | 3.5 |
| 75 | D9 | 22 | ARG | 3.5 |
| 18 | M7 | 178 | ALA | 3.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 62 | C6 | 17 | THR | 3.5 |
| 66 | D0 | 78 | THR | 3.5 |
| 68 | d2 | 46 | TYR | 3.5 |
| 16 | m5 | 121 | VAL | 3.5 |
| 65 | C9 | 113 | ILE | 3.5 |
| 22 | n1 | 46 | GLY | 3.5 |
| 49 | S3 | 205 | ALA | 3.5 |
| 20 | m9 | 177 | VAL | 3.5 |
| 73 | d7 | 80 | ARG | 3.5 |
| 50 | S4 | 58 | GLY | 3.5 |
| 51 | S5 | 150 | GLY | 3.5 |
| 62 | C6 | 46 | PHE | 3.5 |
| 61 | c5 | 6 | ASN | 3.4 |
| 79 | s6 | 139 | ASN | 3.4 |
| 77 | SR | 100 | TYR | 3.4 |
| 62 | C6 | 48 | VAL | 3.4 |
| 41 | Q0 | 83 | LYS | 3.4 |
| 52 | S6 | 77 | LEU | 3.4 |
| 51 | S5 | 101 | GLY | 3.4 |
| 28 | n7 | 75 | VAL | 3.4 |
| 35 | o4 | 62 | TYR | 3.4 |
| 48 | s2 | 222 | TYR | 3.4 |
| 62 | c6 | 79 | TYR | 3.4 |
| 50 | s4 | 228 | ILE | 3.4 |
| 55 | S9 | 97 | LEU | 3.4 |
| 67 | d1 | 34 | ILE | 3.4 |
| 77 | SR | 46 | LYS | 3.4 |
| 47 | S1 | 133 | TYR | 3.4 |
| 77 | sR | 314 | GLN | 3.4 |
| 49 | s3 | 175 | VAL | 3.4 |
| 60 | c4 | 33 | LEU | 3.4 |
| 60 | c4 | 74 | VAL | 3.4 |
| 7 | L5 | 95 | TRP | 3.4 |
| 1 | 1 | 1580 | A | 3.4 |
| 71 | D5 | 58 | ARG | 3.4 |
| 65 | C9 | 37 | VAL | 3.4 |
| 77 | SR | 184 | ASN | 3.4 |
| 62 | C6 | 56 | GLY | 3.4 |
| 51 | S5 | 180 | ARG | 3.4 |
| 65 | C9 | 29 | GLU | 3.4 |
| 68 | d2 | 82 | LYS | 3.4 |
| 25 | n4 | 85 | ALA | 3.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 40 | o9 | 4 | GLN | 3.4 |
| 68 | D2 | 52 | TYR | 3.4 |
| 71 | D5 | 50 | ILE | 3.4 |
| 77 | SR | 192 | PHE | 3.4 |
| 50 | S4 | 51 | ARG | 3.4 |
| 55 | s9 | 3 | ARG | 3.4 |
| 78 | SM | 41 | SER | 3.4 |
| 48 | S2 | 92 | ALA | 3.4 |
| 64 | C8 | 146 | ALA | 3.4 |
| 77 | sR | 8 | VAL | 3.4 |
| 51 | S5 | 172 | ILE | 3.4 |
| 64 | c8 | 119 | ILE | 3.4 |
| 28 | n7 | 135 | ARG | 3.4 |
| 12 | M0 | 171 | TRP | 3.4 |
| 22 | n1 | 91 | LEU | 3.4 |
| 28 | n7 | 114 | VAL | 3.4 |
| 73 | d7 | 82 | LYS | 3.4 |
| 47 | S1 | 122 | GLU | 3.4 |
| 51 | S5 | 98 | MET | 3.4 |
| 12 | M0 | 87 | LEU | 3.4 |
| 18 | M7 | 170 | SER | 3.4 |
| 26 | n5 | 29 | SER | 3.4 |
| 62 | C6 | 44 | LEU | 3.4 |
| 72 | d6 | 53 | LEU | 3.4 |
| 77 | SR | 309 | VAL | 3.4 |
| 49 | S3 | 174 | HIS | 3.4 |
| 50 | S4 | 109 | PHE | 3.4 |
| 62 | C6 | 30 | LYS | 3.4 |
| 62 | C6 | 83 | GLN | 3.4 |
| 62 | C6 | 118 | ILE | 3.4 |
| 47 | s1 | 217 | LEU | 3.4 |
| 61 | C5 | 101 | ALA | 3.4 |
| 79 | s6 | 102 | VAL | 3.4 |
| 51 | s5 | 61 | TYR | 3.4 |
| 47 | s1 | 74 | GLN | 3.4 |
| 62 | C6 | 9 | THR | 3.4 |
| 75 | d9 | 55 | PHE | 3.4 |
| 1 | 5 | 620 | U | 3.4 |
| 10 | l8 | 198 | ALA | 3.4 |
| 51 | S5 | 182 | ALA | 3.4 |
| 51 | s5 | 23 | VAL | 3.4 |
| 54 | S8 | 141 | ARG | 3.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 55 | s9 | 118 | LEU | 3.4 |
| 64 | c8 | 86 | LEU | 3.4 |
| 71 | D5 | 65 | LEU | 3.4 |
| 76 | E0 | 39 | LEU | 3.4 |
| 77 | sR | 234 | LEU | 3.4 |
| 68 | D2 | 53 | ILE | 3.4 |
| 50 | s4 | 24 | SER | 3.4 |
| 53 | s7 | 45 | SER | 3.4 |
| 58 | c2 | 38 | HIS | 3.4 |
| 47 | s1 | 45 | LYS | 3.4 |
| 50 | S4 | 49 | ARG | 3.4 |
| 68 | d2 | 102 | VAL | 3.4 |
| 47 | S1 | 104 | ASP | 3.4 |
| 78 | SM | 43 | ASP | 3.4 |
| 50 | S4 | 121 | TYR | 3.4 |
| 62 | c6 | 15 | SER | 3.4 |
| 70 | d4 | 24 | VAL | 3.3 |
| 77 | SR | 47 | LEU | 3.3 |
| 77 | sR | 145 | LEU | 3.3 |
| 77 | sR | 270 | LEU | 3.3 |
| 49 | s3 | 147 | ALA | 3.3 |
| 77 | SR | 75 | ALA | 3.3 |
| 28 | n7 | 72 | ILE | 3.3 |
| 65 | c9 | 124 | ILE | 3.3 |
| 51 | S5 | 193 | THR | 3.3 |
| 51 | s5 | 25 | LEU | 3.3 |
| 62 | C6 | 75 | VAL | 3.3 |
| 61 | c5 | 12 | PHE | 3.3 |
| 25 | n4 | 82 | ILE | 3.3 |
| 43 | Q2 | 11 | TYR | 3.3 |
| 50 | s4 | 27 | TYR | 3.3 |
| 64 | c8 | 14 | ILE | 3.3 |
| 72 | d6 | 73 | TYR | 3.3 |
| 58 | c2 | 113 | ARG | 3.3 |
| 66 | d0 | 85 | ARG | 3.3 |
| 74 | d8 | 17 | GLY | 3.3 |
| 28 | n7 | 26 | VAL | 3.3 |
| 78 | SM | 85 | SER | 3.3 |
| 67 | d1 | 54 | ALA | 3.3 |
| 47 | s1 | 224 | ASP | 3.3 |
| 68 | D2 | 109 | GLY | 3.3 |
| 53 | s7 | 74 | GLN | 3.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | s1 | 47 | LEU | 3.3 |
| 48 | s2 | 86 | VAL | 3.3 |
| 47 | S1 | 33 | LYS | 3.3 |
| 75 | D9 | 43 | PHE | 3.3 |
| 77 | sR | 36 | ALA | 3.3 |
| 71 | D5 | 67 | ASP | 3.3 |
| 50 | S4 | 52 | LEU | 3.3 |
| 77 | sR | 9 | LEU | 3.3 |
| 48 | S2 | 98 | PHE | 3.3 |
| 32 | O1 | 91 | SER | 3.3 |
| 43 | Q2 | 92 | GLU | 3.3 |
| 61 | C5 | 125 | PRO | 3.3 |
| 65 | C9 | 142 | GLU | 3.3 |
| 77 | SR | 260 | ILE | 3.3 |
| 78 | SM | 81 | THR | 3.3 |
| 51 | S5 | 142 | PRO | 3.3 |
| 70 | D4 | 26 | ASP | 3.3 |
| 46 | S0 | 160 | ILE | 3.3 |
| 49 | s3 | 114 | ALA | 3.3 |
| 8 | l6 | 67 | GLY | 3.3 |
| 62 | c6 | 71 | GLY | 3.3 |
| 77 | sR | 258 | THR | 3.3 |
| 49 | s3 | 96 | LEU | 3.3 |
| 51 | S5 | 127 | GLN | 3.3 |
| 53 | s7 | 93 | LEU | 3.3 |
| 63 | C7 | 26 | LEU | 3.3 |
| 58 | c2 | 131 | ASP | 3.3 |
| 62 | c6 | 78 | VAL | 3.3 |
| 65 | C9 | 130 | ARG | 3.3 |
| 20 | m9 | 179 | GLU | 3.3 |
| 46 | S0 | 49 | ASN | 3.3 |
| 55 | s9 | 72 | GLU | 3.3 |
| 10 | l8 | 253 | SER | 3.3 |
| 74 | D8 | 65 | ARG | 3.3 |
| 51 | S5 | 79 | ASN | 3.3 |
| 61 | c5 | 113 | GLY | 3.3 |
| 74 | d8 | 43 | ASN | 3.3 |
| 26 | n5 | 24 | LEU | 3.3 |
| 50 | s4 | 9 | LEU | 3.3 |
| 53 | S7 | 126 | LEU | 3.3 |
| 55 | s9 | 5 | PRO | 3.3 |
| 63 | C7 | 46 | LEU | 3.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 64 | c8 | 18 | LEU | 3.3 |
| 77 | sR | 222 | LEU | 3.3 |
| 77 | SR | 300 | THR | 3.3 |
| 13 | M1 | 65 | ILE | 3.3 |
| 51 | S5 | 135 | ASP | 3.3 |
| 51 | S5 | 177 | ILE | 3.3 |
| 78 | sM | 68 | ARG | 3.3 |
| 50 | s4 | 207 | LEU | 3.3 |
| 53 | s7 | 41 | LEU | 3.3 |
| 62 | c6 | 62 | ASN | 3.3 |
| 62 | c6 | 105 | LEU | 3.3 |
| 52 | S6 | 67 | VAL | 3.3 |
| 78 | SM | 22 | PRO | 3.3 |
| 77 | SR | 99 | THR | 3.3 |
| 50 | S4 | 240 | LYS | 3.3 |
| 65 | C9 | 67 | MET | 3.3 |
| 78 | SM | 46 | LYS | 3.3 |
| 52 | S6 | 137 | ARG | 3.3 |
| 62 | c6 | 58 | ASP | 3.3 |
| 73 | d7 | 63 | LEU | 3.3 |
| 77 | sR | 47 | LEU | 3.3 |
| 50 | S4 | 111 | VAL | 3.3 |
| 66 | d0 | 121 | ASN | 3.3 |
| 74 | d8 | 45 | LYS | 3.3 |
| 28 | n7 | 11 | ALA | 3.3 |
| 49 | s3 | 95 | GLY | 3.3 |
| 51 | S5 | 97 | LEU | 3.3 |
| 63 | C7 | 73 | LEU | 3.3 |
| 50 | S4 | 225 | VAL | 3.3 |
| 46 | s0 | 207 | PRO | 3.2 |
| 52 | S6 | 65 | GLN | 3.2 |
| 61 | c5 | 80 | MET | 3.2 |
| 64 | c8 | 57 | ARG | 3.2 |
| 62 | C6 | 63 | ILE | 3.2 |
| 65 | c9 | 83 | ALA | 3.2 |
| 62 | C6 | 64 | ASP | 3.2 |
| 4 | l2 | 76 | PHE | 3.2 |
| 47 | s1 | 68 | VAL | 3.2 |
| 61 | c5 | 94 | VAL | 3.2 |
| 65 | C9 | 9 | VAL | 3.2 |
| 71 | D5 | 70 | LYS | 3.2 |
| 55 | s9 | 144 | PRO | 3.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 58 | C2 | 84 | ASN | 3.2 |
| 50 | S4 | 18 | TRP | 3.2 |
| 50 | S4 | 222 | LEU | 3.2 |
| 75 | D9 | 28 | THR | 3.2 |
| 51 | s5 | 162 | VAL | 3.2 |
| 55 | S9 | 104 | PHE | 3.2 |
| 76 | e0 | 43 | ARG | 3.2 |
| 55 | s9 | 33 | GLU | 3.2 |
| 51 | s5 | 151 | GLY | 3.2 |
| 62 | C6 | 27 | GLY | 3.2 |
| 29 | n8 | 149 | ALA | 3.2 |
| 43 | Q2 | 83 | LEU | 3.2 |
| 48 | s2 | 186 | LYS | 3.2 |
| 51 | S5 | 183 | ALA | 3.2 |
| 74 | D8 | 21 | SER | 3.2 |
| 77 | SR | 283 | LYS | 3.2 |
| 51 | S5 | 117 | THR | 3.2 |
| 46 | S0 | 156 | VAL | 3.2 |
| 50 | s4 | 47 | PHE | 3.2 |
| 54 | S8 | 109 | PHE | 3.2 |
| 51 | S5 | 39 | GLU | 3.2 |
| 10 | l8 | 67 | ILE | 3.2 |
| 25 | n4 | 90 | ILE | 3.2 |
| 25 | n4 | 127 | LYS | 3.2 |
| 32 | O1 | 75 | ILE | 3.2 |
| 77 | sR | 177 | MET | 3.2 |
| 26 | n5 | 82 | LEU | 3.2 |
| 28 | n7 | 51 | LEU | 3.2 |
| 58 | c2 | 133 | LEU | 3.2 |
| 64 | c8 | 3 | LEU | 3.2 |
| 77 | sR | 49 | GLY | 3.2 |
| 51 | S5 | 110 | ALA | 3.2 |
| 76 | E0 | 34 | ALA | 3.2 |
| 77 | sR | 2 | ALA | 3.2 |
| 68 | D2 | 101 | TYR | 3.2 |
| 28 | n7 | 52 | LYS | 3.2 |
| 47 | S1 | 85 | LYS | 3.2 |
| 4 | l2 | 138 | GLY | 3.2 |
| 46 | S0 | 185 | ARG | 3.2 |
| 46 | s0 | 162 | CYS | 3.2 |
| 77 | SR | 89 | LEU | 3.2 |
| 28 | n7 | 129 | TRP | 3.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 56 | C0 | 22 | VAL | 3.2 |
| 64 | C8 | 79 | TYR | 3.2 |
| 65 | C9 | 104 | VAL | 3.2 |
| 41 | Q0 | 128 | LYS | 3.2 |
| 48 | s2 | 84 | LYS | 3.2 |
| 70 | D4 | 9 | THR | 3.2 |
| 28 | n7 | 25 | ILE | 3.2 |
| 36 | o5 | 9 | LEU | 3.2 |
| 48 | S2 | 83 | ILE | 3.2 |
| 58 | C2 | 89 | ILE | 3.2 |
| 58 | c2 | 40 | GLY | 3.2 |
| 66 | D0 | 20 | ILE | 3.2 |
| 12 | M0 | 105 | CYS | 3.2 |
| 20 | m9 | 178 | ALA | 3.2 |
| 74 | D8 | 48 | VAL | 3.2 |
| 64 | c8 | 45 | LEU | 3.2 |
| 77 | sR | 23 | LEU | 3.2 |
| 71 | d5 | 91 | PRO | 3.2 |
| 77 | sR | 119 | ALA | 3.2 |
| 29 | N8 | 79 | TRP | 3.2 |
| 47 | s1 | 95 | ASN | 3.2 |
| 65 | c9 | 101 | ASN | 3.2 |
| 77 | SR | 14 | GLU | 3.2 |
| 13 | m1 | 70 | THR | 3.2 |
| 60 | c4 | 105 | LEU | 3.2 |
| 77 | sR | 48 | THR | 3.2 |
| 79 | s6 | 133 | LEU | 3.2 |
| 51 | S5 | 116 | HIS | 3.2 |
| 62 | C6 | 86 | ALA | 3.2 |
| 50 | S4 | 105 | VAL | 3.2 |
| 58 | C2 | 123 | VAL | 3.2 |
| 62 | C6 | 78 | VAL | 3.2 |
| 51 | S5 | 92 | ARG | 3.2 |
| 63 | C7 | 33 | ARG | 3.2 |
| 23 | n2 | 52 | ASN | 3.2 |
| 46 | S0 | 133 | ILE | 3.2 |
| 47 | s1 | 86 | LEU | 3.2 |
| 50 | S4 | 19 | LEU | 3.2 |
| 58 | c2 | 89 | ILE | 3.2 |
| 79 | s6 | 124 | LEU | 3.2 |
| 76 | e0 | 3 | LYS | 3.2 |
| 28 | n7 | 74 | VAL | 3.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 58 | C2 | 56 | GLU | 3.2 |
| 58 | C2 | 129 | GLU | 3.2 |
| 65 | C9 | 86 | ARG | 3.2 |
| 37 | o6 | 77 | LEU | 3.2 |
| 46 | s0 | 18 | LEU | 3.2 |
| 52 | S6 | 54 | GLY | 3.2 |
| 71 | d5 | 88 | ILE | 3.2 |
| 68 | D2 | 111 | MET | 3.2 |
| 49 | s3 | 90 | ARG | 3.2 |
| 60 | C4 | 50 | ALA | 3.2 |
| 61 | C5 | 17 | TYR | 3.2 |
| 79 | s6 | 130 | PRO | 3.2 |
| 45 | 6 | 1052 | U | 3.2 |
| 66 | d0 | 79 | TRP | 3.2 |
| 65 | C9 | 32 | GLY | 3.2 |
| 74 | D8 | 53 | ILE | 3.2 |
| 73 | D7 | 29 | ARG | 3.2 |
| 7 | l5 | 296 | GLN | 3.2 |
| 19 | m8 | 80 | THR | 3.2 |
| 62 | c6 | 97 | VAL | 3.2 |
| 61 | c5 | 118 | GLU | 3.2 |
| 77 | sR | 254 | ALA | 3.2 |
| 13 | M1 | 91 | LEU | 3.1 |
| 37 | o6 | 93 | ILE | 3.1 |
| 47 | S1 | 93 | GLY | 3.1 |
| 50 | S4 | 90 | ILE | 3.1 |
| 64 | C8 | 101 | LEU | 3.1 |
| 51 | S5 | 43 | PHE | 3.1 |
| 43 | q2 | 102 | GLN | 3.1 |
| 47 | S1 | 90 | GLU | 3.1 |
| 49 | s3 | 58 | VAL | 3.1 |
| 67 | D1 | 10 | GLU | 3.1 |
| 79 | s6 | 179 | VAL | 3.1 |
| 32 | O1 | 112 | ASP | 3.1 |
| 55 | s9 | 61 | THR | 3.1 |
| 74 | D8 | 45 | LYS | 3.1 |
| 54 | S8 | 152 | ILE | 3.1 |
| 3 | 4 | 84 | C | 3.1 |
| 52 | S6 | 161 | GLU | 3.1 |
| 67 | D1 | 54 | ALA | 3.1 |
| 78 | SM | 42 | ALA | 3.1 |
| 54 | S8 | 55 | TYR | 3.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 25 | n4 | 87 | LEU | 3.1 |
| 77 | sR | 10 | ARG | 3.1 |
| 68 | D2 | 83 | ILE | 3.1 |
| 61 | c5 | 4 | ALA | 3.1 |
| 61 | c5 | 106 | GLU | 3.1 |
| 79 | s6 | 107 | ALA | 3.1 |
| 46 | s0 | 46 | HIS | 3.1 |
| 47 | s1 | 228 | LEU | 3.1 |
| 71 | D5 | 51 | LEU | 3.1 |
| 51 | S5 | 40 | ILE | 3.1 |
| 51 | s5 | 147 | THR | 3.1 |
| 59 | c3 | 61 | THR | 3.1 |
| 65 | c9 | 113 | ILE | 3.1 |
| 73 | d7 | 46 | VAL | 3.1 |
| 65 | C9 | 107 | ALA | 3.1 |
| 78 | sM | 66 | ALA | 3.1 |
| 52 | S6 | 208 | TYR | 3.1 |
| 53 | s7 | 9 | LEU | 3.1 |
| 58 | C2 | 88 | LEU | 3.1 |
| 22 | n1 | 96 | ILE | 3.1 |
| 47 | s1 | 138 | PHE | 3.1 |
| 48 | s2 | 227 | PRO | 3.1 |
| 47 | S1 | 41 | ARG | 3.1 |
| 77 | SR | 180 | ALA | 3.1 |
| 50 | s4 | 12 | LEU | 3.1 |
| 56 | c0 | 62 | GLN | 3.1 |
| 63 | C7 | 34 | LEU | 3.1 |
| 27 | n6 | 46 | LYS | 3.1 |
| 28 | n7 | 130 | PHE | 3.1 |
| 45 | 2 | 1363 | U | 3.1 |
| 51 | S5 | 41 | LYS | 3.1 |
| 57 | c1 | 73 | GLY | 3.1 |
| 64 | C8 | 85 | PHE | 3.1 |
| 77 | sR | 115 | ILE | 3.1 |
| 77 | sR | 108 | SER | 3.1 |
| 47 | s1 | 57 | ALA | 3.1 |
| 58 | C2 | 128 | ALA | 3.1 |
| 77 | sR | 261 | LYS | 3.1 |
| 61 | c5 | 85 | ILE | 3.1 |
| 62 | c6 | 11 | GLY | 3.1 |
| 77 | SR | 131 | ILE | 3.1 |
| 47 | S1 | 103 | MET | 3.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 61 | c5 | 81 | ARG | 3.1 |
| 67 | d1 | 82 | VAL | 3.1 |
| 77 | sR | 17 | ASN | 3.1 |
| 66 | d0 | 34 | LEU | 3.1 |
| 63 | c7 | 74 | GLN | 3.1 |
| 66 | d0 | 22 | ILE | 3.1 |
| 26 | n5 | 62 | VAL | 3.1 |
| 45 | 2 | 193 | U | 3.1 |
| 50 | S4 | 197 | HIS | 3.1 |
| 47 | s1 | 54 | LEU | 3.1 |
| 48 | S2 | 41 | LEU | 3.1 |
| 50 | S4 | 44 | LEU | 3.1 |
| 55 | S9 | 109 | LEU | 3.1 |
| 77 | SR | 27 | ALA | 3.1 |
| 16 | m5 | 142 | ILE | 3.1 |
| 50 | S4 | 192 | ILE | 3.1 |
| 70 | D4 | 66 | GLY | 3.1 |
| 77 | SR | 61 | PHE | 3.1 |
| 77 | sR | 122 | ILE | 3.1 |
| 48 | s2 | 80 | VAL | 3.1 |
| 68 | d2 | 81 | VAL | 3.1 |
| 63 | c7 | 35 | CYS | 3.1 |
| 76 | E0 | 60 | PRO | 3.1 |
| 77 | SR | 145 | LEU | 3.1 |
| 56 | c0 | 61 | TRP | 3.1 |
| 7 | L5 | 160 | PHE | 3.1 |
| 62 | c6 | 68 | ARG | 3.1 |
| 57 | C1 | 70 | ILE | 3.1 |
| 12 | M0 | 138 | VAL | 3.1 |
| 48 | S2 | 86 | VAL | 3.1 |
| 11 | L9 | 161 | LEU | 3.1 |
| 47 | S1 | 123 | ALA | 3.1 |
| 55 | s9 | 135 | ALA | 3.1 |
| 77 | SR | 301 | LEU | 3.1 |
| 55 | s9 | 54 | ARG | 3.1 |
| 78 | SM | 21 | PRO | 3.1 |
| 62 | c6 | 120 | ASP | 3.1 |
| 67 | D1 | 34 | ILE | 3.1 |
| 74 | d8 | 32 | PHE | 3.1 |
| 22 | n1 | 40 | VAL | 3.1 |
| 52 | S6 | 124 | LEU | 3.1 |
| 63 | c7 | 57 | LEU | 3.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | sR | 81 | LEU | 3.1 |
| 49 | s3 | 107 | PHE | 3.0 |
| 50 | S4 | 175 | PHE | 3.0 |
| 48 | S2 | 69 | ILE | 3.0 |
| 51 | S5 | 128 | ASN | 3.0 |
| 64 | c8 | 125 | ILE | 3.0 |
| 68 | d2 | 45 | GLY | 3.0 |
| 77 | SR | 92 | TRP | 3.0 |
| 51 | S5 | 168 | VAL | 3.0 |
| 79 | s6 | 112 | VAL | 3.0 |
| 50 | S4 | 9 | LEU | 3.0 |
| 78 | sM | 51 | ARG | 3.0 |
| 67 | D1 | 26 | ALA | 3.0 |
| 8 | l6 | 128 | LYS | 3.0 |
| 37 | o6 | 71 | LYS | 3.0 |
| 62 | C6 | 112 | TYR | 3.0 |
| 63 | c7 | 53 | TYR | 3.0 |
| 54 | S8 | 176 | SER | 3.0 |
| 55 | s9 | 142 | ASN | 3.0 |
| 77 | SR | 242 | SER | 3.0 |
| 77 | sR | 181 | TRP | 3.0 |
| 28 | n7 | 98 | THR | 3.0 |
| 74 | d8 | 33 | LEU | 3.0 |
| 50 | S4 | 242 | LYS | 3.0 |
| 52 | S6 | 27 | PHE | 3.0 |
| 47 | S1 | 121 | ILE | 3.0 |
| 55 | s9 | 143 | ILE | 3.0 |
| 68 | D2 | 47 | ILE | 3.0 |
| 12 | m0 | 110 | ARG | 3.0 |
| 36 | o5 | 19 | SER | 3.0 |
| 53 | s7 | 39 | ARG | 3.0 |
| 74 | d8 | 25 | VAL | 3.0 |
| 77 | sR | 205 | SER | 3.0 |
| 53 | S7 | 43 | PHE | 3.0 |
| 79 | s6 | 175 | ILE | 3.0 |
| 13 | m1 | 47 | GLN | 3.0 |
| 29 | n8 | 123 | VAL | 3.0 |
| 51 | S5 | 149 | VAL | 3.0 |
| 51 | s5 | 158 | GLN | 3.0 |
| 54 | s8 | 46 | VAL | 3.0 |
| 49 | S3 | 182 | LEU | 3.0 |
| 50 | S4 | 213 | SER | 3.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 57 | c1 | 29 | LYS | 3.0 |
| 51 | s5 | 48 | PHE | 3.0 |
| 63 | c7 | 28 | PHE | 3.0 |
| 77 | sR | 130 | THR | 3.0 |
| 51 | s5 | 154 | ALA | 3.0 |
| 53 | s7 | 12 | ALA | 3.0 |
| 74 | D8 | 49 | ARG | 3.0 |
| 47 | s1 | 20 | VAL | 3.0 |
| 72 | d6 | 45 | VAL | 3.0 |
| 46 | S0 | 149 | LEU | 3.0 |
| 56 | c0 | 29 | GLN | 3.0 |
| 62 | c6 | 103 | ASN | 3.0 |
| 51 | S5 | 76 | ARG | 3.0 |
| 48 | s2 | 179 | VAL | 3.0 |
| 70 | d4 | 44 | LEU | 3.0 |
| 77 | SR | 265 | LEU | 3.0 |
| 28 | n7 | 48 | ARG | 3.0 |
| 58 | c2 | 107 | ASP | 3.0 |
| 62 | C6 | 114 | ARG | 3.0 |
| 7 | L5 | 217 | GLU | 3.0 |
| 36 | O5 | 2 | ALA | 3.0 |
| 77 | sR | 305 | TYR | 3.0 |
| 79 | s6 | 84 | TYR | 3.0 |
| 28 | n7 | 96 | VAL | 3.0 |
| 28 | n7 | 87 | LEU | 3.0 |
| 55 | S9 | 2 | PRO | 3.0 |
| 77 | SR | 16 | HIS | 3.0 |
| 51 | S5 | 143 | ARG | 3.0 |
| 7 | l5 | 190 | ILE | 3.0 |
| 43 | Q2 | 3 | ASN | 3.0 |
| 51 | S5 | 31 | GLU | 3.0 |
| 68 | D2 | 18 | GLU | 3.0 |
| 77 | sR | 169 | ILE | 3.0 |
| 29 | n8 | 147 | LEU | 3.0 |
| 7 | L5 | 181 | PRO | 3.0 |
| 22 | n1 | 95 | HIS | 3.0 |
| 64 | C8 | 45 | LEU | 3.0 |
| 66 | D0 | 85 | ARG | 3.0 |
| 71 | D5 | 82 | HIS | 3.0 |
| 66 | D0 | 79 | TRP | 3.0 |
| 52 | S6 | 66 | GLY | 3.0 |
| 35 | o4 | 29 | ILE | 3.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 22 | n1 | 93 | VAL | 3.0 |
| 77 | SR | 58 | VAL | 3.0 |
| 77 | SR | 157 | VAL | 3.0 |
| 65 | c9 | 22 | LEU | 3.0 |
| 29 | n8 | 129 | PHE | 3.0 |
| 50 | S4 | 195 | ILE | 3.0 |
| 50 | s4 | 13 | ALA | 3.0 |
| 61 | C5 | 131 | ALA | 3.0 |
| 10 | L8 | 150 | LEU | 3.0 |
| 13 | M1 | 102 | PHE | 3.0 |
| 65 | C9 | 69 | LYS | 3.0 |
| 73 | D7 | 47 | PHE | 3.0 |
| 74 | D8 | 5 | THR | 3.0 |
| 36 | o5 | 16 | GLN | 3.0 |
| 77 | SR | 101 | GLN | 3.0 |
| 79 | s6 | 146 | GLY | 3.0 |
| 1 | 5 | 252 | U | 3.0 |
| 58 | c2 | 30 | VAL | 3.0 |
| 64 | c8 | 58 | ALA | 3.0 |
| 10 | l8 | 186 | LEU | 3.0 |
| 64 | C8 | 97 | ASP | 3.0 |
| 13 | m1 | 174 | LYS | 3.0 |
| 63 | C7 | 14 | LYS | 3.0 |
| 68 | D2 | 124 | LYS | 3.0 |
| 52 | S6 | 50 | PHE | 3.0 |
| 64 | c8 | 11 | PHE | 3.0 |
| 46 | s0 | 147 | THR | 3.0 |
| 49 | s3 | 140 | GLY | 2.9 |
| 51 | S5 | 113 | ILE | 2.9 |
| 62 | C6 | 82 | ARG | 2.9 |
| 67 | D1 | 23 | ILE | 2.9 |
| 50 | S4 | 161 | LYS | 2.9 |
| 50 | s4 | 101 | LEU | 2.9 |
| 59 | c3 | 40 | TYR | 2.9 |
| 61 | C5 | 60 | LEU | 2.9 |
| 61 | C5 | 94 | VAL | 2.9 |
| 32 | O1 | 79 | ARG | 2.9 |
| 55 | s9 | 130 | THR | 2.9 |
| 76 | e0 | 6 | GLY | 2.9 |
| 77 | SR | 98 | GLU | 2.9 |
| 41 | Q0 | 78 | ILE | 2.9 |
| 47 | S1 | 84 | ILE | 2.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 68 | D2 | 72 | CYS | 2.9 |
| 68 | d2 | 125 | ILE | 2.9 |
| 71 | d5 | 71 | ILE | 2.9 |
| 71 | d5 | 78 | ILE | 2.9 |
| 13 | M1 | 12 | LEU | 2.9 |
| 13 | m1 | 115 | LYS | 2.9 |
| 18 | M7 | 166 | VAL | 2.9 |
| 67 | d1 | 55 | LEU | 2.9 |
| 68 | d2 | 69 | LEU | 2.9 |
| 77 | SR | 156 | VAL | 2.9 |
| 77 | SR | 261 | LYS | 2.9 |
| 57 | C1 | 60 | PHE | 2.9 |
| 79 | s6 | 50 | PHE | 2.9 |
| 10 | l8 | 179 | ILE | 2.9 |
| 47 | s1 | 231 | LEU | 2.9 |
| 51 | S5 | 64 | VAL | 2.9 |
| 51 | s5 | 64 | VAL | 2.9 |
| 69 | d3 | 118 | PRO | 2.9 |
| 7 | l5 | 62 | CYS | 2.9 |
| 71 | D5 | 57 | TYR | 2.9 |
| 49 | s3 | 173 | ARG | 2.9 |
| 51 | S5 | 112 | ARG | 2.9 |
| 7 | l5 | 34 | LYS | 2.9 |
| 13 | m1 | 64 | LYS | 2.9 |
| 62 | C6 | 125 | GLU | 2.9 |
| 64 | c8 | 59 | GLY | 2.9 |
| 77 | SR | 117 | LYS | 2.9 |
| 47 | S1 | 215 | VAL | 2.9 |
| 54 | S8 | 43 | ILE | 2.9 |
| 49 | S3 | 201 | ALA | 2.9 |
| 49 | s3 | 39 | VAL | 2.9 |
| 64 | C8 | 69 | ILE | 2.9 |
| 49 | s3 | 72 | LEU | 2.9 |
| 63 | c7 | 26 | LEU | 2.9 |
| 73 | D7 | 33 | LEU | 2.9 |
| 66 | D0 | 82 | TYR | 2.9 |
| 77 | SR | 135 | THR | 2.9 |
| 58 | C2 | 100 | TRP | 2.9 |
| 49 | s3 | 134 | CYS | 2.9 |
| 50 | S4 | 221 | ARG | 2.9 |
| 66 | d0 | 83 | GLU | 2.9 |
| 62 | C6 | 71 | GLY | 2.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 50 | S4 | 56 | LEU | 2.9 |
| 61 | C5 | 53 | PRO | 2.9 |
| 62 | c6 | 21 | HIS | 2.9 |
| 67 | D1 | 55 | LEU | 2.9 |
| 70 | D4 | 18 | LEU | 2.9 |
| 74 | D8 | 54 | LEU | 2.9 |
| 77 | SR | 23 | LEU | 2.9 |
| 77 | sR | 26 | SER | 2.9 |
| 52 | S6 | 100 | ALA | 2.9 |
| 62 | c6 | 142 | TYR | 2.9 |
| 64 | c8 | 42 | TYR | 2.9 |
| 77 | sR | 317 | THR | 2.9 |
| 74 | D8 | 50 | GLU | 2.9 |
| 77 | sR | 146 | GLY | 2.9 |
| 18 | M7 | 176 | ILE | 2.9 |
| 19 | m8 | 138 | LEU | 2.9 |
| 50 | S4 | 160 | VAL | 2.9 |
| 63 | C7 | 9 | VAL | 2.9 |
| 62 | c6 | 16 | ALA | 2.9 |
| 65 | C9 | 134 | ARG | 2.9 |
| 13 | M1 | 163 | PHE | 2.9 |
| 48 | S2 | 96 | THR | 2.9 |
| 71 | d5 | 105 | THR | 2.9 |
| 57 | c1 | 4 | GLU | 2.9 |
| 28 | n7 | 42 | LEU | 2.9 |
| 28 | n7 | 134 | LEU | 2.9 |
| 52 | S6 | 92 | ARG | 2.9 |
| 65 | c9 | 8 | ASP | 2.9 |
| 68 | d2 | 121 | VAL | 2.9 |
| 13 | m1 | 96 | PHE | 2.9 |
| 43 | Q2 | 81 | ALA | 2.9 |
| 58 | C2 | 85 | LYS | 2.9 |
| 65 | C9 | 66 | TYR | 2.9 |
| 65 | c9 | 19 | ALA | 2.9 |
| 46 | s0 | 35 | PRO | 2.9 |
| 16 | m5 | 120 | TRP | 2.9 |
| 58 | C2 | 126 | TRP | 2.9 |
| 49 | S3 | 183 | GLY | 2.9 |
| 29 | n8 | 75 | LEU | 2.9 |
| 48 | s2 | 76 | LEU | 2.9 |
| 49 | s3 | 94 | ARG | 2.9 |
| 55 | s9 | 141 | VAL | 2.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 64 | c8 | 81 | ILE | 2.9 |
| 67 | d1 | 9 | VAL | 2.9 |
| 70 | D4 | 17 | LEU | 2.9 |
| 65 | C9 | 101 | ASN | 2.9 |
| 22 | n1 | 29 | THR | 2.9 |
| 54 | S8 | 48 | THR | 2.9 |
| 56 | c0 | 67 | THR | 2.9 |
| 68 | d2 | 68 | ARG | 2.9 |
| 77 | sR | 256 | THR | 2.9 |
| 10 | l8 | 43 | LYS | 2.9 |
| 62 | C6 | 69 | VAL | 2.9 |
| 68 | D2 | 60 | LYS | 2.9 |
| 70 | D4 | 44 | LEU | 2.9 |
| 12 | m0 | 220 | GLN | 2.9 |
| 20 | m9 | 188 | ASP | 2.9 |
| 55 | S9 | 164 | PHE | 2.9 |
| 58 | C2 | 69 | ALA | 2.9 |
| 64 | c8 | 136 | GLN | 2.9 |
| 62 | c6 | 49 | TYR | 2.9 |
| 56 | C0 | 25 | LYS | 2.9 |
| 76 | e0 | 36 | LYS | 2.9 |
| 77 | sR | 19 | TRP | 2.9 |
| 6 | l4 | 290 | ILE | 2.9 |
| 22 | n1 | 75 | ILE | 2.9 |
| 48 | s2 | 81 | MET | 2.9 |
| 55 | s9 | 113 | VAL | 2.9 |
| 68 | D2 | 128 | PHE | 2.9 |
| 63 | C7 | 65 | PRO | 2.9 |
| 79 | s6 | 173 | PRO | 2.9 |
| 10 | l8 | 252 | ASN | 2.9 |
| 73 | D7 | 24 | LEU | 2.9 |
| 19 | m8 | 99 | THR | 2.9 |
| 57 | c1 | 27 | THR | 2.9 |
| 62 | C6 | 37 | THR | 2.9 |
| 73 | D7 | 65 | THR | 2.9 |
| 68 | D2 | 51 | GLU | 2.9 |
| 66 | D0 | 61 | LYS | 2.9 |
| 71 | d5 | 52 | LYS | 2.9 |
| 13 | m1 | 45 | PRO | 2.9 |
| 16 | M5 | 58 | GLY | 2.9 |
| 48 | s2 | 154 | LEU | 2.9 |
| 59 | C3 | 28 | LEU | 2.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | SR | 270 | LEU | 2.9 |
| 52 | S6 | 32 | ILE | 2.8 |
| 62 | C6 | 15 | SER | 2.8 |
| 65 | C9 | 100 | ILE | 2.8 |
| 67 | d1 | 39 | VAL | 2.8 |
| 75 | D9 | 55 | PHE | 2.8 |
| 79 | s6 | 4 | ASN | 2.8 |
| 4 | l2 | 59 | ALA | 2.8 |
| 20 | m9 | 11 | ALA | 2.8 |
| 49 | s3 | 61 | GLU | 2.8 |
| 62 | C6 | 140 | LYS | 2.8 |
| 78 | sM | 123 | ALA | 2.8 |
| 7 | l5 | 171 | LEU | 2.8 |
| 43 | Q2 | 93 | LEU | 2.8 |
| 45 | 2 | 754 | A | 2.8 |
| 47 | S1 | 171 | ILE | 2.8 |
| 52 | S6 | 141 | ILE | 2.8 |
| 52 | S6 | 175 | ILE | 2.8 |
| 66 | d0 | 65 | ILE | 2.8 |
| 75 | D9 | 31 | ILE | 2.8 |
| 13 | M1 | 41 | SER | 2.8 |
| 79 | s6 | 92 | ARG | 2.8 |
| 47 | S1 | 50 | LYS | 2.8 |
| 1 | 5 | 3278 | C | 2.8 |
| 36 | o5 | 85 | THR | 2.8 |
| 51 | S5 | 61 | TYR | 2.8 |
| 54 | s8 | 97 | THR | 2.8 |
| 46 | s0 | 9 | LEU | 2.8 |
| 71 | D5 | 73 | GLY | 2.8 |
| 10 | l8 | 50 | VAL | 2.8 |
| 47 | S1 | 140 | ILE | 2.8 |
| 50 | S4 | 102 | VAL | 2.8 |
| 53 | S7 | 172 | VAL | 2.8 |
| 62 | c6 | 69 | VAL | 2.8 |
| 28 | n7 | 65 | ARG | 2.8 |
| 68 | D2 | 103 | ILE | 2.8 |
| 45 | 2 | 506 | A | 2.8 |
| 49 | S3 | 8 | LYS | 2.8 |
| 66 | d0 | 64 | LYS | 2.8 |
| 13 | m1 | 20 | ASN | 2.8 |
| 79 | s6 | 140 | ASN | 2.8 |
| 77 | sR | 25 | THR | 2.8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 52 | S6 | 99 | GLY | 2.8 |
| 27 | N6 | 125 | LYS | 2.8 |
| 37 | o6 | 41 | ARG | 2.8 |
| 50 | S4 | 210 | ILE | 2.8 |
| 77 | sR | 154 | VAL | 2.8 |
| 79 | s6 | 162 | VAL | 2.8 |
| 51 | S5 | 129 | PRO | 2.8 |
| 77 | SR | 57 | PRO | 2.8 |
| 28 | n7 | 44 | ALA | 2.8 |
| 63 | C7 | 62 | GLN | 2.8 |
| 7 | L5 | 153 | THR | 2.8 |
| 37 | o6 | 11 | LEU | 2.8 |
| 47 | S1 | 86 | LEU | 2.8 |
| 65 | c9 | 108 | LEU | 2.8 |
| 60 | c4 | 92 | LYS | 2.8 |
| 77 | SR | 203 | THR | 2.8 |
| 3 | 8 | 82 | U | 2.8 |
| 12 | m0 | 197 | VAL | 2.8 |
| 50 | S4 | 76 | VAL | 2.8 |
| 62 | c6 | 5 | PRO | 2.8 |
| 63 | C7 | 58 | MET | 2.8 |
| 75 | d9 | 52 | PHE | 2.8 |
| 46 | S0 | 158 | VAL | 2.8 |
| 65 | C9 | 36 | ILE | 2.8 |
| 50 | S4 | 35 | PRO | 2.8 |
| 73 | D7 | 66 | PRO | 2.8 |
| 25 | n4 | 128 | ALA | 2.8 |
| 7 | L5 | 163 | LEU | 2.8 |
| 12 | M0 | 103 | LEU | 2.8 |
| 23 | n2 | 70 | LYS | 2.8 |
| 56 | c0 | 15 | LEU | 2.8 |
| 68 | d2 | 104 | LEU | 2.8 |
| 68 | d2 | 130 | TYR | 2.8 |
| 70 | D4 | 40 | LEU | 2.8 |
| 10 | L8 | 195 | SER | 2.8 |
| 62 | c6 | 4 | VAL | 2.8 |
| 68 | D2 | 125 | ILE | 2.8 |
| 47 | s1 | 37 | THR | 2.8 |
| 58 | c2 | 34 | THR | 2.8 |
| 76 | E0 | 56 | MET | 2.8 |
| 48 | S2 | 95 | ARG | 2.8 |
| 48 | s2 | 97 | ARG | 2.8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | s5 | 164 | PRO | 2.8 |
| 52 | S6 | 135 | PRO | 2.8 |
| 62 | C6 | 124 | PRO | 2.8 |
| 64 | c8 | 76 | PRO | 2.8 |
| 78 | SM | 40 | PRO | 2.8 |
| 22 | n1 | 151 | LEU | 2.8 |
| 43 | q2 | 72 | LEU | 2.8 |
| 58 | C2 | 57 | ALA | 2.8 |
| 58 | c2 | 74 | LEU | 2.8 |
| 60 | c4 | 20 | TYR | 2.8 |
| 51 | S5 | 68 | ILE | 2.8 |
| 53 | S7 | 90 | VAL | 2.8 |
| 53 | S7 | 92 | PHE | 2.8 |
| 71 | d5 | 89 | ILE | 2.8 |
| 74 | d8 | 15 | VAL | 2.8 |
| 77 | SR | 213 | SER | 2.8 |
| 77 | sR | 312 | VAL | 2.8 |
| 51 | S5 | 95 | ASN | 2.8 |
| 77 | SR | 200 | ASN | 2.8 |
| 47 | s1 | 234 | GLU | 2.8 |
| 28 | n7 | 82 | PRO | 2.8 |
| 22 | n1 | 30 | TYR | 2.8 |
| 32 | O1 | 51 | LEU | 2.8 |
| 55 | s9 | 93 | LEU | 2.8 |
| 62 | c6 | 44 | LEU | 2.8 |
| 68 | D2 | 126 | LEU | 2.8 |
| 77 | SR | 208 | GLY | 2.8 |
| 77 | sR | 32 | LEU | 2.8 |
| 43 | Q2 | 91 | PHE | 2.8 |
| 72 | d6 | 50 | VAL | 2.8 |
| 77 | SR | 104 | VAL | 2.8 |
| 49 | S3 | 158 | ILE | 2.8 |
| 8 | l6 | 129 | GLU | 2.8 |
| 29 | N8 | 95 | SER | 2.8 |
| 51 | S5 | 104 | ASN | 2.8 |
| 60 | c4 | 43 | THR | 2.8 |
| 50 | S4 | 207 | LEU | 2.8 |
| 64 | c8 | 32 | LEU | 2.8 |
| 71 | d5 | 55 | PRO | 2.8 |
| 77 | SR | 222 | LEU | 2.8 |
| 47 | S1 | 100 | PHE | 2.8 |
| 51 | S5 | 162 | VAL | 2.8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | s5 | 24 | VAL | 2.8 |
| 66 | D0 | 105 | GLN | 2.8 |
| 10 | l8 | 143 | ILE | 2.8 |
| 60 | c4 | 83 | ILE | 2.8 |
| 77 | SR | 263 | PHE | 2.8 |
| 71 | D5 | 94 | LYS | 2.8 |
| 77 | sR | 43 | ILE | 2.8 |
| 14 | M3 | 134 | GLU | 2.8 |
| 68 | D2 | 30 | SER | 2.8 |
| 7 | l5 | 129 | TYR | 2.8 |
| 37 | o6 | 95 | ALA | 2.8 |
| 49 | s3 | 69 | LEU | 2.8 |
| 49 | s3 | 149 | ALA | 2.8 |
| 53 | s7 | 38 | LEU | 2.8 |
| 55 | S9 | 28 | LEU | 2.8 |
| 51 | S5 | 178 | GLY | 2.8 |
| 59 | C3 | 63 | ALA | 2.8 |
| 12 | M0 | 50 | VAL | 2.8 |
| 12 | M0 | 85 | PHE | 2.8 |
| 64 | C8 | 71 | GLN | 2.8 |
| 77 | sR | 109 | ASP | 2.8 |
| 13 | M1 | 114 | ILE | 2.8 |
| 52 | S6 | 79 | LYS | 2.8 |
| 74 | D8 | 18 | ARG | 2.8 |
| 79 | s6 | 136 | LYS | 2.8 |
| 45 | 6 | 194 | U | 2.8 |
| 77 | sR | 189 | GLU | 2.8 |
| 75 | d9 | 36 | LEU | 2.8 |
| 25 | n4 | 94 | ARG | 2.8 |
| 54 | S8 | 182 | TYR | 2.8 |
| 77 | SR | 78 | ALA | 2.8 |
| 73 | D7 | 2 | VAL | 2.8 |
| 76 | E0 | 29 | LYS | 2.8 |
| 77 | SR | 167 | VAL | 2.8 |
| 77 | sR | 54 | PHE | 2.8 |
| 75 | d9 | 38 | ILE | 2.7 |
| 45 | 6 | 648 | G | 2.7 |
| 41 | Q0 | 82 | LEU | 2.7 |
| 49 | S3 | 69 | LEU | 2.7 |
| 51 | s5 | 97 | LEU | 2.7 |
| 55 | s9 | 36 | LEU | 2.7 |
| 7 | l5 | 179 | ARG | 2.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 45 | 6 | 793 | A | 2.7 |
| 51 | S5 | 74 | ALA | 2.7 |
| 65 | C9 | 119 | LYS | 2.7 |
| 67 | D1 | 84 | SER | 2.7 |
| 78 | sM | 85 | SER | 2.7 |
| 29 | N8 | 121 | VAL | 2.7 |
| 51 | S5 | 82 | PHE | 2.7 |
| 78 | sM | 119 | ALA | 2.7 |
| 7 | l5 | 109 | THR | 2.7 |
| 13 | M1 | 134 | PRO | 2.7 |
| 66 | D0 | 117 | VAL | 2.7 |
| 50 | S4 | 184 | THR | 2.7 |
| 53 | S7 | 149 | ILE | 2.7 |
| 77 | SR | 30 | PRO | 2.7 |
| 47 | S1 | 188 | LEU | 2.7 |
| 50 | s4 | 107 | GLY | 2.7 |
| 49 | s3 | 16 | VAL | 2.7 |
| 64 | c8 | 2 | SER | 2.7 |
| 74 | D8 | 28 | VAL | 2.7 |
| 76 | e0 | 61 | SER | 2.7 |
| 77 | sR | 240 | VAL | 2.7 |
| 11 | L9 | 30 | PRO | 2.7 |
| 66 | D0 | 41 | ILE | 2.7 |
| 26 | n5 | 37 | THR | 2.7 |
| 65 | c9 | 131 | ASP | 2.7 |
| 7 | l5 | 150 | LEU | 2.7 |
| 52 | S6 | 216 | LEU | 2.7 |
| 55 | s9 | 174 | ARG | 2.7 |
| 62 | C6 | 14 | LYS | 2.7 |
| 25 | n4 | 103 | ALA | 2.7 |
| 37 | o6 | 8 | ALA | 2.7 |
| 71 | D5 | 76 | ALA | 2.7 |
| 53 | S7 | 134 | GLU | 2.7 |
| 77 | SR | 209 | THR | 2.7 |
| 50 | S4 | 189 | LEU | 2.7 |
| 4 | l2 | 62 | VAL | 2.7 |
| 7 | l5 | 200 | PHE | 2.7 |
| 68 | D2 | 21 | GLY | 2.7 |
| 62 | c6 | 96 | TYR | 2.7 |
| 73 | D7 | 35 | VAL | 2.7 |
| 78 | sM | 42 | ALA | 2.7 |
| 74 | d8 | 40 | ILE | 2.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 64 | C8 | 48 | LYS | 2.7 |
| 65 | C9 | 7 | ARG | 2.7 |
| 65 | c9 | 110 | LYS | 2.7 |
| 68 | d2 | 95 | PRO | 2.7 |
| 71 | D5 | 98 | GLN | 2.7 |
| 79 | s6 | 93 | LYS | 2.7 |
| 32 | O1 | 89 | LEU | 2.7 |
| 46 | s0 | 164 | ASN | 2.7 |
| 47 | s1 | 42 | ASN | 2.7 |
| 47 | s1 | 99 | ASN | 2.7 |
| 50 | s4 | 18 | TRP | 2.7 |
| 55 | S9 | 146 | PHE | 2.7 |
| 56 | c0 | 19 | GLY | 2.7 |
| 70 | D4 | 64 | PHE | 2.7 |
| 49 | S3 | 37 | VAL | 2.7 |
| 66 | D0 | 56 | VAL | 2.7 |
| 77 | sR | 318 | ALA | 2.7 |
| 41 | q0 | 77 | ILE | 2.7 |
| 60 | c4 | 36 | LYS | 2.7 |
| 68 | d2 | 117 | ARG | 2.7 |
| 71 | D5 | 89 | ILE | 2.7 |
| 79 | s6 | 32 | ILE | 2.7 |
| 45 | 2 | 504 | U | 2.7 |
| 45 | 6 | 239 | C | 2.7 |
| 63 | C7 | 74 | GLN | 2.7 |
| 65 | c9 | 12 | GLN | 2.7 |
| 68 | D2 | 104 | LEU | 2.7 |
| 73 | d7 | 41 | LEU | 2.7 |
| 76 | e0 | 49 | LEU | 2.7 |
| 79 | s6 | 12 | SER | 2.7 |
| 77 | SR | 182 | ASN | 2.7 |
| 7 | l5 | 180 | PHE | 2.7 |
| 68 | D2 | 67 | GLY | 2.7 |
| 50 | s4 | 84 | ALA | 2.7 |
| 50 | s4 | 149 | TYR | 2.7 |
| 51 | s5 | 32 | GLU | 2.7 |
| 55 | s9 | 4 | ALA | 2.7 |
| 65 | C9 | 122 | ARG | 2.7 |
| 70 | d4 | 20 | ARG | 2.7 |
| 61 | c5 | 109 | PRO | 2.7 |
| 62 | C6 | 53 | LEU | 2.7 |
| 13 | M1 | 96 | PHE | 2.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 28 | n7 | 27 | LYS | 2.7 |
| 47 | S1 | 223 | PHE | 2.7 |
| 77 | SR | 125 | GLY | 2.7 |
| 52 | S6 | 81 | VAL | 2.7 |
| 60 | c4 | 103 | ARG | 2.7 |
| 67 | D1 | 32 | VAL | 2.7 |
| 51 | S5 | 49 | GLU | 2.7 |
| 39 | o8 | 31 | LEU | 2.7 |
| 47 | S1 | 47 | LEU | 2.7 |
| 61 | C5 | 112 | LEU | 2.7 |
| 7 | L5 | 223 | PHE | 2.7 |
| 25 | n4 | 70 | LYS | 2.7 |
| 46 | S0 | 162 | CYS | 2.7 |
| 49 | S3 | 7 | LYS | 2.7 |
| 62 | C6 | 47 | LYS | 2.7 |
| 78 | sM | 54 | PRO | 2.7 |
| 36 | o5 | 57 | VAL | 2.7 |
| 65 | C9 | 68 | ARG | 2.7 |
| 62 | C6 | 103 | ASN | 2.7 |
| 68 | D2 | 74 | VAL | 2.7 |
| 71 | D5 | 81 | ARG | 2.7 |
| 77 | sR | 309 | VAL | 2.7 |
| 1 | 5 | 2539 | C | 2.7 |
| 51 | S5 | 94 | THR | 2.7 |
| 77 | SR | 149 | ASP | 2.7 |
| 49 | S3 | 202 | LEU | 2.7 |
| 53 | S7 | 81 | LEU | 2.7 |
| 66 | d0 | 26 | LEU | 2.7 |
| 35 | o4 | 59 | PRO | 2.7 |
| 54 | S8 | 65 | PHE | 2.7 |
| 77 | SR | 237 | GLN | 2.7 |
| 19 | m8 | 101 | VAL | 2.7 |
| 48 | s2 | 208 | GLU | 2.7 |
| 49 | s3 | 47 | GLU | 2.7 |
| 55 | S9 | 145 | SER | 2.7 |
| 59 | C3 | 21 | ASN | 2.7 |
| 71 | d5 | 104 | ALA | 2.7 |
| 64 | c8 | 91 | ASP | 2.7 |
| 77 | SR | 114 | ASP | 2.7 |
| 25 | n4 | 129 | LYS | 2.7 |
| 46 | s0 | 201 | LEU | 2.7 |
| 49 | s3 | 29 | LEU | 2.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 67 | D1 | 8 | LEU | 2.7 |
| 49 | S3 | 105 | MET | 2.7 |
| 64 | C8 | 74 | GLN | 2.7 |
| 25 | n4 | 66 | GLU | 2.7 |
| 50 | s4 | 5 | PRO | 2.7 |
| 77 | SR | 77 | GLY | 2.7 |
| 7 | l5 | 44 | TYR | 2.7 |
| 7 | l5 | 61 | ILE | 2.7 |
| 37 | o6 | 9 | ILE | 2.7 |
| 61 | c5 | 90 | ILE | 2.7 |
| 77 | SR | 24 | ALA | 2.7 |
| 77 | SR | 170 | ILE | 2.7 |
| 45 | 2 | 1573 | A | 2.7 |
| 48 | S2 | 225 | LEU | 2.7 |
| 58 | c2 | 43 | ARG | 2.7 |
| 61 | C5 | 65 | LEU | 2.7 |
| 66 | d0 | 27 | THR | 2.7 |
| 74 | D8 | 16 | LEU | 2.7 |
| 16 | m5 | 130 | PHE | 2.7 |
| 45 | 2 | 655 | G | 2.7 |
| 47 | s1 | 225 | VAL | 2.7 |
| 50 | S4 | 208 | VAL | 2.7 |
| 54 | S8 | 102 | VAL | 2.7 |
| 50 | s4 | 147 | ILE | 2.7 |
| 54 | s8 | 192 | TYR | 2.6 |
| 60 | c4 | 115 | ILE | 2.7 |
| 48 | s2 | 113 | LEU | 2.6 |
| 51 | S5 | 198 | LEU | 2.6 |
| 77 | sR | 210 | LEU | 2.6 |
| 55 | s9 | 157 | ASP | 2.6 |
| 7 | L5 | 180 | PHE | 2.6 |
| 74 | d8 | 39 | THR | 2.6 |
| 77 | sR | 103 | PHE | 2.6 |
| 37 | o6 | 72 | VAL | 2.6 |
| 60 | C4 | 42 | VAL | 2.6 |
| 79 | s6 | 11 | GLY | 2.6 |
| 11 | L9 | 2 | LYS | 2.6 |
| 50 | s4 | 22 | LYS | 2.6 |
| 55 | s9 | 37 | LYS | 2.6 |
| 20 | m9 | 173 | ARG | 2.6 |
| 20 | m9 | 183 | ALA | 2.6 |
| 50 | s4 | 92 | LEU | 2.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | S5 | 81 | ARG | 2.6 |
| 54 | S8 | 184 | LEU | 2.6 |
| 63 | C7 | 24 | LEU | 2.6 |
| 75 | D9 | 40 | ARG | 2.6 |
| 77 | SR | 171 | SER | 2.6 |
| 50 | S4 | 157 | ASN | 2.6 |
| 35 | o4 | 72 | VAL | 2.6 |
| 49 | S3 | 44 | THR | 2.6 |
| 50 | S4 | 134 | LYS | 2.6 |
| 50 | S4 | 211 | LYS | 2.6 |
| 51 | S5 | 23 | VAL | 2.6 |
| 56 | c0 | 58 | GLN | 2.6 |
| 60 | c4 | 88 | GLY | 2.6 |
| 62 | C6 | 33 | GLY | 2.6 |
| 64 | C8 | 20 | THR | 2.6 |
| 71 | D5 | 52 | LYS | 2.6 |
| 78 | sM | 64 | LYS | 2.6 |
| 14 | m3 | 89 | TYR | 2.6 |
| 26 | n5 | 38 | LEU | 2.6 |
| 50 | S4 | 147 | ILE | 2.6 |
| 66 | d0 | 95 | ALA | 2.6 |
| 61 | c5 | 45 | PHE | 2.6 |
| 51 | S5 | 99 | MET | 2.6 |
| 55 | S9 | 91 | LYS | 2.6 |
| 60 | c4 | 10 | ASN | 2.6 |
| 68 | D2 | 123 | GLY | 2.6 |
| 78 | sM | 23 | LYS | 2.6 |
| 48 | S2 | 91 | ARG | 2.6 |
| 62 | c6 | 100 | GLN | 2.6 |
| 45 | 6 | 1688 | U | 2.6 |
| 10 | l8 | 199 | ALA | 2.6 |
| 51 | S5 | 114 | ILE | 2.6 |
| 53 | S7 | 135 | ILE | 2.6 |
| 55 | S9 | 129 | ILE | 2.6 |
| 77 | SR | 234 | LEU | 2.6 |
| 79 | s6 | 5 | ILE | 2.6 |
| 53 | S7 | 24 | PHE | 2.6 |
| 77 | sR | 61 | PHE | 2.6 |
| 68 | D2 | 58 | SER | 2.6 |
| 77 | sR | 120 | SER | 2.6 |
| 43 | q2 | 75 | VAL | 2.6 |
| 48 | s2 | 167 | VAL | 2.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 66 | D0 | 92 | ASP | 2.6 |
| 72 | D6 | 42 | ARG | 2.6 |
| 72 | d6 | 84 | VAL | 2.6 |
| 77 | SR | 113 | VAL | 2.6 |
| 26 | n5 | 57 | LEU | 2.6 |
| 51 | S5 | 121 | ILE | 2.6 |
| 51 | S5 | 136 | ALA | 2.6 |
| 55 | S9 | 36 | LEU | 2.6 |
| 55 | S9 | 76 | LEU | 2.6 |
| 66 | D0 | 22 | ILE | 2.6 |
| 77 | SR | 169 | ILE | 2.6 |
| 77 | sR | 310 | ILE | 2.6 |
| 29 | n8 | 119 | PRO | 2.6 |
| 51 | S5 | 46 | TRP | 2.6 |
| 58 | c2 | 120 | VAL | 2.6 |
| 65 | c9 | 134 | ARG | 2.6 |
| 67 | d1 | 65 | SER | 2.6 |
| 29 | n8 | 65 | GLN | 2.6 |
| 51 | s5 | 35 | GLN | 2.6 |
| 59 | C3 | 16 | ILE | 2.6 |
| 16 | m5 | 43 | THR | 2.6 |
| 55 | s9 | 183 | ALA | 2.6 |
| 64 | c8 | 132 | ARG | 2.6 |
| 65 | c9 | 21 | PHE | 2.6 |
| 77 | SR | 103 | PHE | 2.6 |
| 79 | s6 | 149 | LYS | 2.6 |
| 29 | N8 | 117 | ARG | 2.6 |
| 77 | sR | 155 | ARG | 2.6 |
| 71 | d5 | 53 | GLU | 2.6 |
| 79 | s6 | 134 | GLY | 2.6 |
| 29 | n8 | 118 | ILE | 2.6 |
| 31 | O0 | 101 | LEU | 2.6 |
| 58 | c2 | 142 | GLN | 2.6 |
| 59 | C3 | 50 | ILE | 2.6 |
| 60 | c4 | 19 | ILE | 2.6 |
| 65 | C9 | 79 | LEU | 2.6 |
| 66 | D0 | 86 | ILE | 2.6 |
| 74 | d8 | 56 | LEU | 2.6 |
| 77 | SR | 299 | GLN | 2.6 |
| 12 | m0 | 108 | ALA | 2.6 |
| 13 | M1 | 20 | ASN | 2.6 |
| 35 | o4 | 92 | ALA | 2.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 58 | c2 | 92 | ALA | 2.6 |
| 59 | C3 | 40 | TYR | 2.6 |
| 65 | C9 | 77 | ASN | 2.6 |
| 67 | D1 | 22 | ARG | 2.6 |
| 77 | sR | 178 | VAL | 2.6 |
| 61 | c5 | 83 | MET | 2.6 |
| 64 | C8 | 73 | MET | 2.6 |
| 53 | s7 | 77 | LEU | 2.6 |
| 64 | c8 | 66 | LEU | 2.6 |
| 66 | D0 | 24 | ILE | 2.6 |
| 79 | s6 | 190 | GLN | 2.6 |
| 4 | l2 | 70 | ARG | 2.6 |
| 11 | L9 | 92 | TYR | 2.6 |
| 47 | s1 | 41 | ARG | 2.6 |
| 1 | 1 | 2971 | A | 2.6 |
| 79 | s6 | 56 | ASN | 2.6 |
| 57 | C1 | 61 | THR | 2.6 |
| 7 | L5 | 156 | GLY | 2.6 |
| 28 | n7 | 89 | VAL | 2.6 |
| 48 | s2 | 105 | GLY | 2.6 |
| 50 | S4 | 36 | HIS | 2.6 |
| 71 | D5 | 54 | VAL | 2.6 |
| 79 | s6 | 97 | VAL | 2.6 |
| 22 | n1 | 31 | LEU | 2.6 |
| 36 | o5 | 55 | LEU | 2.6 |
| 58 | c2 | 126 | TRP | 2.6 |
| 49 | S3 | 54 | ARG | 2.6 |
| 53 | S7 | 60 | ILE | 2.6 |
| 70 | d4 | 125 | LEU | 2.6 |
| 62 | c6 | 139 | GLN | 2.6 |
| 13 | M1 | 167 | TYR | 2.6 |
| 73 | d7 | 64 | CYS | 2.6 |
| 62 | c6 | 98 | ASP | 2.6 |
| 22 | n1 | 50 | LYS | 2.6 |
| 28 | n7 | 69 | LYS | 2.6 |
| 51 | s5 | 149 | VAL | 2.6 |
| 55 | S9 | 35 | GLY | 2.6 |
| 58 | c2 | 75 | VAL | 2.6 |
| 60 | C4 | 28 | VAL | 2.6 |
| 65 | C9 | 92 | LYS | 2.6 |
| 77 | sR | 233 | THR | 2.6 |
| 1 | 5 | 1351 | U | 2.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 15 | M4 | 38 | ILE | 2.6 |
| 63 | C7 | 16 | LEU | 2.6 |
| 14 | m3 | 160 | GLN | 2.6 |
| 12 | M0 | 108 | ALA | 2.6 |
| 25 | n4 | 125 | ALA | 2.6 |
| 6 | l4 | 177 | ASP | 2.6 |
| 77 | SR | 152 | SER | 2.6 |
| 7 | l5 | 43 | LYS | 2.6 |
| 39 | o8 | 13 | GLU | 2.6 |
| 47 | s1 | 150 | VAL | 2.6 |
| 48 | S2 | 49 | LYS | 2.6 |
| 66 | d0 | 30 | LYS | 2.6 |
| 77 | SR | 238 | ASP | 2.6 |
| 49 | s3 | 62 | ASN | 2.6 |
| 55 | S9 | 141 | VAL | 2.6 |
| 48 | s2 | 91 | ARG | 2.6 |
| 30 | n9 | 48 | HIS | 2.6 |
| 53 | s7 | 81 | LEU | 2.6 |
| 64 | C8 | 61 | LEU | 2.6 |
| 48 | s2 | 218 | ILE | 2.6 |
| 49 | s3 | 50 | ILE | 2.6 |
| 51 | S5 | 89 | ILE | 2.6 |
| 55 | S9 | 140 | ILE | 2.6 |
| 1 | 5 | 3276 | G | 2.6 |
| 4 | l2 | 34 | TYR | 2.6 |
| 12 | M0 | 106 | ALA | 2.6 |
| 30 | N9 | 56 | ALA | 2.6 |
| 51 | S5 | 86 | GLN | 2.6 |
| 61 | C5 | 56 | PHE | 2.6 |
| 60 | c4 | 60 | ALA | 2.6 |
| 61 | c5 | 74 | ALA | 2.6 |
| 50 | S4 | 185 | GLY | 2.6 |
| 51 | s5 | 39 | GLU | 2.6 |
| 62 | C6 | 13 | LYS | 2.6 |
| 77 | SR | 20 | VAL | 2.6 |
| 77 | SR | 138 | GLY | 2.6 |
| 77 | SR | 286 | GLU | 2.6 |
| 50 | S4 | 196 | VAL | 2.6 |
| 51 | s5 | 145 | ASP | 2.6 |
| 58 | c2 | 122 | VAL | 2.6 |
| 79 | s6 | 6 | SER | 2.6 |
| 79 | s6 | 67 | VAL | 2.6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | L9 | 112 | ILE | 2.6 |
| 28 | N7 | 66 | THR | 2.6 |
| 46 | s0 | 6 | THR | 2.6 |
| 50 | S4 | 244 | ILE | 2.6 |
| 51 | s5 | 90 | ILE | 2.6 |
| 72 | d6 | 83 | ILE | 2.6 |
| 77 | SR | 231 | MET | 2.6 |
| 62 | c6 | 109 | PHE | 2.5 |
| 12 | m0 | 219 | ALA | 2.5 |
| 23 | N2 | 10 | LYS | 2.5 |
| 54 | S8 | 74 | LYS | 2.5 |
| 65 | c9 | 17 | ALA | 2.5 |
| 7 | l5 | 216 | GLU | 2.5 |
| 58 | c2 | 83 | GLU | 2.5 |
| 75 | D9 | 34 | TYR | 2.5 |
| 45 | 6 | 230 | C | 2.5 |
| 70 | D4 | 27 | VAL | 2.5 |
| 77 | SR | 68 | VAL | 2.5 |
| 74 | d8 | 9 | LEU | 2.5 |
| 4 | l2 | 97 | ASN | 2.5 |
| 11 | L9 | 4 | ILE | 2.5 |
| 26 | n5 | 63 | ILE | 2.5 |
| 54 | S8 | 60 | ILE | 2.5 |
| 50 | S4 | 75 | LYS | 2.5 |
| 50 | S4 | 218 | PHE | 2.5 |
| 59 | C3 | 26 | PHE | 2.5 |
| 67 | D1 | 21 | ASN | 2.5 |
| 71 | d5 | 50 | ILE | 2.5 |
| 51 | S5 | 176 | THR | 2.5 |
| 68 | D2 | 119 | LYS | 2.5 |
| 75 | d9 | 54 | LYS | 2.5 |
| 28 | N7 | 2 | ALA | 2.5 |
| 13 | m1 | 124 | GLY | 2.5 |
| 58 | c2 | 104 | GLY | 2.5 |
| 74 | d8 | 24 | GLY | 2.5 |
| 41 | q0 | 82 | LEU | 2.5 |
| 45 | 6 | 558 | U | 2.5 |
| 45 | 6 | 1687 | U | 2.5 |
| 46 | s0 | 146 | LEU | 2.5 |
| 22 | n1 | 48 | ILE | 2.5 |
| 36 | o5 | 78 | LYS | 2.5 |
| 45 | 6 | 237 | C | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 65 | c9 | 5 | SER | 2.5 |
| 47 | S1 | 83 | LYS | 2.5 |
| 70 | D4 | 11 | LYS | 2.5 |
| 78 | sM | 84 | LYS | 2.5 |
| 45 | 6 | 228 | G | 2.5 |
| 47 | S1 | 99 | ASN | 2.5 |
| 50 | S4 | 153 | ASN | 2.5 |
| 29 | n8 | 98 | THR | 2.5 |
| 51 | S5 | 66 | GLN | 2.5 |
| 56 | C0 | 66 | TYR | 2.5 |
| 62 | c6 | 143 | ARG | 2.5 |
| 66 | D0 | 90 | TYR | 2.5 |
| 77 | sR | 139 | GLN | 2.5 |
| 79 | s6 | 110 | ALA | 2.5 |
| 6 | l4 | 303 | GLY | 2.5 |
| 54 | s8 | 102 | VAL | 2.5 |
| 13 | M1 | 40 | LEU | 2.5 |
| 57 | c1 | 69 | LYS | 2.5 |
| 59 | c3 | 45 | LEU | 2.5 |
| 27 | n6 | 45 | ILE | 2.5 |
| 29 | N8 | 118 | ILE | 2.5 |
| 39 | O8 | 56 | ILE | 2.5 |
| 58 | c2 | 71 | ILE | 2.5 |
| 73 | d7 | 47 | PHE | 2.5 |
| 79 | s6 | 29 | ASP | 2.5 |
| 4 | l2 | 149 | ARG | 2.5 |
| 10 | l8 | 44 | ARG | 2.5 |
| 32 | o1 | 31 | ARG | 2.5 |
| 47 | S1 | 46 | THR | 2.5 |
| 50 | S4 | 231 | GLN | 2.5 |
| 60 | C4 | 21 | ALA | 2.5 |
| 60 | c4 | 80 | HIS | 2.5 |
| 62 | C6 | 88 | GLY | 2.5 |
| 67 | D1 | 33 | GLN | 2.5 |
| 70 | d4 | 55 | VAL | 2.5 |
| 77 | SR | 201 | THR | 2.5 |
| 7 | L5 | 236 | LEU | 2.5 |
| 49 | s3 | 59 | LEU | 2.5 |
| 55 | S9 | 10 | LYS | 2.5 |
| 57 | C1 | 40 | LEU | 2.5 |
| 50 | S4 | 236 | ILE | 2.5 |
| 52 | S6 | 101 | ILE | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 12 | M0 | 47 | PRO | 2.5 |
| 12 | M0 | 104 | SER | 2.5 |
| 22 | n1 | 86 | GLU | 2.5 |
| 45 | 2 | 238 | U | 2.5 |
| 58 | C2 | 119 | SER | 2.5 |
| 65 | c9 | 126 | GLU | 2.5 |
| 10 | l8 | 39 | ALA | 2.5 |
| 13 | M1 | 70 | THR | 2.5 |
| 22 | n1 | 25 | VAL | 2.5 |
| 47 | s1 | 21 | VAL | 2.5 |
| 50 | S4 | 126 | VAL | 2.5 |
| 51 | S5 | 35 | GLN | 2.5 |
| 56 | C0 | 12 | HIS | 2.5 |
| 60 | c4 | 42 | VAL | 2.5 |
| 60 | c4 | 81 | VAL | 2.5 |
| 77 | SR | 133 | VAL | 2.5 |
| 13 | m1 | 60 | ARG | 2.5 |
| 29 | N8 | 124 | ILE | 2.5 |
| 46 | S0 | 170 | ILE | 2.5 |
| 13 | m1 | 26 | SER | 2.5 |
| 27 | n6 | 53 | ASP | 2.5 |
| 56 | c0 | 60 | SER | 2.5 |
| 7 | l5 | 122 | VAL | 2.5 |
| 10 | l8 | 114 | ALA | 2.5 |
| 11 | L9 | 93 | VAL | 2.5 |
| 58 | c2 | 42 | ALA | 2.5 |
| 60 | c4 | 47 | LYS | 2.5 |
| 55 | s9 | 112 | GLN | 2.5 |
| 61 | C5 | 116 | LEU | 2.5 |
| 7 | l5 | 153 | THR | 2.5 |
| 72 | d6 | 51 | ARG | 2.5 |
| 77 | SR | 233 | THR | 2.5 |
| 54 | s8 | 60 | ILE | 2.5 |
| 28 | n7 | 9 | LYS | 2.5 |
| 51 | s5 | 213 | LYS | 2.5 |
| 52 | S6 | 222 | GLU | 2.5 |
| 62 | C6 | 113 | ASP | 2.5 |
| 79 | s6 | 51 | LYS | 2.5 |
| 11 | L9 | 3 | TYR | 2.5 |
| 16 | m5 | 6 | TYR | 2.5 |
| 46 | S0 | 36 | TYR | 2.5 |
| 63 | c7 | 65 | PRO | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 73 | d7 | 54 | VAL | 2.5 |
| 28 | n7 | 103 | GLN | 2.5 |
| 34 | O3 | 60 | ARG | 2.5 |
| 47 | S1 | 218 | LEU | 2.5 |
| 50 | S4 | 238 | LEU | 2.5 |
| 54 | s8 | 44 | HIS | 2.5 |
| 74 | d8 | 61 | ARG | 2.5 |
| 4 | l2 | 100 | ASN | 2.5 |
| 46 | S0 | 173 | ILE | 2.5 |
| 49 | s3 | 152 | PHE | 2.5 |
| 55 | s9 | 146 | PHE | 2.5 |
| 57 | C1 | 20 | PHE | 2.5 |
| 58 | c2 | 140 | PHE | 2.5 |
| 77 | SR | 224 | ASN | 2.5 |
| 77 | sR | 182 | ASN | 2.5 |
| 53 | S7 | 98 | ILE | 2.5 |
| 62 | c6 | 17 | THR | 2.5 |
| 11 | L9 | 189 | GLU | 2.5 |
| 62 | c6 | 99 | GLU | 2.5 |
| 70 | D4 | 37 | LYS | 2.5 |
| 10 | L8 | 189 | LEU | 2.5 |
| 28 | N7 | 44 | ALA | 2.5 |
| 28 | N7 | 62 | VAL | 2.5 |
| 48 | s2 | 196 | VAL | 2.5 |
| 51 | s5 | 56 | ALA | 2.5 |
| 52 | S6 | 177 | ARG | 2.5 |
| 58 | c2 | 20 | ALA | 2.5 |
| 77 | sR | 83 | ALA | 2.5 |
| 27 | N6 | 42 | GLN | 2.5 |
| 56 | c0 | 12 | HIS | 2.5 |
| 64 | c8 | 122 | HIS | 2.5 |
| 16 | m5 | 122 | ASN | 2.5 |
| 43 | q2 | 24 | LYS | 2.5 |
| 62 | c6 | 70 | THR | 2.5 |
| 77 | sR | 46 | LYS | 2.5 |
| 35 | o4 | 110 | GLU | 2.5 |
| 13 | m1 | 128 | TYR | 2.5 |
| 14 | M3 | 119 | TYR | 2.5 |
| 29 | n8 | 127 | ALA | 2.5 |
| 43 | q2 | 35 | LEU | 2.5 |
| 49 | S3 | 73 | VAL | 2.5 |
| 49 | s3 | 60 | GLY | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | c7 | 80 | ARG | 2.5 |
| 55 | s9 | 128 | LEU | 2.5 |
| 66 | d0 | 31 | VAL | 2.5 |
| 71 | d5 | 62 | VAL | 2.5 |
| 76 | E0 | 42 | ARG | 2.5 |
| 48 | S2 | 138 | PRO | 2.5 |
| 52 | S6 | 8 | PRO | 2.5 |
| 10 | l8 | 121 | SER | 2.5 |
| 54 | s8 | 170 | SER | 2.5 |
| 65 | c9 | 25 | GLN | 2.5 |
| 68 | D2 | 37 | PHE | 2.5 |
| 77 | sR | 87 | LYS | 2.5 |
| 11 | l9 | 59 | ASN | 2.5 |
| 13 | m1 | 63 | GLU | 2.5 |
| 35 | o4 | 60 | ARG | 2.5 |
| 61 | c5 | 108 | ARG | 2.5 |
| 64 | c8 | 19 | ASN | 2.5 |
| 7 | L5 | 51 | LEU | 2.5 |
| 28 | n7 | 113 | VAL | 2.5 |
| 29 | N8 | 130 | VAL | 2.5 |
| 61 | C5 | 63 | ALA | 2.5 |
| 63 | c7 | 73 | LEU | 2.5 |
| 79 | s6 | 129 | VAL | 2.5 |
| 47 | S1 | 128 | LYS | 2.5 |
| 57 | C1 | 16 | GLN | 2.5 |
| 77 | SR | 247 | PRO | 2.5 |
| 4 | l2 | 135 | ILE | 2.5 |
| 13 | M1 | 14 | ILE | 2.5 |
| 28 | N7 | 105 | SER | 2.5 |
| 30 | n9 | 21 | ILE | 2.5 |
| 48 | s2 | 139 | ILE | 2.5 |
| 7 | l5 | 154 | THR | 2.5 |
| 27 | N6 | 104 | LEU | 2.5 |
| 56 | c0 | 68 | LEU | 2.5 |
| 76 | E0 | 4 | VAL | 2.5 |
| 49 | s3 | 141 | LYS | 2.5 |
| 54 | s8 | 182 | TYR | 2.5 |
| 59 | C3 | 27 | LYS | 2.5 |
| 62 | c6 | 8 | GLN | 2.5 |
| 48 | s2 | 110 | HIS | 2.5 |
| 61 | c5 | 40 | ARG | 2.5 |
| 63 | c7 | 41 | ILE | 2.5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | L5 | 171 | LEU | 2.4 |
| 47 | s1 | 124 | ASN | 2.4 |
| 51 | s5 | 165 | LEU | 2.4 |
| 58 | c2 | 103 | LEU | 2.4 |
| 62 | C6 | 90 | VAL | 2.4 |
| 66 | D0 | 63 | LEU | 2.4 |
| 51 | S5 | 210 | ALA | 2.4 |
| 60 | c4 | 26 | THR | 2.4 |
| 62 | c6 | 46 | PHE | 2.4 |
| 46 | s0 | 160 | ILE | 2.4 |
| 49 | s3 | 84 | ILE | 2.4 |
| 51 | s5 | 121 | ILE | 2.4 |
| 64 | c8 | 69 | ILE | 2.4 |
| 74 | d8 | 64 | ARG | 2.4 |
| 77 | SR | 266 | ASP | 2.4 |
| 27 | N6 | 105 | VAL | 2.4 |
| 28 | n7 | 21 | LYS | 2.4 |
| 35 | O4 | 66 | SER | 2.4 |
| 46 | s0 | 176 | LEU | 2.4 |
| 50 | S4 | 42 | LEU | 2.4 |
| 50 | s4 | 6 | LYS | 2.4 |
| 52 | S6 | 109 | LEU | 2.4 |
| 58 | C2 | 58 | LEU | 2.4 |
| 62 | c6 | 57 | LEU | 2.4 |
| 64 | c8 | 130 | GLY | 2.4 |
| 66 | D0 | 51 | VAL | 2.4 |
| 71 | D5 | 72 | GLY | 2.4 |
| 25 | n4 | 104 | ASN | 2.4 |
| 39 | O8 | 15 | THR | 2.4 |
| 47 | S1 | 42 | ASN | 2.4 |
| 50 | S4 | 99 | PHE | 2.4 |
| 76 | E0 | 35 | TYR | 2.4 |
| 10 | l8 | 153 | ILE | 2.4 |
| 13 | m1 | 21 | ILE | 2.4 |
| 51 | s5 | 144 | GLU | 2.4 |
| 55 | S9 | 138 | LYS | 2.4 |
| 20 | m9 | 18 | GLY | 2.4 |
| 49 | s3 | 136 | VAL | 2.4 |
| 51 | s5 | 205 | SER | 2.4 |
| 58 | C2 | 116 | VAL | 2.4 |
| 58 | c2 | 78 | LEU | 2.4 |
| 68 | D2 | 7 | LEU | 2.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 70 | d4 | 56 | SER | 2.4 |
| 51 | s5 | 82 | PHE | 2.4 |
| 58 | c2 | 101 | ALA | 2.4 |
| 67 | d1 | 53 | TYR | 2.4 |
| 70 | D4 | 60 | PHE | 2.4 |
| 62 | C6 | 62 | ASN | 2.4 |
| 13 | m1 | 108 | GLU | 2.4 |
| 22 | N1 | 100 | LYS | 2.4 |
| 25 | n4 | 77 | LYS | 2.4 |
| 45 | 2 | 1060 | U | 2.4 |
| 49 | S3 | 115 | ILE | 2.4 |
| 62 | c6 | 106 | LYS | 2.4 |
| 63 | c7 | 29 | GLN | 2.4 |
| 65 | c9 | 84 | LYS | 2.4 |
| 68 | D2 | 86 | ILE | 2.4 |
| 10 | l8 | 203 | VAL | 2.4 |
| 11 | L9 | 85 | GLY | 2.4 |
| 12 | M0 | 48 | LEU | 2.4 |
| 30 | n9 | 45 | HIS | 2.4 |
| 55 | s9 | 85 | VAL | 2.4 |
| 62 | c6 | 33 | GLY | 2.4 |
| 77 | sR | 68 | VAL | 2.4 |
| 79 | s6 | 88 | ARG | 2.4 |
| 30 | n9 | 27 | TYR | 2.4 |
| 65 | C9 | 33 | TYR | 2.4 |
| 22 | n1 | 42 | ILE | 2.4 |
| 49 | S3 | 185 | LYS | 2.4 |
| 54 | S8 | 137 | LYS | 2.4 |
| 77 | SR | 277 | GLU | 2.4 |
| 46 | S0 | 147 | THR | 2.4 |
| 60 | c4 | 89 | THR | 2.4 |
| 21 | N0 | 76 | GLY | 2.4 |
| 46 | s0 | 166 | GLY | 2.4 |
| 47 | s1 | 61 | LEU | 2.4 |
| 50 | s4 | 46 | VAL | 2.4 |
| 50 | s4 | 136 | VAL | 2.4 |
| 56 | c0 | 76 | LEU | 2.4 |
| 59 | C3 | 60 | VAL | 2.4 |
| 65 | c9 | 121 | GLY | 2.4 |
| 71 | d5 | 69 | LEU | 2.4 |
| 76 | e0 | 54 | ARG | 2.4 |
| 79 | s6 | 54 | GLY | 2.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 31 | o0 | 105 | ALA | 2.4 |
| 49 | s3 | 92 | GLN | 2.4 |
| 10 | l8 | 197 | VAL | 2.4 |
| 51 | S5 | 102 | ARG | 2.4 |
| 51 | s5 | 125 | THR | 2.4 |
| 52 | S6 | 68 | LEU | 2.4 |
| 62 | c6 | 90 | VAL | 2.4 |
| 62 | c6 | 110 | THR | 2.4 |
| 63 | c7 | 16 | LEU | 2.4 |
| 76 | E0 | 41 | THR | 2.4 |
| 77 | SR | 194 | GLY | 2.4 |
| 45 | 2 | 192 | U | 2.4 |
| 79 | s6 | 28 | PHE | 2.4 |
| 7 | l5 | 183 | TRP | 2.4 |
| 21 | N0 | 2 | ALA | 2.4 |
| 36 | o5 | 51 | ILE | 2.4 |
| 51 | s5 | 57 | SER | 2.4 |
| 22 | n1 | 89 | LEU | 2.4 |
| 24 | n3 | 7 | GLN | 2.4 |
| 22 | n1 | 61 | THR | 2.4 |
| 49 | s3 | 55 | THR | 2.4 |
| 50 | S4 | 135 | GLY | 2.4 |
| 51 | S5 | 67 | PRO | 2.4 |
| 59 | C3 | 67 | THR | 2.4 |
| 64 | c8 | 75 | ASN | 2.4 |
| 62 | c6 | 102 | LYS | 2.4 |
| 62 | c6 | 133 | GLY | 2.4 |
| 74 | D8 | 30 | VAL | 2.4 |
| 78 | SM | 50 | ASN | 2.4 |
| 79 | s6 | 41 | VAL | 2.4 |
| 54 | S8 | 53 | LYS | 2.4 |
| 23 | n2 | 33 | TYR | 2.4 |
| 8 | l6 | 130 | ILE | 2.4 |
| 13 | M1 | 79 | ILE | 2.4 |
| 19 | m8 | 69 | ARG | 2.4 |
| 29 | N8 | 82 | ILE | 2.4 |
| 56 | c0 | 77 | ARG | 2.4 |
| 29 | n8 | 105 | LEU | 2.4 |
| 46 | S0 | 73 | VAL | 2.4 |
| 70 | d4 | 96 | LEU | 2.4 |
| 79 | s6 | 3 | LEU | 2.4 |
| 14 | m3 | 76 | THR | 2.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | N0 | 4 | PHE | 2.4 |
| 46 | S0 | 39 | ASN | 2.4 |
| 68 | D2 | 48 | GLY | 2.4 |
| 49 | s3 | 25 | PHE | 2.4 |
| 49 | s3 | 70 | THR | 2.4 |
| 55 | s9 | 169 | PRO | 2.4 |
| 13 | M1 | 66 | ALA | 2.4 |
| 4 | l2 | 88 | ILE | 2.4 |
| 13 | M1 | 59 | ILE | 2.4 |
| 50 | S4 | 212 | ASP | 2.4 |
| 73 | d7 | 53 | ALA | 2.4 |
| 45 | 6 | 1491 | U | 2.4 |
| 63 | C7 | 50 | ILE | 2.4 |
| 29 | n8 | 101 | VAL | 2.4 |
| 56 | c0 | 44 | LYS | 2.4 |
| 68 | D2 | 39 | GLN | 2.4 |
| 77 | SR | 71 | CYS | 2.4 |
| 35 | o4 | 93 | PHE | 2.4 |
| 55 | S9 | 32 | GLY | 2.4 |
| 27 | N6 | 43 | TYR | 2.4 |
| 46 | S0 | 53 | THR | 2.4 |
| 51 | S5 | 73 | THR | 2.4 |
| 74 | D8 | 22 | ARG | 2.4 |
| 45 | 6 | 503 | G | 2.4 |
| 53 | S7 | 91 | ILE | 2.4 |
| 53 | s7 | 91 | ILE | 2.4 |
| 58 | c2 | 93 | ASP | 2.4 |
| 64 | C8 | 28 | ILE | 2.4 |
| 64 | C8 | 80 | LYS | 2.4 |
| 66 | d0 | 77 | LYS | 2.4 |
| 71 | D5 | 43 | ASP | 2.4 |
| 55 | S9 | 99 | LEU | 2.4 |
| 13 | m1 | 34 | SER | 2.4 |
| 43 | Q2 | 106 | PHE | 2.4 |
| 63 | c7 | 42 | GLN | 2.4 |
| 37 | o6 | 62 | ARG | 2.4 |
| 36 | o5 | 84 | LYS | 2.4 |
| 38 | o7 | 86 | ALA | 2.4 |
| 57 | c1 | 146 | ALA | 2.4 |
| 61 | c5 | 88 | GLU | 2.4 |
| 65 | C9 | 127 | ASN | 2.4 |
| 71 | d5 | 100 | ILE | 2.4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | sR | 41 | THR | 2.4 |
| 13 | M1 | 17 | LEU | 2.4 |
| 65 | c9 | 28 | LEU | 2.4 |
| 4 | L2 | 248 | GLY | 2.4 |
| 22 | N1 | 40 | VAL | 2.4 |
| 68 | D2 | 129 | VAL | 2.4 |
| 10 | l8 | 94 | PHE | 2.4 |
| 26 | n5 | 32 | PHE | 2.4 |
| 50 | S4 | 41 | SER | 2.4 |
| 77 | SR | 166 | SER | 2.4 |
| 10 | l8 | 245 | LYS | 2.4 |
| 48 | s2 | 85 | PRO | 2.4 |
| 65 | C9 | 136 | ALA | 2.4 |
| 71 | D5 | 85 | LYS | 2.4 |
| 77 | SR | 53 | LYS | 2.4 |
| 78 | sM | 49 | LYS | 2.4 |
| 19 | m8 | 100 | THR | 2.4 |
| 29 | N8 | 102 | ILE | 2.4 |
| 35 | O4 | 54 | ILE | 2.4 |
| 51 | S5 | 103 | ASN | 2.4 |
| 53 | S7 | 46 | ILE | 2.4 |
| 41 | Q0 | 127 | LEU | 2.4 |
| 46 | S0 | 172 | LEU | 2.4 |
| 53 | S7 | 154 | LEU | 2.4 |
| 12 | M0 | 114 | GLY | 2.3 |
| 75 | D9 | 52 | PHE | 2.3 |
| 58 | c2 | 132 | GLU | 2.3 |
| 66 | D0 | 66 | SER | 2.3 |
| 77 | SR | 132 | LYS | 2.3 |
| 1 | 1 | 2522 | G | 2.3 |
| 7 | l5 | 92 | LEU | 2.3 |
| 47 | S1 | 168 | ILE | 2.3 |
| 74 | d8 | 10 | ALA | 2.3 |
| 77 | sR | 255 | ALA | 2.3 |
| 79 | s6 | 100 | ALA | 2.3 |
| 1 | 1 | 2539 | C | 2.3 |
| 13 | m1 | 130 | VAL | 2.3 |
| 22 | n1 | 45 | ASN | 2.3 |
| 48 | s2 | 184 | VAL | 2.3 |
| 50 | S4 | 11 | ARG | 2.3 |
| 57 | C1 | 135 | VAL | 2.3 |
| 64 | c8 | 120 | ARG | 2.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 73 | D7 | 49 | HIS | 2.3 |
| 74 | d8 | 30 | VAL | 2.3 |
| 74 | d8 | 51 | ASN | 2.3 |
| 26 | n5 | 84 | PHE | 2.3 |
| 39 | O8 | 43 | PHE | 2.3 |
| 77 | SR | 19 | TRP | 2.3 |
| 77 | SR | 294 | TRP | 2.3 |
| 12 | M0 | 76 | MET | 2.3 |
| 77 | SR | 87 | LYS | 2.3 |
| 1 | 5 | 1763 | U | 2.3 |
| 4 | l2 | 96 | LEU | 2.3 |
| 10 | l8 | 237 | ILE | 2.3 |
| 15 | m4 | 58 | ILE | 2.3 |
| 25 | n4 | 80 | ARG | 2.3 |
| 50 | S4 | 239 | PRO | 2.3 |
| 55 | s9 | 140 | ILE | 2.3 |
| 63 | C7 | 38 | ILE | 2.3 |
| 61 | c5 | 127 | ARG | 2.3 |
| 64 | c8 | 126 | ARG | 2.3 |
| 67 | d1 | 69 | LEU | 2.3 |
| 30 | N9 | 52 | LYS | 2.3 |
| 51 | S5 | 80 | LYS | 2.3 |
| 54 | S8 | 138 | ASN | 2.3 |
| 61 | c5 | 100 | LYS | 2.3 |
| 63 | C7 | 31 | ASN | 2.3 |
| 65 | C9 | 14 | PHE | 2.3 |
| 66 | d0 | 70 | THR | 2.3 |
| 74 | d8 | 8 | THR | 2.3 |
| 18 | M7 | 179 | GLN | 2.3 |
| 51 | s5 | 50 | GLU | 2.3 |
| 1 | 5 | 1814 | A | 2.3 |
| 7 | l5 | 77 | ALA | 2.3 |
| 47 | S1 | 172 | LEU | 2.3 |
| 48 | s2 | 143 | TYR | 2.3 |
| 48 | s2 | 169 | LEU | 2.3 |
| 50 | S4 | 169 | ILE | 2.3 |
| 51 | s5 | 29 | ILE | 2.3 |
| 54 | s8 | 43 | ILE | 2.3 |
| 62 | C6 | 96 | TYR | 2.3 |
| 77 | SR | 295 | SER | 2.3 |
| 45 | 2 | 1682 | U | 2.3 |
| 23 | N2 | 28 | PHE | 2.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | S2 | 88 | LYS | 2.3 |
| 49 | S3 | 161 | GLY | 2.3 |
| 50 | s4 | 208 | VAL | 2.3 |
| 77 | sR | 283 | LYS | 2.3 |
| 78 | SM | 67 | GLY | 2.3 |
| 14 | M3 | 92 | THR | 2.3 |
| 47 | S1 | 229 | MET | 2.3 |
| 43 | Q2 | 105 | GLN | 2.3 |
| 47 | S1 | 220 | GLN | 2.3 |
| 49 | s3 | 38 | GLU | 2.3 |
| 55 | S9 | 33 | GLU | 2.3 |
| 1 | 1 | 1578 | C | 2.3 |
| 1 | 5 | 1812 | G | 2.3 |
| 37 | o6 | 70 | ARG | 2.3 |
| 49 | s3 | 190 | ARG | 2.3 |
| 64 | C8 | 145 | ARG | 2.3 |
| 74 | d8 | 42 | ARG | 2.3 |
| 47 | s1 | 218 | LEU | 2.3 |
| 49 | s3 | 176 | LEU | 2.3 |
| 49 | s3 | 205 | ALA | 2.3 |
| 77 | sR | 232 | TYR | 2.3 |
| 11 | L9 | 55 | VAL | 2.3 |
| 48 | S2 | 101 | VAL | 2.3 |
| 49 | s3 | 126 | VAL | 2.3 |
| 50 | S4 | 31 | PRO | 2.3 |
| 58 | C2 | 90 | LYS | 2.3 |
| 65 | c9 | 20 | SER | 2.3 |
| 66 | D0 | 118 | VAL | 2.3 |
| 69 | d3 | 145 | SER | 2.3 |
| 77 | sR | 37 | SER | 2.3 |
| 7 | L5 | 170 | GLY | 2.3 |
| 22 | N1 | 146 | ASN | 2.3 |
| 49 | s3 | 103 | GLU | 2.3 |
| 63 | C7 | 76 | GLU | 2.3 |
| 50 | S4 | 159 | THR | 2.3 |
| 28 | n7 | 73 | LYS | 2.3 |
| 48 | s2 | 187 | LEU | 2.3 |
| 56 | c0 | 11 | ILE | 2.3 |
| 61 | c5 | 123 | TYR | 2.3 |
| 63 | C7 | 41 | ILE | 2.3 |
| 74 | D8 | 40 | ILE | 2.3 |
| 32 | O1 | 107 | VAL | 2.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 64 | c8 | 128 | PHE | 2.3 |
| 77 | SR | 290 | VAL | 2.3 |
| 45 | 2 | 143 | G | 2.3 |
| 53 | s7 | 106 | SER | 2.3 |
| 7 | l5 | 186 | GLU | 2.3 |
| 51 | S5 | 192 | GLU | 2.3 |
| 55 | S9 | 126 | ARG | 2.3 |
| 59 | c3 | 58 | HIS | 2.3 |
| 62 | c6 | 82 | ARG | 2.3 |
| 37 | o6 | 91 | ASN | 2.3 |
| 7 | l5 | 49 | TYR | 2.3 |
| 7 | l5 | 163 | LEU | 2.3 |
| 18 | M7 | 180 | LYS | 2.3 |
| 10 | l8 | 75 | ILE | 2.3 |
| 50 | s4 | 45 | ILE | 2.3 |
| 51 | s5 | 174 | LEU | 2.3 |
| 58 | c2 | 124 | LYS | 2.3 |
| 79 | s6 | 115 | LYS | 2.3 |
| 57 | C1 | 131 | ILE | 2.3 |
| 77 | sR | 238 | ASP | 2.3 |
| 10 | l8 | 151 | VAL | 2.3 |
| 11 | L9 | 167 | VAL | 2.3 |
| 23 | n2 | 96 | VAL | 2.3 |
| 32 | O1 | 93 | VAL | 2.3 |
| 59 | c3 | 60 | VAL | 2.3 |
| 60 | c4 | 44 | GLY | 2.3 |
| 77 | SR | 97 | GLY | 2.3 |
| 29 | N8 | 93 | SER | 2.3 |
| 32 | O1 | 11 | GLU | 2.3 |
| 51 | s5 | 143 | ARG | 2.3 |
| 66 | D0 | 76 | SER | 2.3 |
| 66 | d0 | 68 | ARG | 2.3 |
| 66 | d0 | 76 | SER | 2.3 |
| 71 | d5 | 68 | ARG | 2.3 |
| 7 | l5 | 120 | LYS | 2.3 |
| 47 | s1 | 216 | LYS | 2.3 |
| 19 | m8 | 140 | LEU | 2.3 |
| 27 | N6 | 45 | ILE | 2.3 |
| 7 | L5 | 215 | ASP | 2.3 |
| 7 | l5 | 76 | ALA | 2.3 |
| 33 | O2 | 2 | ALA | 2.3 |
| 35 | O4 | 89 | ILE | 2.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 43 | Q2 | 70 | LEU | 2.3 |
| 46 | s0 | 184 | LEU | 2.3 |
| 65 | C9 | 138 | GLN | 2.3 |
| 58 | c2 | 27 | ALA | 2.3 |
| 65 | C9 | 131 | ASP | 2.3 |
| 68 | D2 | 20 | THR | 2.3 |
| 68 | D2 | 27 | ILE | 2.3 |
| 79 | s6 | 111 | LEU | 2.3 |
| 34 | o3 | 59 | VAL | 2.3 |
| 46 | s0 | 14 | ALA | 2.3 |
| 78 | SM | 100 | THR | 2.3 |
| 68 | D2 | 121 | VAL | 2.3 |
| 57 | c1 | 87 | ARG | 2.3 |
| 77 | sR | 298 | GLY | 2.3 |
| 47 | s1 | 85 | LYS | 2.3 |
| 55 | s9 | 21 | SER | 2.3 |
| 7 | l5 | 131 | LEU | 2.3 |
| 50 | s4 | 44 | LEU | 2.3 |
| 8 | l6 | 9 | TRP | 2.3 |
| 51 | S5 | 63 | GLN | 2.3 |
| 64 | c8 | 12 | GLN | 2.3 |
| 70 | D4 | 74 | LEU | 2.3 |
| 77 | SR | 195 | HIS | 2.3 |
| 77 | sR | 64 | HIS | 2.3 |
| 11 | L9 | 181 | VAL | 2.3 |
| 46 | S0 | 187 | ALA | 2.3 |
| 56 | C0 | 16 | PHE | 2.3 |
| 56 | c0 | 54 | TYR | 2.3 |
| 49 | S3 | 124 | ARG | 2.3 |
| 64 | c8 | 123 | ARG | 2.3 |
| 70 | D4 | 33 | ALA | 2.3 |
| 77 | SR | 36 | ALA | 2.3 |
| 51 | S5 | 141 | GLY | 2.3 |
| 1 | 1 | 2535 | A | 2.3 |
| 48 | s2 | 79 | GLU | 2.3 |
| 77 | sR | 179 | LYS | 2.3 |
| 13 | m1 | 91 | LEU | 2.3 |
| 62 | c6 | 53 | LEU | 2.3 |
| 64 | C8 | 131 | LEU | 2.3 |
| 77 | SR | 33 | LEU | 2.3 |
| 77 | SR | 42 | LEU | 2.3 |
| 77 | sR | 246 | SER | 2.3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | l5 | 69 | ILE | 2.3 |
| 10 | l8 | 52 | TRP | 2.3 |
| 13 | M1 | 109 | HIS | 2.3 |
| 43 | q2 | 81 | ALA | 2.3 |
| 49 | s3 | 65 | ARG | 2.3 |
| 51 | S5 | 65 | ARG | 2.3 |
| 51 | s5 | 77 | TYR | 2.3 |
| 54 | s8 | 21 | PHE | 2.3 |
| 73 | D7 | 32 | PHE | 2.3 |
| 77 | sR | 113 | VAL | 2.3 |
| 22 | n1 | 60 | LYS | 2.3 |
| 49 | S3 | 187 | LYS | 2.3 |
| 57 | C1 | 43 | LYS | 2.3 |
| 77 | sR | 194 | GLY | 2.3 |
| 53 | s7 | 134 | GLU | 2.3 |
| 46 | S0 | 182 | LEU | 2.3 |
| 60 | C4 | 112 | ILE | 2.3 |
| 12 | m0 | 95 | HIS | 2.3 |
| 46 | S0 | 74 | VAL | 2.3 |
| 50 | S4 | 13 | ALA | 2.3 |
| 51 | S5 | 171 | ALA | 2.3 |
| 52 | S6 | 131 | LYS | 2.3 |
| 77 | sR | 236 | ALA | 2.3 |
| 79 | s6 | 7 | TYR | 2.3 |
| 16 | m5 | 131 | GLU | 2.3 |
| 48 | s2 | 194 | GLU | 2.3 |
| 1 | 5 | 1023 | C | 2.3 |
| 22 | n1 | 77 | ASN | 2.3 |
| 22 | n1 | 90 | ASN | 2.3 |
| 50 | S4 | 151 | ASP | 2.3 |
| 51 | s5 | 60 | ASP | 2.3 |
| 63 | c7 | 25 | THR | 2.3 |
| 46 | S0 | 120 | LEU | 2.3 |
| 63 | c7 | 24 | LEU | 2.3 |
| 71 | D5 | 68 | ARG | 2.3 |
| 6 | l4 | 299 | ILE | 2.3 |
| 11 | L9 | 187 | ILE | 2.3 |
| 61 | C5 | 58 | LYS | 2.3 |
| 70 | d4 | 128 | LYS | 2.3 |
| 78 | SM | 23 | LYS | 2.3 |
| 6 | l4 | 142 | VAL | 2.3 |
| 12 | m0 | 114 | GLY | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 21 | N0 | 88 | HIS | 2.3 |
| 33 | o2 | 77 | ALA | 2.3 |
| 51 | s5 | 163 | SER | 2.3 |
| 54 | s8 | 82 | VAL | 2.3 |
| 48 | s2 | 230 | TRP | 2.2 |
| 54 | s8 | 167 | ALA | 2.3 |
| 58 | c2 | 61 | VAL | 2.3 |
| 60 | C4 | 121 | VAL | 2.3 |
| 62 | c6 | 131 | GLY | 2.2 |
| 77 | SR | 289 | ALA | 2.3 |
| 25 | n4 | 92 | GLU | 2.2 |
| 45 | 2 | 1364 | G | 2.2 |
| 45 | 6 | 235 | G | 2.2 |
| 77 | sR | 160 | GLU | 2.2 |
| 11 | L9 | 91 | ARG | 2.2 |
| 27 | n6 | 109 | LEU | 2.2 |
| 36 | o5 | 17 | LEU | 2.2 |
| 38 | o7 | 73 | ARG | 2.2 |
| 47 | S1 | 37 | THR | 2.2 |
| 51 | S5 | 60 | ASP | 2.2 |
| 52 | S6 | 69 | LEU | 2.2 |
| 45 | 6 | 1686 | C | 2.2 |
| 46 | S0 | 141 | ILE | 2.2 |
| 47 | s1 | 193 | ILE | 2.2 |
| 48 | s2 | 69 | ILE | 2.2 |
| 48 | s2 | 83 | ILE | 2.2 |
| 52 | S6 | 64 | LYS | 2.2 |
| 54 | s8 | 101 | ILE | 2.2 |
| 56 | C0 | 11 | ILE | 2.2 |
| 62 | C6 | 109 | PHE | 2.2 |
| 71 | D5 | 78 | ILE | 2.2 |
| 15 | M4 | 44 | VAL | 2.2 |
| 20 | m9 | 17 | VAL | 2.2 |
| 12 | m0 | 195 | ALA | 2.2 |
| 27 | n6 | 81 | GLN | 2.2 |
| 51 | S5 | 132 | VAL | 2.2 |
| 74 | D8 | 41 | VAL | 2.2 |
| 25 | n4 | 114 | GLU | 2.2 |
| 76 | e0 | 59 | GLY | 2.2 |
| 25 | n4 | 74 | LYS | 2.2 |
| 28 | N7 | 87 | LEU | 2.2 |
| 47 | s1 | 96 | LEU | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 71 | D5 | 75 | LEU | 2.2 |
| 76 | e0 | 39 | LEU | 2.2 |
| 27 | N6 | 98 | ASN | 2.2 |
| 7 | l5 | 64 | ILE | 2.2 |
| 14 | M3 | 95 | ILE | 2.2 |
| 39 | o8 | 22 | THR | 2.2 |
| 45 | 2 | 503 | G | 2.2 |
| 49 | s3 | 57 | ASP | 2.2 |
| 61 | c5 | 82 | ASN | 2.2 |
| 78 | sM | 43 | ASP | 2.2 |
| 79 | s6 | 18 | ILE | 2.2 |
| 43 | Q2 | 4 | VAL | 2.2 |
| 58 | c2 | 22 | VAL | 2.2 |
| 10 | L8 | 131 | ALA | 2.2 |
| 13 | M1 | 98 | ALA | 2.2 |
| 46 | s0 | 99 | ALA | 2.2 |
| 62 | C6 | 133 | GLY | 2.2 |
| 79 | s6 | 40 | ALA | 2.2 |
| 12 | M0 | 143 | SER | 2.2 |
| 37 | o6 | 64 | SER | 2.2 |
| 47 | s1 | 87 | ARG | 2.2 |
| 55 | s9 | 184 | SER | 2.2 |
| 64 | C8 | 10 | SER | 2.2 |
| 72 | d6 | 82 | ARG | 2.2 |
| 77 | SR | 147 | HIS | 2.2 |
| 10 | l8 | 109 | LEU | 2.2 |
| 39 | o8 | 73 | LEU | 2.2 |
| 64 | C8 | 49 | LYS | 2.2 |
| 77 | sR | 40 | LYS | 2.2 |
| 28 | n7 | 101 | PHE | 2.2 |
| 35 | o4 | 54 | ILE | 2.2 |
| 48 | S2 | 66 | PHE | 2.2 |
| 28 | n7 | 70 | PRO | 2.2 |
| 46 | S0 | 121 | VAL | 2.2 |
| 51 | s5 | 33 | VAL | 2.2 |
| 51 | s5 | 146 | THR | 2.2 |
| 61 | C5 | 84 | ILE | 2.2 |
| 64 | C8 | 21 | ASN | 2.2 |
| 72 | d6 | 79 | ILE | 2.2 |
| 74 | d8 | 7 | VAL | 2.2 |
| 77 | SR | 94 | VAL | 2.2 |
| 15 | M4 | 41 | GLN | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 16 | m5 | 129 | TYR | 2.2 |
| 49 | s3 | 23 | GLU | 2.2 |
| 51 | S5 | 195 | ALA | 2.2 |
| 53 | S7 | 95 | GLU | 2.2 |
| 54 | S8 | 117 | TYR | 2.2 |
| 66 | D0 | 74 | GLU | 2.2 |
| 69 | d3 | 29 | TYR | 2.2 |
| 75 | D9 | 26 | SER | 2.2 |
| 77 | SR | 66 | HIS | 2.2 |
| 26 | n5 | 126 | LEU | 2.2 |
| 46 | S0 | 17 | LEU | 2.2 |
| 48 | s2 | 190 | LEU | 2.2 |
| 64 | c8 | 61 | LEU | 2.2 |
| 48 | s2 | 115 | ILE | 2.2 |
| 68 | D2 | 50 | PHE | 2.2 |
| 14 | m3 | 188 | ARG | 2.2 |
| 28 | N7 | 45 | GLY | 2.2 |
| 51 | S5 | 139 | ASN | 2.2 |
| 61 | c5 | 41 | VAL | 2.2 |
| 66 | d0 | 62 | VAL | 2.2 |
| 36 | o5 | 20 | GLN | 2.2 |
| 36 | o5 | 83 | LYS | 2.2 |
| 54 | s8 | 55 | TYR | 2.2 |
| 60 | c4 | 91 | THR | 2.2 |
| 71 | d5 | 58 | ARG | 2.2 |
| 61 | C5 | 54 | ALA | 2.2 |
| 73 | D7 | 64 | CYS | 2.2 |
| 79 | s6 | 2 | LYS | 2.2 |
| 1 | 1 | 2206 | G | 2.2 |
| 8 | L6 | 9 | TRP | 2.2 |
| 45 | 6 | 647 | G | 2.2 |
| 48 | S2 | 248 | SER | 2.2 |
| 1 | 1 | 2572 | C | 2.2 |
| 45 | 2 | 1359 | C | 2.2 |
| 16 | M5 | 60 | VAL | 2.2 |
| 41 | Q0 | 106 | ARG | 2.2 |
| 47 | S1 | 64 | ARG | 2.2 |
| 47 | s1 | 88 | VAL | 2.2 |
| 57 | c1 | 86 | ILE | 2.2 |
| 60 | C4 | 83 | ILE | 2.2 |
| 72 | D6 | 22 | ARG | 2.2 |
| 77 | SR | 56 | VAL | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 77 | SR | 193 | ILE | 2.2 |
| 77 | sR | 131 | ILE | 2.2 |
| 79 | s6 | 191 | ARG | 2.2 |
| 26 | n5 | 60 | TYR | 2.2 |
| 27 | N6 | 86 | THR | 2.2 |
| 30 | n9 | 24 | PRO | 2.2 |
| 55 | S9 | 89 | ASP | 2.2 |
| 77 | SR | 105 | GLY | 2.2 |
| 49 | S3 | 172 | THR | 2.2 |
| 51 | S5 | 131 | GLN | 2.2 |
| 62 | C6 | 8 | GLN | 2.2 |
| 4 | l2 | 71 | LEU | 2.2 |
| 7 | L5 | 222 | LEU | 2.2 |
| 10 | l8 | 189 | LEU | 2.2 |
| 13 | m1 | 30 | LEU | 2.2 |
| 26 | n5 | 40 | LEU | 2.2 |
| 46 | s0 | 17 | LEU | 2.2 |
| 13 | M1 | 115 | LYS | 2.2 |
| 13 | m1 | 161 | SER | 2.2 |
| 33 | o2 | 117 | ILE | 2.2 |
| 39 | O8 | 45 | VAL | 2.2 |
| 39 | o8 | 5 | ILE | 2.2 |
| 59 | C3 | 65 | VAL | 2.2 |
| 63 | C7 | 120 | SER | 2.2 |
| 70 | d4 | 21 | LYS | 2.2 |
| 71 | D5 | 46 | LYS | 2.2 |
| 1 | 5 | 1803 | C | 2.2 |
| 22 | n1 | 94 | GLU | 2.2 |
| 28 | n7 | 18 | TYR | 2.2 |
| 7 | L5 | 151 | GLN | 2.2 |
| 7 | L5 | 233 | ALA | 2.2 |
| 13 | M1 | 93 | ASP | 2.2 |
| 49 | s3 | 93 | ASP | 2.2 |
| 69 | d3 | 113 | ALA | 2.2 |
| 48 | s2 | 156 | THR | 2.2 |
| 52 | S6 | 56 | ASN | 2.2 |
| 55 | S9 | 93 | LEU | 2.2 |
| 64 | C8 | 86 | LEU | 2.2 |
| 77 | sR | 209 | THR | 2.2 |
| 54 | S8 | 8 | ARG | 2.2 |
| 14 | m3 | 95 | ILE | 2.2 |
| 22 | n1 | 71 | SER | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 35 | O4 | 105 | VAL | 2.2 |
| 48 | s2 | 178 | ILE | 2.2 |
| 66 | D0 | 69 | LYS | 2.2 |
| 51 | s5 | 206 | SER | 2.2 |
| 10 | l8 | 178 | ALA | 2.2 |
| 23 | n2 | 78 | TYR | 2.2 |
| 22 | n1 | 106 | LEU | 2.2 |
| 55 | s9 | 139 | GLN | 2.2 |
| 75 | D9 | 41 | GLN | 2.2 |
| 28 | n7 | 133 | LYS | 2.2 |
| 48 | s2 | 49 | LYS | 2.2 |
| 58 | c2 | 49 | THR | 2.2 |
| 62 | c6 | 128 | LYS | 2.2 |
| 66 | d0 | 78 | THR | 2.2 |
| 70 | D4 | 119 | PHE | 2.2 |
| 79 | s6 | 30 | LYS | 2.2 |
| 13 | m1 | 157 | GLU | 2.2 |
| 39 | o8 | 45 | VAL | 2.2 |
| 64 | c8 | 92 | ILE | 2.2 |
| 70 | D4 | 25 | VAL | 2.2 |
| 70 | D4 | 57 | VAL | 2.2 |
| 77 | SR | 219 | GLU | 2.2 |
| 77 | sR | 290 | VAL | 2.2 |
| 79 | s6 | 49 | VAL | 2.2 |
| 47 | s1 | 233 | GLY | 2.2 |
| 30 | n9 | 57 | ALA | 2.2 |
| 58 | c2 | 94 | ALA | 2.2 |
| 59 | C3 | 45 | LEU | 2.2 |
| 63 | C7 | 15 | ALA | 2.2 |
| 67 | D1 | 58 | TYR | 2.2 |
| 50 | S4 | 20 | LEU | 2.2 |
| 10 | l8 | 42 | PRO | 2.2 |
| 59 | c3 | 62 | GLN | 2.2 |
| 66 | D0 | 77 | LYS | 2.2 |
| 67 | D1 | 87 | ARG | 2.2 |
| 79 | s6 | 182 | GLN | 2.2 |
| 48 | s2 | 226 | THR | 2.2 |
| 77 | SR | 130 | THR | 2.2 |
| 77 | SR | 159 | ASN | 2.2 |
| 13 | M1 | 148 | VAL | 2.2 |
| 35 | o4 | 34 | HIS | 2.2 |
| 50 | s4 | 36 | HIS | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 55 | S9 | 72 | GLU | 2.2 |
| 62 | c6 | 55 | VAL | 2.2 |
| 65 | c9 | 64 | HIS | 2.2 |
| 50 | s4 | 124 | GLY | 2.2 |
| 14 | M3 | 132 | ALA | 2.2 |
| 19 | m8 | 76 | ALA | 2.2 |
| 26 | N5 | 87 | SER | 2.2 |
| 48 | S2 | 222 | TYR | 2.2 |
| 49 | s3 | 108 | LYS | 2.2 |
| 51 | S5 | 209 | TYR | 2.2 |
| 51 | s5 | 175 | LEU | 2.2 |
| 53 | S7 | 52 | ALA | 2.2 |
| 68 | D2 | 68 | ARG | 2.2 |
| 70 | d4 | 117 | LYS | 2.2 |
| 7 | L5 | 232 | ASP | 2.2 |
| 27 | N6 | 58 | VAL | 2.2 |
| 46 | S0 | 58 | VAL | 2.2 |
| 47 | s1 | 43 | VAL | 2.2 |
| 54 | s8 | 169 | ILE | 2.2 |
| 65 | c9 | 16 | ASN | 2.2 |
| 70 | D4 | 24 | VAL | 2.2 |
| 74 | D8 | 44 | VAL | 2.2 |
| 35 | o4 | 78 | GLY | 2.2 |
| 50 | s4 | 4 | GLY | 2.2 |
| 55 | s9 | 73 | GLY | 2.2 |
| 29 | n8 | 117 | ARG | 2.2 |
| 7 | l5 | 195 | LEU | 2.2 |
| 10 | l8 | 169 | LEU | 2.2 |
| 13 | M1 | 75 | LYS | 2.2 |
| 14 | m3 | 193 | ALA | 2.2 |
| 55 | s9 | 109 | LEU | 2.2 |
| 56 | C0 | 15 | LEU | 2.2 |
| 77 | SR | 281 | TYR | 2.2 |
| 21 | N0 | 75 | PHE | 2.2 |
| 53 | s7 | 42 | GLN | 2.2 |
| 37 | o6 | 88 | GLU | 2.2 |
| 57 | c1 | 121 | ASP | 2.2 |
| 60 | c4 | 28 | VAL | 2.2 |
| 60 | c4 | 112 | ILE | 2.2 |
| 63 | C7 | 18 | GLU | 2.2 |
| 77 | SR | 262 | VAL | 2.2 |
| 39 | o8 | 6 | THR | 2.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 51 | S5 | 109 | LYS | 2.2 |
| 52 | S6 | 174 | LYS | 2.2 |
| 57 | C1 | 6 | THR | 2.2 |
| 61 | C5 | 64 | LYS | 2.2 |
| 61 | c5 | 98 | ASN | 2.2 |
| 64 | c8 | 20 | THR | 2.2 |
| 64 | c8 | 144 | ARG | 2.2 |
| 54 | S8 | 96 | LEU | 2.1 |
| 4 | L2 | 90 | ALA | 2.1 |
| 16 | m5 | 110 | ALA | 2.1 |
| 78 | SM | 80 | ALA | 2.1 |
| 10 | l8 | 79 | GLN | 2.1 |
| 18 | M7 | 172 | GLN | 2.1 |
| 35 | o4 | 73 | SER | 2.1 |
| 47 | S1 | 30 | PHE | 2.1 |
| 47 | S1 | 138 | PHE | 2.1 |
| 53 | s7 | 24 | PHE | 2.1 |
| 77 | sR | 235 | SER | 2.1 |
| 43 | q2 | 73 | GLU | 2.1 |
| 47 | S1 | 59 | ASP | 2.1 |
| 49 | S3 | 58 | VAL | 2.1 |
| 43 | q2 | 76 | LYS | 2.1 |
| 50 | S4 | 122 | LYS | 2.1 |
| 50 | s4 | 39 | ARG | 2.1 |
| 51 | s5 | 148 | ARG | 2.1 |
| 56 | c0 | 43 | ILE | 2.1 |
| 57 | c1 | 122 | ILE | 2.1 |
| 66 | d0 | 13 | GLU | 2.1 |
| 70 | D4 | 35 | VAL | 2.1 |
| 76 | E0 | 23 | LYS | 2.1 |
| 77 | sR | 297 | ASP | 2.1 |
| 23 | N2 | 33 | TYR | 2.1 |
| 32 | O1 | 16 | LEU | 2.1 |
| 45 | 6 | 1800 | A | 2.1 |
| 46 | S0 | 202 | TYR | 2.1 |
| 51 | s5 | 21 | THR | 2.1 |
| 52 | S6 | 180 | THR | 2.1 |
| 59 | C3 | 61 | THR | 2.1 |
| 61 | c5 | 15 | HIS | 2.1 |
| 66 | D0 | 27 | THR | 2.1 |
| 55 | S9 | 159 | ALA | 2.1 |
| 61 | C5 | 37 | ALA | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | S2 | 57 | PHE | 2.1 |
| 23 | n2 | 77 | LYS | 2.1 |
| 25 | n4 | 73 | ARG | 2.1 |
| 25 | n4 | 110 | LYS | 2.1 |
| 26 | n5 | 25 | LYS | 2.1 |
| 47 | S1 | 165 | ARG | 2.1 |
| 54 | S8 | 78 | ILE | 2.1 |
| 58 | C2 | 83 | GLU | 2.1 |
| 63 | C7 | 23 | LYS | 2.1 |
| 63 | C7 | 79 | GLU | 2.1 |
| 72 | D6 | 2 | PRO | 2.1 |
| 25 | n4 | 84 | GLY | 2.1 |
| 77 | sR | 97 | GLY | 2.1 |
| 39 | O8 | 54 | LEU | 2.1 |
| 47 | s1 | 70 | LEU | 2.1 |
| 50 | s4 | 123 | LEU | 2.1 |
| 7 | L5 | 55 | PHE | 2.1 |
| 39 | o8 | 23 | ALA | 2.1 |
| 51 | s5 | 72 | HIS | 2.1 |
| 50 | S4 | 226 | PHE | 2.1 |
| 53 | S7 | 78 | THR | 2.1 |
| 62 | C6 | 115 | THR | 2.1 |
| 74 | d8 | 19 | THR | 2.1 |
| 77 | SR | 319 | ASN | 2.1 |
| 79 | s6 | 16 | PHE | 2.1 |
| 22 | n1 | 92 | ARG | 2.1 |
| 15 | M4 | 58 | ILE | 2.1 |
| 28 | n7 | 12 | VAL | 2.1 |
| 35 | O4 | 108 | GLN | 2.1 |
| 47 | S1 | 55 | LYS | 2.1 |
| 51 | s5 | 114 | ILE | 2.1 |
| 51 | s5 | 170 | GLN | 2.1 |
| 64 | C8 | 57 | ARG | 2.1 |
| 67 | d1 | 33 | GLN | 2.1 |
| 77 | SR | 69 | GLN | 2.1 |
| 7 | l5 | 182 | GLY | 2.1 |
| 52 | S6 | 90 | GLY | 2.1 |
| 77 | SR | 291 | SER | 2.1 |
| 77 | SR | 316 | MET | 2.1 |
| 10 | l8 | 238 | LEU | 2.1 |
| 36 | o5 | 21 | LEU | 2.1 |
| 43 | Q2 | 85 | LEU | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 55 | s9 | 76 | LEU | 2.1 |
| 4 | l2 | 115 | ASN | 2.1 |
| 22 | n1 | 35 | LYS | 2.1 |
| 27 | N6 | 87 | LYS | 2.1 |
| 32 | O1 | 50 | ARG | 2.1 |
| 43 | Q2 | 71 | ARG | 2.1 |
| 54 | S8 | 139 | ALA | 2.1 |
| 57 | c1 | 138 | ASN | 2.1 |
| 58 | c2 | 130 | THR | 2.1 |
| 64 | C8 | 16 | ARG | 2.1 |
| 64 | C8 | 96 | LYS | 2.1 |
| 74 | d8 | 11 | LYS | 2.1 |
| 77 | SR | 285 | ALA | 2.1 |
| 77 | sR | 12 | THR | 2.1 |
| 27 | N6 | 88 | GLU | 2.1 |
| 46 | s0 | 121 | VAL | 2.1 |
| 55 | s9 | 110 | GLN | 2.1 |
| 65 | c9 | 111 | ILE | 2.1 |
| 29 | n8 | 116 | GLY | 2.1 |
| 34 | o3 | 61 | GLY | 2.1 |
| 46 | S0 | 44 | GLY | 2.1 |
| 48 | S2 | 154 | LEU | 2.1 |
| 50 | S4 | 167 | GLY | 2.1 |
| 58 | c2 | 82 | PRO | 2.1 |
| 70 | D4 | 125 | LEU | 2.1 |
| 7 | L5 | 78 | ALA | 2.1 |
| 35 | o4 | 43 | LYS | 2.1 |
| 49 | s3 | 102 | ALA | 2.1 |
| 49 | s3 | 225 | TYR | 2.1 |
| 50 | S4 | 108 | ARG | 2.1 |
| 61 | C5 | 123 | TYR | 2.1 |
| 73 | D7 | 82 | LYS | 2.1 |
| 74 | D8 | 10 | ALA | 2.1 |
| 47 | s1 | 215 | VAL | 2.1 |
| 48 | s2 | 96 | THR | 2.1 |
| 68 | d2 | 70 | ASN | 2.1 |
| 4 | l2 | 102 | LEU | 2.1 |
| 7 | l5 | 146 | LEU | 2.1 |
| 13 | m1 | 103 | GLY | 2.1 |
| 61 | c5 | 91 | GLY | 2.1 |
| 63 | C7 | 57 | LEU | 2.1 |
| 66 | D0 | 26 | LEU | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 13 | M1 | 119 | SER | 2.1 |
| 47 | s1 | 51 | SER | 2.1 |
| 77 | sR | 166 | SER | 2.1 |
| 70 | D4 | 85 | PHE | 2.1 |
| 17 | M6 | 185 | ALA | 2.1 |
| 58 | c2 | 35 | ALA | 2.1 |
| 58 | c2 | 128 | ALA | 2.1 |
| 77 | sR | 284 | ALA | 2.1 |
| 16 | m5 | 91 | GLU | 2.1 |
| 50 | S4 | 17 | HIS | 2.1 |
| 56 | c0 | 22 | VAL | 2.1 |
| 64 | c8 | 137 | HIS | 2.1 |
| 58 | C2 | 130 | THR | 2.1 |
| 62 | C6 | 70 | THR | 2.1 |
| 65 | c9 | 100 | ILE | 2.1 |
| 66 | D0 | 62 | VAL | 2.1 |
| 68 | d2 | 63 | VAL | 2.1 |
| 78 | sM | 58 | GLU | 2.1 |
| 11 | l9 | 144 | ILE | 2.1 |
| 39 | o8 | 40 | GLN | 2.1 |
| 22 | n1 | 85 | LEU | 2.1 |
| 12 | M0 | 49 | CYS | 2.1 |
| 43 | Q2 | 89 | LYS | 2.1 |
| 47 | S1 | 219 | LYS | 2.1 |
| 48 | s2 | 133 | LYS | 2.1 |
| 49 | S3 | 21 | LEU | 2.1 |
| 53 | s7 | 40 | PRO | 2.1 |
| 54 | S8 | 168 | CYS | 2.1 |
| 55 | s9 | 39 | LYS | 2.1 |
| 77 | SR | 107 | LYS | 2.1 |
| 79 | s6 | 137 | ARG | 2.1 |
| 58 | c2 | 87 | PRO | 2.1 |
| 53 | S7 | 115 | SER | 2.1 |
| 7 | L5 | 76 | ALA | 2.1 |
| 53 | S7 | 94 | ALA | 2.1 |
| 54 | S8 | 106 | ALA | 2.1 |
| 59 | C3 | 90 | TYR | 2.1 |
| 16 | m5 | 66 | VAL | 2.1 |
| 28 | n7 | 24 | VAL | 2.1 |
| 10 | l8 | 65 | LEU | 2.1 |
| 50 | S4 | 39 | ARG | 2.1 |
| 51 | S5 | 106 | LYS | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 54 | s8 | 138 | ASN | 2.1 |
| 55 | S9 | 79 | ARG | 2.1 |
| 63 | C7 | 29 | GLN | 2.1 |
| 46 | S0 | 142 | PRO | 2.1 |
| 46 | s0 | 155 | PHE | 2.1 |
| 51 | s5 | 129 | PRO | 2.1 |
| 19 | M8 | 65 | SER | 2.1 |
| 62 | C6 | 6 | SER | 2.1 |
| 65 | C9 | 58 | ALA | 2.1 |
| 7 | l5 | 37 | VAL | 2.1 |
| 13 | M1 | 110 | ILE | 2.1 |
| 27 | n6 | 108 | LYS | 2.1 |
| 28 | n7 | 64 | LYS | 2.1 |
| 29 | n8 | 138 | ILE | 2.1 |
| 4 | l2 | 58 | LEU | 2.1 |
| 22 | N1 | 151 | LEU | 2.1 |
| 37 | o6 | 82 | ARG | 2.1 |
| 46 | S0 | 122 | ILE | 2.1 |
| 47 | S1 | 214 | LYS | 2.1 |
| 47 | s1 | 62 | LYS | 2.1 |
| 49 | S3 | 204 | ASP | 2.1 |
| 51 | s5 | 168 | VAL | 2.1 |
| 53 | s7 | 90 | VAL | 2.1 |
| 55 | s9 | 138 | LYS | 2.1 |
| 62 | C6 | 74 | HIS | 2.1 |
| 64 | C8 | 127 | HIS | 2.1 |
| 77 | SR | 176 | LYS | 2.1 |
| 31 | O0 | 14 | LEU | 2.1 |
| 31 | o0 | 12 | GLN | 2.1 |
| 48 | s2 | 114 | GLY | 2.1 |
| 49 | s3 | 21 | LEU | 2.1 |
| 77 | sR | 223 | TRP | 2.1 |
| 35 | o4 | 25 | THR | 2.1 |
| 46 | s0 | 49 | ASN | 2.1 |
| 1 | 1 | 1562 | C | 2.1 |
| 16 | m5 | 30 | TYR | 2.1 |
| 78 | SM | 38 | PRO | 2.1 |
| 58 | c2 | 90 | LYS | 2.1 |
| 62 | c6 | 119 | ALA | 2.1 |
| 77 | sR | 14 | GLU | 2.1 |
| 51 | S5 | 111 | VAL | 2.1 |
| 53 | s7 | 51 | VAL | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 63 | C7 | 80 | ARG | 2.1 |
| 64 | c8 | 72 | ILE | 2.1 |
| 67 | D1 | 39 | VAL | 2.1 |
| 70 | d4 | 8 | ARG | 2.1 |
| 74 | D8 | 29 | ARG | 2.1 |
| 76 | e0 | 45 | VAL | 2.1 |
| 7 | l5 | 170 | GLY | 2.1 |
| 13 | m1 | 24 | GLY | 2.1 |
| 14 | m3 | 153 | ASP | 2.1 |
| 46 | S0 | 157 | ASP | 2.1 |
| 67 | d1 | 66 | ASP | 2.1 |
| 77 | sR | 136 | ILE | 2.1 |
| 73 | D7 | 21 | LEU | 2.1 |
| 77 | sR | 202 | LEU | 2.1 |
| 48 | S2 | 87 | GLN | 2.1 |
| 77 | SR | 177 | MET | 2.1 |
| 47 | S1 | 119 | THR | 2.1 |
| 51 | S5 | 122 | ASN | 2.1 |
| 64 | C8 | 11 | PHE | 2.1 |
| 77 | SR | 174 | ASN | 2.1 |
| 16 | m5 | 119 | TYR | 2.1 |
| 45 | 6 | 225 | A | 2.1 |
| 53 | S7 | 148 | LYS | 2.1 |
| 57 | C1 | 17 | PRO | 2.1 |
| 65 | c9 | 144 | GLU | 2.1 |
| 77 | sR | 30 | PRO | 2.1 |
| 7 | l5 | 53 | VAL | 2.1 |
| 46 | s0 | 73 | VAL | 2.1 |
| 28 | n7 | 68 | ILE | 2.1 |
| 33 | o2 | 128 | LEU | 2.1 |
| 50 | s4 | 206 | ASP | 2.1 |
| 55 | s9 | 97 | LEU | 2.1 |
| 59 | c3 | 54 | LEU | 2.1 |
| 67 | D1 | 18 | SER | 2.1 |
| 28 | n7 | 122 | HIS | 2.1 |
| 68 | D2 | 127 | GLY | 2.1 |
| 39 | o8 | 10 | GLN | 2.1 |
| 65 | c9 | 23 | GLN | 2.1 |
| 10 | l8 | 125 | ALA | 2.1 |
| 12 | M0 | 140 | THR | 2.1 |
| 19 | M8 | 123 | THR | 2.1 |
| 25 | N4 | 47 | ARG | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 47 | s1 | 82 | ARG | 2.1 |
| 49 | S3 | 67 | ASN | 2.1 |
| 54 | S8 | 54 | LYS | 2.1 |
| 79 | s6 | 174 | LYS | 2.1 |
| 28 | N7 | 59 | ALA | 2.1 |
| 32 | O1 | 40 | ALA | 2.1 |
| 46 | s0 | 22 | THR | 2.1 |
| 49 | s3 | 18 | TYR | 2.1 |
| 50 | s4 | 15 | PRO | 2.1 |
| 52 | S6 | 157 | VAL | 2.1 |
| 54 | s8 | 100 | ALA | 2.1 |
| 56 | C0 | 57 | THR | 2.1 |
| 77 | SR | 204 | ALA | 2.1 |
| 11 | L9 | 41 | ILE | 2.1 |
| 16 | M5 | 133 | ILE | 2.1 |
| 39 | o8 | 54 | LEU | 2.1 |
| 49 | s3 | 110 | LEU | 2.1 |
| 55 | s9 | 137 | GLY | 2.1 |
| 59 | c3 | 139 | TRP | 2.0 |
| 62 | c6 | 138 | PHE | 2.0 |
| 63 | c7 | 58 | MET | 2.1 |
| 77 | sR | 70 | ASP | 2.1 |
| 23 | n2 | 90 | ARG | 2.0 |
| 37 | o6 | 75 | LYS | 2.0 |
| 45 | 6 | 234 | G | 2.0 |
| 49 | S3 | 61 | GLU | 2.0 |
| 12 | M0 | 68 | ALA | 2.0 |
| 13 | M1 | 45 | PRO | 2.0 |
| 35 | o4 | 68 | THR | 2.0 |
| 77 | sR | 151 | VAL | 2.0 |
| 79 | s6 | 128 | THR | 2.0 |
| 14 | M3 | 130 | GLY | 2.0 |
| 28 | n7 | 80 | LEU | 2.0 |
| 29 | n8 | 148 | ILE | 2.0 |
| 32 | o1 | 75 | ILE | 2.0 |
| 63 | c7 | 50 | ILE | 2.0 |
| 35 | o4 | 3 | GLN | 2.0 |
| 46 | S0 | 23 | HIS | 2.0 |
| 52 | S6 | 31 | ARG | 2.0 |
| 52 | S6 | 142 | ARG | 2.0 |
| 54 | S8 | 56 | ARG | 2.0 |
| 64 | c8 | 78 | HIS | 2.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 32 | O1 | 68 | GLU | 2.0 |
| 45 | 2 | 239 | C | 2.0 |
| 55 | s9 | 186 | GLU | 2.0 |
| 4 | l2 | 35 | ALA | 2.0 |
| 48 | S2 | 249 | ALA | 2.0 |
| 69 | D3 | 12 | ALA | 2.0 |
| 75 | D9 | 6 | VAL | 2.0 |
| 77 | SR | 232 | TYR | 2.0 |
| 77 | sR | 226 | ALA | 2.0 |
| 46 | S0 | 103 | THR | 2.0 |
| 47 | S1 | 49 | ASN | 2.0 |
| 51 | s5 | 142 | PRO | 2.0 |
| 63 | C7 | 100 | LEU | 2.0 |
| 77 | SR | 310 | ILE | 2.0 |
| 11 | L9 | 174 | LYS | 2.0 |
| 28 | n7 | 118 | PHE | 2.0 |
| 45 | 2 | 766 | U | 2.0 |
| 70 | d4 | 122 | GLY | 2.0 |
| 79 | s6 | 116 | LYS | 2.0 |
| 53 | S7 | 70 | PHE | 2.0 |
| 68 | D2 | 79 | PHE | 2.0 |
| 77 | sR | 241 | PHE | 2.0 |
| 10 | l8 | 41 | GLN | 2.0 |
| 50 | S4 | 142 | HIS | 2.0 |
| 63 | C7 | 20 | TYR | 2.0 |
| 27 | n6 | 39 | LEU | 2.0 |
| 32 | O1 | 4 | LEU | 2.0 |
| 37 | o6 | 86 | LYS | 2.0 |
| 46 | S0 | 76 | ILE | 2.0 |
| 46 | S0 | 146 | LEU | 2.0 |
| 49 | s3 | 151 | LYS | 2.0 |
| 50 | s4 | 173 | ILE | 2.0 |
| 54 | S8 | 165 | LEU | 2.0 |
| 55 | S9 | 118 | LEU | 2.0 |
| 63 | C7 | 39 | ALA | 2.0 |
| 68 | D2 | 82 | LYS | 2.0 |
| 19 | m8 | 92 | ARG | 2.0 |
| 32 | O1 | 39 | PHE | 2.0 |
| 36 | o5 | 105 | ARG | 2.0 |
| 72 | d6 | 69 | ASN | 2.0 |
| 75 | D9 | 56 | ARG | 2.0 |
| 79 | s6 | 83 | CYS | 2.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 5 | 2542 | U | 2.0 |
| 4 | l2 | 109 | GLU | 2.0 |
| 62 | c6 | 77 | GLN | 2.0 |
| 50 | S4 | 209 | HIS | 2.0 |
| 57 | C1 | 92 | HIS | 2.0 |
| 77 | SR | 112 | SER | 2.0 |
| 77 | SR | 205 | SER | 2.0 |
| 77 | sR | 92 | TRP | 2.0 |
| 20 | m9 | 45 | VAL | 2.0 |
| 41 | Q0 | 107 | ALA | 2.0 |
| 46 | S0 | 98 | ILE | 2.0 |
| 47 | S1 | 137 | ILE | 2.0 |
| 49 | S3 | 50 | ILE | 2.0 |
| 50 | S4 | 22 | LYS | 2.0 |
| 56 | C0 | 75 | TYR | 2.0 |
| 62 | c6 | 48 | VAL | 2.0 |
| 62 | c6 | 91 | ALA | 2.0 |
| 66 | d0 | 90 | TYR | 2.0 |
| 69 | d3 | 72 | VAL | 2.0 |
| 49 | S3 | 76 | ARG | 2.0 |
| 50 | S4 | 162 | ILE | 2.0 |
| 51 | s5 | 76 | ARG | 2.0 |
| 53 | s7 | 16 | LEU | 2.0 |
| 54 | s8 | 96 | LEU | 2.0 |
| 66 | d0 | 86 | ILE | 2.0 |
| 51 | s5 | 69 | PHE | 2.0 |
| 57 | C1 | 137 | PHE | 2.0 |
| 48 | S2 | 82 | ASN | 2.0 |
| 48 | S2 | 90 | THR | 2.0 |
| 69 | d3 | 27 | ASN | 2.0 |
| 64 | C8 | 8 | GLN | 2.0 |
| 65 | C9 | 141 | GLU | 2.0 |
| 73 | d7 | 51 | GLN | 2.0 |
| 78 | sM | 120 | GLU | 2.0 |
| 11 | L9 | 54 | LYS | 2.0 |
| 45 | 2 | 1473 | U | 2.0 |
| 45 | 6 | 499 | U | 2.0 |
| 13 | M1 | 18 | VAL | 2.0 |
| 13 | m1 | 153 | LYS | 2.0 |
| 29 | n8 | 99 | ALA | 2.0 |
| 30 | N9 | 57 | ALA | 2.0 |
| 40 | o9 | 36 | ARG | 2.0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 48 | S2 | 240 | LEU | 2.0 |
| 50 | s4 | 82 | TYR | 2.0 |
| 76 | e0 | 21 | VAL | 2.0 |
| 77 | SR | 312 | VAL | 2.0 |
| 77 | sR | 229 | LYS | 2.0 |
| 54 | S8 | 99 | ALA | 2.0 |
| 63 | C7 | 17 | ILE | 2.0 |
| 78 | SM | 20 | LEU | 2.0 |
| 79 | s6 | 154 | ARG | 2.0 |
| 5 | l3 | 298 | PHE | 2.0 |
| 45 | 2 | 539 | G | 2.0 |
| 43 | Q2 | 5 | PRO | 2.0 |
| 77 | sR | 276 | PRO | 2.0 |
| 21 | N0 | 8 | GLN | 2.0 |
| 53 | s7 | 108 | GLN | 2.0 |
| 14 | m3 | 159 | VAL | 2.0 |
| 23 | n2 | 79 | LEU | 2.0 |
| 46 | s0 | 37 | VAL | 2.0 |
| 49 | s3 | 182 | LEU | 2.0 |
| 61 | C5 | 26 | LEU | 2.0 |
| 61 | c5 | 115 | TYR | 2.0 |
| 71 | d5 | 40 | VAL | 2.0 |
| 74 | D8 | 55 | VAL | 2.0 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3796 | 1/1 | -0.24 | 0.33 | 165,165,165,165 | 0 |
| 81 | MG | 8 | 220 | 1/1 | 0.09 | 0.42 | 88,88,88,88 | 0 |
| 81 | MG | 2 | 2059 | 1/1 | 0.13 | 0.58 | 114,114,114,114 | 0 |
| 81 | MG | 5 | 3878 | 1/1 | 0.18 | 0.62 | 118,118,118,118 | 0 |
| 81 | MG | 2 | 1947 | 1/1 | 0.18 | 0.27 | 110,110,110,110 | 0 |
| 81 | MG | 5 | 4057 | 1/1 | 0.19 | 0.62 | 117,117,117,117 | 0 |
| 81 | MG | 1 | 4093 | 1/1 | 0.23 | 0.32 | 86,86,86,86 | 0 |
| 81 | MG | 1 | 4118 | 1/1 | 0.26 | 0.45 | 88,88,88,88 | 0 |
| 81 | MG | 2 | 2084 | 1/1 | 0.26 | 0.35 | 105,105,105,105 | 0 |
| 81 | MG | 1 | 3968 | 1/1 | 0.27 | 0.18 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3853 | 1/1 | 0.27 | 0.28 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3944 | 1/1 | 0.31 | 0.26 | 118,118,118,118 | 0 |
| 81 | MG | 5 | 3839 | 1/1 | 0.36 | 1.23 | 88,88,88,88 | 0 |
| 81 | MG | 2 | 2048 | 1/1 | 0.38 | 0.83 | 84,84,84,84 | 0 |
| 81 | MG | 6 | 2009 | 1/1 | 0.39 | 0.17 | 126,126,126,126 | 0 |
| 81 | MG | 5 | 3983 | 1/1 | 0.39 | 0.46 | 92,92,92,92 | 0 |
| 81 | MG | m5 | 302 | 1/1 | 0.40 | 0.39 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3942 | 1/1 | 0.40 | 0.29 | 108,108,108,108 | 0 |
| 81 | MG | 1 | 4155 | 1/1 | 0.40 | 0.76 | 40,40,40,40 | 1 |
| 81 | MG | 1 | 4043 | 1/1 | 0.40 | 0.17 | 91,91,91,91 | 0 |
| 81 | MG | 5 | 4090 | 1/1 | 0.42 | 0.76 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 4036 | 1/1 | 0.43 | 0.34 | 80,80,80,80 | 0 |
| 81 | MG | 8 | 213 | 1/1 | 0.43 | 0.38 | 67,67,67,67 | 0 |
| 81 | MG | l8 | 301 | 1/1 | 0.44 | 0.39 | 109,109,109,109 | 0 |
| 81 | MG | 5 | 3536 | 1/1 | 0.44 | 0.57 | 51,51,51,51 | 1 |
| 81 | MG | 5 | 3893 | 1/1 | 0.44 | 0.30 | 68,68,68,68 | 0 |
| 81 | MG | 6 | 1944 | 1/1 | 0.45 | 0.34 | 95,95,95,95 | 0 |
| 81 | MG | 1 | 3998 | 1/1 | 0.45 | 0.50 | 86,86,86,86 | 0 |
| 81 | MG | 5 | 3966 | 1/1 | 0.45 | 0.62 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 4079 | 1/1 | 0.46 | 0.55 | 105,105,105,105 | 0 |
| 81 | MG | 2 | 2007 | 1/1 | 0.46 | 0.33 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3851 | 1/1 | 0.47 | 0.28 | 86,86,86,86 | 0 |
| 81 | MG | 3 | 206 | 1/1 | 0.47 | 0.27 | 87,87,87,87 | 0 |
| 81 | MG | 1 | 3903 | 1/1 | 0.47 | 0.50 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3967 | 1/1 | 0.47 | 0.31 | 100,100,100,100 | 0 |
| 81 | MG | 6 | 1943 | 1/1 | 0.48 | 0.29 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 4100 | 1/1 | 0.48 | 0.63 | 94,94,94,94 | 0 |
| 81 | MG | 1 | 4117 | 1/1 | 0.50 | 0.16 | 114,114,114,114 | 0 |
| 81 | MG | D3 | 202 | 1/1 | 0.51 | 0.45 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 4035 | 1/1 | 0.52 | 0.18 | 98,98,98,98 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3507 | 1/1 | 0.52 | 0.23 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3789 | 1/1 | 0.52 | 0.37 | 70,70,70,70 | 0 |
| 81 | MG | c9 | 201 | 1/1 | 0.53 | 0.09 | 115,115,115,115 | 0 |
| 81 | MG | 1 | 3857 | 1/1 | 0.53 | 0.30 | 57,57,57,57 | 0 |
| 81 | MG | 6 | 2028 | 1/1 | 0.53 | 0.24 | 126,126,126,126 | 0 |
| 81 | MG | 5 | 4059 | 1/1 | 0.53 | 0.43 | 98,98,98,98 | 0 |
| 81 | MG | 1 | 4099 | 1/1 | 0.53 | 0.58 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 4114 | 1/1 | 0.53 | 0.38 | 76,76,76,76 | 0 |
| 81 | MG | 6 | 1952 | 1/1 | 0.54 | 0.17 | 103,103,103,103 | 0 |
| 81 | MG | 6 | 1946 | 1/1 | 0.54 | 0.23 | 84,84,84,84 | 0 |
| 81 | MG | 1 | 3502 | 1/1 | 0.54 | 0.22 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 4091 | 1/1 | 0.55 | 0.55 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3521 | 1/1 | 0.55 | 0.41 | 49,49,49,49 | 1 |
| 81 | MG | 1 | 3849 | 1/1 | 0.55 | 0.20 | 56,56,56,56 | 0 |
| 81 | MG | 6 | 2063 | 1/1 | 0.55 | 0.37 | 88,88,88,88 | 0 |
| 81 | MG | 2 | 2069 | 1/1 | 0.55 | 0.28 | 96,96,96,96 | 0 |
| 81 | MG | 5 | 4033 | 1/1 | 0.56 | 0.18 | 88,88,88,88 | 0 |
| 81 | MG | c1 | 201 | 1/1 | 0.56 | 0.35 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3685 | 1/1 | 0.56 | 0.64 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 4025 | 1/1 | 0.56 | 0.50 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3914 | 1/1 | 0.57 | 0.34 | 97,97,97,97 | 0 |
| 81 | MG | 5 | 4019 | 1/1 | 0.57 | 0.80 | 86,86,86,86 | 0 |
| 81 | MG | 2 | 2061 | 1/1 | 0.57 | 0.50 | 105,105,105,105 | 0 |
| 81 | MG | 1 | 3924 | 1/1 | 0.57 | 0.56 | 58,58,58,58 | 0 |
| 81 | MG | d3 | 202 | 1/1 | 0.57 | 0.27 | 87,87,87,87 | 0 |
| 81 | MG | 5 | 3999 | 1/1 | 0.57 | 0.47 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 4085 | 1/1 | 0.57 | 0.42 | 88,88,88,88 | 0 |
| 81 | MG | 6 | 1937 | 1/1 | 0.57 | 0.76 | 72,72,72,72 | 0 |
| 81 | MG | 8 | 223 | 1/1 | 0.57 | 0.53 | 99,99,99,99 | 0 |
| 81 | MG | 6 | 2064 | 1/1 | 0.57 | 0.95 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 4105 | 1/1 | 0.58 | 0.59 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3647 | 1/1 | 0.58 | 0.29 | 56,56,56,56 | 0 |
| 81 | MG | 6 | 2045 | 1/1 | 0.58 | 0.24 | 117,117,117,117 | 0 |
| 81 | MG | 5 | 3896 | 1/1 | 0.58 | 0.19 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3646 | 1/1 | 0.58 | 0.15 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3927 | 1/1 | 0.59 | 0.67 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 4009 | 1/1 | 0.59 | 0.20 | 97,97,97,97 | 0 |
| 81 | MG | 5 | 3619 | 1/1 | 0.59 | 0.36 | 70,70,70,70 | 0 |
| 81 | MG | 5 | 3874 | 1/1 | 0.59 | 0.35 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3752 | 1/1 | 0.59 | 0.36 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 4133 | 1/1 | 0.59 | 0.31 | 69,69,69,69 | 0 |
| 81 | MG | 3 | 209 | 1/1 | 0.59 | 0.26 | 80,80,80,80 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | q3 | 502 | 1/1 | 0.59 | 0.41 | 81,81,81,81 | 0 |
| 81 | MG | n0 | 206 | 1/1 | 0.59 | 0.27 | 72,72,72,72 | 0 |
| 81 | MG | o1 | 201 | 1/1 | 0.59 | 0.21 | 72,72,72,72 | 0 |
| 81 | MG | L7 | 302 | 1/1 | 0.59 | 0.56 | 62,62,62,62 | 0 |
| 81 | MG | 6 | 2075 | 1/1 | 0.60 | 0.23 | 98,98,98,98 | 0 |
| 81 | MG | 1 | 3632 | 1/1 | 0.60 | 0.55 | 45,45,45,45 | 0 |
| 81 | MG | 2 | 1954 | 1/1 | 0.60 | 0.11 | 133,133,133,133 | 0 |
| 81 | MG | 2 | 2043 | 1/1 | 0.60 | 0.20 | 85,85,85,85 | 0 |
| 81 | MG | l7 | 305 | 1/1 | 0.60 | 0.30 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3855 | 1/1 | 0.60 | 0.40 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3963 | 1/1 | 0.60 | 0.45 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 4033 | 1/1 | 0.60 | 0.41 | 55,55,55,55 | 0 |
| 81 | MG | 8 | 216 | 1/1 | 0.60 | 0.28 | 82,82,82,82 | 0 |
| 81 | MG | 2 | 2044 | 1/1 | 0.61 | 0.55 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 4107 | 1/1 | 0.61 | 0.45 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3906 | 1/1 | 0.61 | 0.32 | 92,92,92,92 | 0 |
| 81 | MG | N8 | 203 | 1/1 | 0.61 | 0.43 | 61,61,61,61 | 1 |
| 81 | MG | 5 | 3794 | 1/1 | 0.61 | 0.95 | 124,124,124,124 | 0 |
| 81 | MG | 5 | 4068 | 1/1 | 0.61 | 0.47 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3640 | 1/1 | 0.61 | 0.27 | 57,57,57,57 | 0 |
| 81 | MG | 2 | 1929 | 1/1 | 0.61 | 0.23 | 78,78,78,78 | 0 |
| 81 | MG | 6 | 2054 | 1/1 | 0.61 | 0.18 | 110,110,110,110 | 0 |
| 81 | MG | 1 | 3605 | 1/1 | 0.61 | 0.25 | 61,61,61,61 | 0 |
| 81 | MG | L5 | 301 | 1/1 | 0.61 | 0.34 | 84,84,84,84 | 0 |
| 81 | MG | 5 | 3840 | 1/1 | 0.61 | 0.91 | 89,89,89,89 | 0 |
| 81 | MG | 5 | 4099 | 1/1 | 0.61 | 0.59 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3945 | 1/1 | 0.62 | 0.18 | 103,103,103,103 | 0 |
| 81 | MG | 5 | 4066 | 1/1 | 0.62 | 0.68 | 88,88,88,88 | 0 |
| 81 | MG | 1 | 3593 | 1/1 | 0.62 | 0.63 | 50,50,50,50 | 0 |
| 81 | MG | 2 | 2025 | 1/1 | 0.62 | 0.41 | 75,75,75,75 | 0 |
| 81 | MG | 8 | 225 | 1/1 | 0.62 | 0.22 | 77,77,77,77 | 0 |
| 81 | MG | 5 | 4044 | 1/1 | 0.62 | 0.33 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3994 | 1/1 | 0.62 | 0.51 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3654 | 1/1 | 0.62 | 0.35 | 47,47,47,47 | 0 |
| 81 | MG | 2 | 2020 | 1/1 | 0.62 | 0.37 | 83,83,83,83 | 0 |
| 81 | MG | 5 | 3890 | 1/1 | 0.62 | 0.36 | 78,78,78,78 | 0 |
| 81 | MG | 2 | 2054 | 1/1 | 0.62 | 0.28 | 86,86,86,86 | 0 |
| 81 | MG | O1 | 202 | 1/1 | 0.62 | 0.33 | 63,63,63,63 | 0 |
| 81 | MG | l3 | 408 | 1/1 | 0.62 | 0.25 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 4020 | 1/1 | 0.62 | 0.49 | 49,49,49,49 | 1 |
| 81 | MG | 1 | 3526 | 1/1 | 0.63 | 0.36 | 48,48,48,48 | 0 |
| 81 | MG | L9 | 201 | 1/1 | 0.63 | 0.14 | 80,80,80,80 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | m9 | 204 | 1/1 | 0.63 | 0.52 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 4091 | 1/1 | 0.63 | 0.36 | 82,82,82,82 | 0 |
| 81 | MG | m8 | 201 | 1/1 | 0.63 | 0.36 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 4004 | 1/1 | 0.63 | 0.21 | 89,89,89,89 | 0 |
| 81 | MG | 5 | 4070 | 1/1 | 0.63 | 0.30 | 113,113,113,113 | 0 |
| 81 | MG | 2 | 2070 | 1/1 | 0.63 | 0.31 | 119,119,119,119 | 0 |
| 81 | MG | 1 | 3982 | 1/1 | 0.63 | 0.48 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4184 | 1/1 | 0.63 | 0.87 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3957 | 1/1 | 0.64 | 0.41 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 4121 | 1/1 | 0.64 | 0.56 | 88,88,88,88 | 0 |
| 81 | MG | 5 | 3887 | 1/1 | 0.64 | 0.37 | 79,79,79,79 | 0 |
| 81 | MG | n6 | 204 | 1/1 | 0.64 | 0.21 | 83,83,83,83 | 0 |
| 81 | MG | 5 | 3660 | 1/1 | 0.64 | 0.18 | 86,86,86,86 | 0 |
| 81 | MG | 1 | 3840 | 1/1 | 0.64 | 0.39 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4180 | 1/1 | 0.64 | 0.49 | 55,55,55,55 | 1 |
| 81 | MG | 5 | 3877 | 1/1 | 0.64 | 0.39 | 66,66,66,66 | 0 |
| 81 | MG | 2 | 2074 | 1/1 | 0.64 | 0.22 | 89,89,89,89 | 0 |
| 81 | MG | 6 | 2037 | 1/1 | 0.65 | 0.33 | 102,102,102,102 | 0 |
| 81 | MG | 8 | 222 | 1/1 | 0.65 | 0.42 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4067 | 1/1 | 0.65 | 0.80 | 94,94,94,94 | 0 |
| 81 | MG | 5 | 4125 | 1/1 | 0.65 | 0.21 | 78,78,78,78 | 0 |
| 81 | MG | 8 | 215 | 1/1 | 0.65 | 0.32 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 4113 | 1/1 | 0.65 | 0.39 | 79,79,79,79 | 0 |
| 81 | MG | 8 | 212 | 1/1 | 0.65 | 0.54 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 4037 | 1/1 | 0.65 | 0.23 | 65,65,65,65 | 0 |
| 81 | MG | 2 | 1932 | 1/1 | 0.65 | 0.47 | 83,83,83,83 | 0 |
| 81 | MG | 1 | 3711 | 1/1 | 0.65 | 0.41 | 44,44,44,44 | 0 |
| 81 | MG | 2 | 2083 | 1/1 | 0.65 | 0.38 | 101,101,101,101 | 0 |
| 81 | MG | 5 | 4073 | 1/1 | 0.65 | 0.25 | 77,77,77,77 | 0 |
| 81 | MG | 5 | 3841 | 1/1 | 0.65 | 1.24 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3581 | 1/1 | 0.65 | 0.40 | 55,55,55,55 | 0 |
| 81 | MG | N1 | 202 | 1/1 | 0.66 | 0.33 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 4065 | 1/1 | 0.66 | 0.37 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3903 | 1/1 | 0.66 | 0.35 | 87,87,87,87 | 0 |
| 81 | MG | 7 | 213 | 1/1 | 0.66 | 0.34 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3559 | 1/1 | 0.66 | 0.39 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4160 | 1/1 | 0.66 | 0.34 | 65,65,65,65 | 0 |
| 81 | MG | 6 | 1915 | 1/1 | 0.66 | 0.25 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 4186 | 1/1 | 0.66 | 0.74 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3989 | 1/1 | 0.66 | 0.60 | 77,77,77,77 | 0 |
| 81 | MG | 7 | 204 | 1/1 | 0.66 | 0.44 | 65,65,65,65 | 0 |
| 81 | MG | 2 | 1931 | 1/1 | 0.66 | 0.25 | 98,98,98,98 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3827 | 1/1 | 0.66 | 0.90 | 70,70,70,70 | 0 |
| 81 | MG | 5 | 3901 | 1/1 | 0.66 | 0.29 | 94,94,94,94 | 0 |
| 81 | MG | 6 | 1981 | 1/1 | 0.66 | 0.33 | 77,77,77,77 | 0 |
| 81 | MG | 6 | 2067 | 1/1 | 0.66 | 0.78 | 75,75,75,75 | 0 |
| 81 | MG | 6 | 1998 | 1/1 | 0.66 | 0.39 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3842 | 1/1 | 0.67 | 1.44 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3677 | 1/1 | 0.67 | 0.70 | 55,55,55,55 | 0 |
| 81 | MG | 4 | 230 | 1/1 | 0.67 | 0.24 | 61,61,61,61 | 0 |
| 81 | MG | 6 | 1972 | 1/1 | 0.67 | 0.15 | 107,107,107,107 | 0 |
| 81 | MG | L4 | 402 | 1/1 | 0.67 | 0.33 | 54,54,54,54 | 0 |
| 81 | MG | 6 | 2060 | 1/1 | 0.67 | 0.60 | 88,88,88,88 | 0 |
| 81 | MG | 2 | 2103 | 1/1 | 0.67 | 0.49 | 73,73,73,73 | 0 |
| 81 | MG | 2 | 2081 | 1/1 | 0.67 | 0.31 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 4000 | 1/1 | 0.67 | 0.44 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4034 | 1/1 | 0.67 | 0.09 | 102,102,102,102 | 0 |
| 81 | MG | 5 | 3871 | 1/1 | 0.68 | 0.32 | 75,75,75,75 | 0 |
| 81 | MG | 6 | 1921 | 1/1 | 0.68 | 0.42 | 70,70,70,70 | 0 |
| 81 | MG | 1 | 3795 | 1/1 | 0.68 | 0.79 | 68,68,68,68 | 1 |
| 81 | MG | 4 | 223 | 1/1 | 0.68 | 0.33 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3911 | 1/1 | 0.68 | 0.33 | 63,63,63,63 | 0 |
| 81 | MG | 6 | 2065 | 1/1 | 0.68 | 0.59 | 66,66,66,66 | 0 |
| 81 | MG | 6 | 1966 | 1/1 | 0.68 | 0.41 | 88,88,88,88 | 0 |
| 81 | MG | 8 | 219 | 1/1 | 0.68 | 0.45 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 4038 | 1/1 | 0.68 | 0.32 | 83,83,83,83 | 0 |
| 81 | MG | 2 | 2111 | 1/1 | 0.68 | 0.58 | 72,72,72,72 | 0 |
| 81 | MG | 2 | 2113 | 1/1 | 0.68 | 0.40 | 95,95,95,95 | 0 |
| 81 | MG | 5 | 4108 | 1/1 | 0.68 | 0.31 | 70,70,70,70 | 0 |
| 81 | MG | 1 | 4166 | 1/1 | 0.69 | 0.36 | 77,77,77,77 | 0 |
| 81 | MG | O1 | 201 | 1/1 | 0.69 | 0.30 | 64,64,64,64 | 0 |
| 81 | MG | 2 | 2094 | 1/1 | 0.69 | 0.43 | 95,95,95,95 | 0 |
| 81 | MG | 1 | 3847 | 1/1 | 0.69 | 0.43 | 77,77,77,77 | 0 |
| 81 | MG | d3 | 204 | 1/1 | 0.69 | 0.47 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3853 | 1/1 | 0.69 | 0.63 | 68,68,68,68 | 0 |
| 81 | MG | o0 | 203 | 1/1 | 0.69 | 0.23 | 102,102,102,102 | 0 |
| 81 | MG | 5 | 3910 | 1/1 | 0.69 | 0.57 | 74,74,74,74 | 0 |
| 81 | MG | 6 | 2071 | 1/1 | 0.69 | 0.91 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3591 | 1/1 | 0.69 | 1.09 | 77,77,77,77 | 0 |
| 81 | MG | 1 | 3884 | 1/1 | 0.69 | 0.42 | 62,62,62,62 | 0 |
| 81 | MG | 6 | 2020 | 1/1 | 0.69 | 0.40 | 101,101,101,101 | 0 |
| 81 | MG | 5 | 4119 | 1/1 | 0.69 | 0.18 | 89,89,89,89 | 0 |
| 81 | MG | 2 | 1950 | 1/1 | 0.70 | 0.14 | 133,133,133,133 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 4098 | 1/1 | 0.70 | 0.46 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3529 | 1/1 | 0.70 | 0.58 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3701 | 1/1 | 0.70 | 0.72 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 2115 | 1/1 | 0.70 | 0.38 | 118,118,118,118 | 0 |
| 81 | MG | 3 | 215 | 1/1 | 0.70 | 0.31 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 4076 | 1/1 | 0.70 | 0.14 | 99,99,99,99 | 0 |
| 81 | MG | 1 | 4018 | 1/1 | 0.70 | 0.46 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 4057 | 1/1 | 0.70 | 0.11 | 89,89,89,89 | 0 |
| 81 | MG | 5 | 3729 | 1/1 | 0.70 | 0.42 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 4089 | 1/1 | 0.71 | 0.43 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 3975 | 1/1 | 0.71 | 0.49 | 71,71,71,71 | 0 |
| 81 | MG | 2 | 2024 | 1/1 | 0.71 | 0.23 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3876 | 1/1 | 0.71 | 0.19 | 66,66,66,66 | 1 |
| 81 | MG | 5 | 3955 | 1/1 | 0.71 | 0.29 | 54,54,54,54 | 0 |
| 81 | MG | 2 | 1937 | 1/1 | 0.71 | 0.42 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3559 | 1/1 | 0.71 | 0.22 | 75,75,75,75 | 0 |
| 81 | MG | 2 | 1976 | 1/1 | 0.71 | 0.17 | 113,113,113,113 | 0 |
| 81 | MG | 5 | 3700 | 1/1 | 0.71 | 0.90 | 62,62,62,62 | 0 |
| 81 | MG | 3 | 210 | 1/1 | 0.71 | 0.13 | 91,91,91,91 | 0 |
| 81 | MG | 2 | 1940 | 1/1 | 0.71 | 0.96 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3625 | 1/1 | 0.71 | 0.34 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3828 | 1/1 | 0.71 | 0.62 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 4013 | 1/1 | 0.71 | 0.42 | 87,87,87,87 | 0 |
| 81 | MG | 1 | 3860 | 1/1 | 0.71 | 0.43 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 4061 | 1/1 | 0.71 | 0.32 | 64,64,64,64 | 0 |
| 81 | MG | 6 | 1953 | 1/1 | 0.71 | 0.23 | 96,96,96,96 | 0 |
| 81 | MG | 1 | 4123 | 1/1 | 0.72 | 0.25 | 70,70,70,70 | 1 |
| 81 | MG | 1 | 4095 | 1/1 | 0.72 | 0.41 | 86,86,86,86 | 0 |
| 81 | MG | 2 | 1986 | 1/1 | 0.72 | 0.32 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3561 | 1/1 | 0.72 | 0.68 | 81,81,81,81 | 0 |
| 81 | MG | o1 | 203 | 1/1 | 0.72 | 0.14 | 74,74,74,74 | 0 |
| 81 | MG | 6 | 1947 | 1/1 | 0.72 | 0.20 | 113,113,113,113 | 0 |
| 81 | MG | 2 | 2019 | 1/1 | 0.72 | 0.50 | 81,81,81,81 | 0 |
| 81 | MG | 5 | 3875 | 1/1 | 0.72 | 0.34 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3965 | 1/1 | 0.72 | 0.27 | 53,53,53,53 | 1 |
| 81 | MG | 5 | 4045 | 1/1 | 0.72 | 0.24 | 67,67,67,67 | 0 |
| 81 | MG | 2 | 2091 | 1/1 | 0.72 | 0.20 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3548 | 1/1 | 0.72 | 0.46 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 4131 | 1/1 | 0.72 | 0.20 | 71,71,71,71 | 0 |
| 81 | MG | 6 | 1965 | 1/1 | 0.72 | 0.24 | 104,104,104,104 | 0 |
| 81 | MG | 2 | 2016 | 1/1 | 0.72 | 0.32 | 84,84,84,84 | 0 |
| 81 | MG | 6 | 2070 | 1/1 | 0.72 | 0.79 | 94,94,94,94 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 6 | 2029 | 1/1 | 0.72 | 0.31 | 77,77,77,77 | 0 |
| 81 | MG | 1 | 4183 | 1/1 | 0.72 | 0.16 | 96,96,96,96 | 0 |
| 81 | MG | l7 | 304 | 1/1 | 0.72 | 0.24 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3615 | 1/1 | 0.72 | 0.31 | 82,82,82,82 | 0 |
| 81 | MG | 6 | 2041 | 1/1 | 0.72 | 0.18 | 101,101,101,101 | 0 |
| 81 | MG | 5 | 3846 | 1/1 | 0.72 | 1.03 | 89,89,89,89 | 0 |
| 81 | MG | o2 | 204 | 1/1 | 0.72 | 0.41 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3960 | 1/1 | 0.72 | 0.39 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3967 | 1/1 | 0.72 | 0.18 | 77,77,77,77 | 0 |
| 81 | MG | 6 | 2011 | 1/1 | 0.72 | 0.52 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 3634 | 1/1 | 0.73 | 0.72 | 48,48,48,48 | 0 |
| 81 | MG | 6 | 1941 | 1/1 | 0.73 | 0.30 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 3955 | 1/1 | 0.73 | 0.25 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3785 | 1/1 | 0.73 | 0.32 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3980 | 1/1 | 0.73 | 0.28 | 97,97,97,97 | 0 |
| 81 | MG | 1 | 4187 | 1/1 | 0.73 | 0.29 | 50,50,50,50 | 0 |
| 81 | MG | 6 | 1992 | 1/1 | 0.73 | 0.32 | 86,86,86,86 | 0 |
| 81 | MG | 2 | 2078 | 1/1 | 0.73 | 0.11 | 100,100,100,100 | 0 |
| 81 | MG | 6 | 1924 | 1/1 | 0.73 | 0.33 | 83,83,83,83 | 0 |
| 81 | MG | O2 | 202 | 1/1 | 0.73 | 0.64 | 44,44,44,44 | 0 |
| 81 | MG | m9 | 203 | 1/1 | 0.73 | 0.14 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4038 | 1/1 | 0.73 | 0.51 | 68,68,68,68 | 0 |
| 81 | MG | 2 | 1991 | 1/1 | 0.73 | 0.33 | 91,91,91,91 | 0 |
| 81 | MG | 6 | 2053 | 1/1 | 0.73 | 0.26 | 123,123,123,123 | 0 |
| 81 | MG | 2 | 2071 | 1/1 | 0.73 | 0.25 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3572 | 1/1 | 0.73 | 0.29 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 3959 | 1/1 | 0.73 | 0.43 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 4070 | 1/1 | 0.73 | 0.17 | 84,84,84,84 | 0 |
| 81 | MG | 5 | 3998 | 1/1 | 0.73 | 0.56 | 63,63,63,63 | 0 |
| 81 | MG | n8 | 201 | 1/1 | 0.73 | 0.18 | 55,55,55,55 | 0 |
| 81 | MG | 2 | 2026 | 1/1 | 0.73 | 0.46 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3769 | 1/1 | 0.73 | 0.58 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3622 | 1/1 | 0.73 | 0.31 | 69,69,69,69 | 0 |
| 81 | MG | n6 | 201 | 1/1 | 0.73 | 0.31 | 71,71,71,71 | 0 |
| 81 | MG | 6 | 2024 | 1/1 | 0.73 | 0.11 | 119,119,119,119 | 0 |
| 81 | MG | 6 | 2014 | 1/1 | 0.73 | 0.37 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 3806 | 1/1 | 0.73 | 0.35 | 50,50,50,50 | 0 |
| 81 | MG | 2 | 2010 | 1/1 | 0.74 | 0.48 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 4173 | 1/1 | 0.74 | 0.41 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4098 | 1/1 | 0.74 | 0.83 | 89,89,89,89 | 0 |
| 81 | MG | 5 | 4087 | 1/1 | 0.74 | 0.26 | 85,85,85,85 | 0 |
| 81 | MG | 2 | 1923 | 1/1 | 0.74 | 0.41 | 55,55,55,55 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 4116 | 1/1 | 0.74 | 0.49 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3952 | 1/1 | 0.74 | 0.60 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3951 | 1/1 | 0.74 | 0.48 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3812 | 1/1 | 0.74 | 0.34 | 55,55,55,55 | 0 |
| 81 | MG | 6 | 2034 | 1/1 | 0.74 | 0.36 | 70,70,70,70 | 0 |
| 81 | MG | 5 | 3679 | 1/1 | 0.74 | 0.50 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 4085 | 1/1 | 0.74 | 0.36 | 62,62,62,62 | 0 |
| 80 | PAR | 5 | 3423 | 42/42 | 0.74 | 0.41 | 86,86,86,86 | 42 |
| 81 | MG | 2 | 1912 | 1/1 | 0.74 | 0.23 | 92,92,92,92 | 0 |
| 81 | MG | 1 | 3715 | 1/1 | 0.74 | 0.37 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3974 | 1/1 | 0.74 | 0.39 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4198 | 1/1 | 0.74 | 0.49 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 4174 | 1/1 | 0.74 | 0.34 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3586 | 1/1 | 0.74 | 0.30 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 3904 | 1/1 | 0.74 | 0.40 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 4079 | 1/1 | 0.74 | 0.28 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 4126 | 1/1 | 0.75 | 0.30 | 78,78,78,78 | 0 |
| 81 | MG | 2 | 2011 | 1/1 | 0.75 | 0.48 | 101,101,101,101 | 0 |
| 81 | MG | d3 | 205 | 1/1 | 0.75 | 0.34 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4115 | 1/1 | 0.75 | 0.70 | 74,74,74,74 | 0 |
| 81 | MG | 3 | 216 | 1/1 | 0.75 | 0.13 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 4092 | 1/1 | 0.75 | 0.29 | 67,67,67,67 | 0 |
| 81 | MG | 2 | 2108 | 1/1 | 0.75 | 0.22 | 110,110,110,110 | 0 |
| 81 | MG | 5 | 3844 | 1/1 | 0.75 | 0.89 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 4111 | 1/1 | 0.75 | 0.35 | 65,65,65,65 | 0 |
| 81 | MG | l3 | 405 | 1/1 | 0.75 | 0.37 | 66,66,66,66 | 0 |
| 81 | MG | Q2 | 505 | 1/1 | 0.75 | 0.28 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3993 | 1/1 | 0.75 | 0.41 | 46,46,46,46 | 0 |
| 81 | MG | 6 | 1949 | 1/1 | 0.75 | 0.21 | 83,83,83,83 | 0 |
| 81 | MG | 5 | 3631 | 1/1 | 0.75 | 0.32 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 4050 | 1/1 | 0.75 | 0.26 | 57,57,57,57 | 1 |
| 81 | MG | 5 | 4082 | 1/1 | 0.75 | 0.51 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 4139 | 1/1 | 0.75 | 0.46 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3979 | 1/1 | 0.75 | 0.40 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 4111 | 1/1 | 0.75 | 1.12 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3987 | 1/1 | 0.75 | 0.69 | 77,77,77,77 | 0 |
| 81 | MG | 5 | 3924 | 1/1 | 0.75 | 0.31 | 75,75,75,75 | 0 |
| 81 | MG | 6 | 1919 | 1/1 | 0.75 | 0.35 | 85,85,85,85 | 1 |
| 81 | MG | 1 | 4115 | 1/1 | 0.75 | 0.22 | 98,98,98,98 | 0 |
| 81 | MG | 4 | 236 | 1/1 | 0.75 | 0.35 | 50,50,50,50 | 0 |
| 81 | MG | 6 | 1956 | 1/1 | 0.75 | 0.14 | 105,105,105,105 | 0 |
| 81 | MG | 1 | 4062 | 1/1 | 0.75 | 0.44 | 48,48,48,48 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3964 | 1/1 | 0.75 | 0.27 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3708 | 1/1 | 0.75 | 0.59 | 59,59,59,59 | 0 |
| 80 | PAR | 6 | 1902 | 42/42 | 0.76 | 0.38 | 87,87,87,87 | 42 |
| 81 | MG | 5 | 4031 | 1/1 | 0.76 | 0.16 | 91,91,91,91 | 0 |
| 81 | MG | 1 | 4031 | 1/1 | 0.76 | 0.32 | 44,44,44,44 | 1 |
| 81 | MG | 1 | 3660 | 1/1 | 0.76 | 0.25 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3728 | 1/1 | 0.76 | 0.39 | 49,49,49,49 | 0 |
| 81 | MG | 8 | 209 | 1/1 | 0.76 | 0.40 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3756 | 1/1 | 0.76 | 0.32 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 4112 | 1/1 | 0.76 | 0.32 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3873 | 1/1 | 0.76 | 0.32 | 69,69,69,69 | 0 |
| 81 | MG | 3 | 214 | 1/1 | 0.76 | 0.14 | 73,73,73,73 | 0 |
| 82 | ZN | d7 | 101 | 1/1 | 0.76 | 0.14 | 261,261,261,261 | 0 |
| 81 | MG | S2 | 302 | 1/1 | 0.76 | 0.15 | 84,84,84,84 | 0 |
| 81 | MG | l3 | 404 | 1/1 | 0.76 | 0.21 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3633 | 1/1 | 0.76 | 0.38 | 56,56,56,56 | 0 |
| 81 | MG | 2 | 1992 | 1/1 | 0.76 | 0.38 | 75,75,75,75 | 0 |
| 81 | MG | 6 | 1922 | 1/1 | 0.76 | 0.49 | 73,73,73,73 | 0 |
| 81 | MG | 5 | 3915 | 1/1 | 0.76 | 0.41 | 97,97,97,97 | 0 |
| 81 | MG | 5 | 4123 | 1/1 | 0.76 | 0.21 | 84,84,84,84 | 0 |
| 81 | MG | m0 | 303 | 1/1 | 0.76 | 0.32 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 3513 | 1/1 | 0.76 | 0.25 | 56,56,56,56 | 0 |
| 81 | MG | 2 | 2085 | 1/1 | 0.77 | 0.39 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3590 | 1/1 | 0.77 | 0.40 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3962 | 1/1 | 0.77 | 0.18 | 81,81,81,81 | 0 |
| 81 | MG | 2 | 1982 | 1/1 | 0.77 | 0.46 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3658 | 1/1 | 0.77 | 0.55 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 4108 | 1/1 | 0.77 | 0.70 | 83,83,83,83 | 0 |
| 81 | MG | 2 | 2062 | 1/1 | 0.77 | 0.27 | 124,124,124,124 | 0 |
| 81 | MG | 5 | 3913 | 1/1 | 0.77 | 0.32 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3845 | 1/1 | 0.77 | 0.91 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3909 | 1/1 | 0.77 | 0.38 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4034 | 1/1 | 0.77 | 0.31 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3614 | 1/1 | 0.77 | 0.24 | 94,94,94,94 | 0 |
| 81 | MG | 6 | 2026 | 1/1 | 0.77 | 0.25 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3969 | 1/1 | 0.77 | 0.31 | 77,77,77,77 | 0 |
| 81 | MG | 1 | 3989 | 1/1 | 0.77 | 0.32 | 60,60,60,60 | 0 |
| 80 | PAR | 5 | 3403 | 42/42 | 0.77 | 0.34 | 84,84,84,84 | 42 |
| 81 | MG | 5 | 3953 | 1/1 | 0.77 | 0.51 | 49,49,49,49 | 0 |
| 81 | MG | L3 | 402 | 1/1 | 0.77 | 0.52 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3793 | 1/1 | 0.77 | 0.67 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 4109 | 1/1 | 0.77 | 0.50 | 78,78,78,78 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3681 | 1/1 | 0.77 | 0.91 | 56,56,56,56 | 0 |
| 81 | MG | 6 | 1986 | 1/1 | 0.77 | 0.41 | 81,81,81,81 | 0 |
| 81 | MG | 5 | 3928 | 1/1 | 0.77 | 0.47 | 76,76,76,76 | 0 |
| 81 | MG | n9 | 101 | 1/1 | 0.77 | 0.37 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3988 | 1/1 | 0.77 | 0.36 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 4026 | 1/1 | 0.77 | 0.43 | 37,37,37,37 | 1 |
| 81 | MG | 5 | 4012 | 1/1 | 0.77 | 0.42 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 3905 | 1/1 | 0.77 | 0.62 | 44,44,44,44 | 1 |
| 81 | MG | 6 | 2058 | 1/1 | 0.77 | 0.40 | 121,121,121,121 | 0 |
| 81 | MG | 2 | 2093 | 1/1 | 0.77 | 0.34 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 4062 | 1/1 | 0.77 | 0.55 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 3830 | 1/1 | 0.77 | 0.51 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3982 | 1/1 | 0.77 | 0.19 | 75,75,75,75 | 0 |
| 80 | PAR | 5 | 3428 | 42/42 | 0.78 | 0.23 | 120,120,120,120 | 0 |
| 81 | MG | 7 | 214 | 1/1 | 0.78 | 0.21 | 89,89,89,89 | 0 |
| 81 | MG | 6 | 2062 | 1/1 | 0.78 | 0.14 | 108,108,108,108 | 0 |
| 81 | MG | 1 | 3890 | 1/1 | 0.78 | 0.11 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 4058 | 1/1 | 0.78 | 0.41 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3537 | 1/1 | 0.78 | 0.41 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3621 | 1/1 | 0.78 | 0.37 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4136 | 1/1 | 0.78 | 0.44 | 47,47,47,47 | 1 |
| 81 | MG | 1 | 3914 | 1/1 | 0.78 | 0.40 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 4119 | 1/1 | 0.78 | 0.23 | 80,80,80,80 | 0 |
| 81 | MG | 3 | 213 | 1/1 | 0.78 | 0.14 | 89,89,89,89 | 0 |
| 81 | MG | M6 | 202 | 1/1 | 0.78 | 0.31 | 52,52,52,52 | 0 |
| 81 | MG | Q2 | 506 | 1/1 | 0.78 | 0.29 | 51,51,51,51 | 0 |
| 81 | MG | 6 | 2013 | 1/1 | 0.78 | 0.43 | 83,83,83,83 | 0 |
| 81 | MG | 1 | 3900 | 1/1 | 0.78 | 0.12 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 1961 | 1/1 | 0.78 | 0.31 | 76,76,76,76 | 0 |
| 81 | MG | N7 | 202 | 1/1 | 0.78 | 0.14 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 3669 | 1/1 | 0.78 | 0.35 | 55,55,55,55 | 0 |
| 81 | MG | 4 | 226 | 1/1 | 0.78 | 0.38 | 60,60,60,60 | 0 |
| 81 | MG | N6 | 204 | 1/1 | 0.78 | 0.23 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4056 | 1/1 | 0.78 | 0.21 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3937 | 1/1 | 0.78 | 0.24 | 76,76,76,76 | 0 |
| 81 | MG | 2 | 1963 | 1/1 | 0.78 | 0.26 | 112,112,112,112 | 0 |
| 80 | PAR | 3 | 201 | 42/42 | 0.78 | 0.20 | 95,95,95,95 | 42 |
| 81 | MG | 5 | 4030 | 1/1 | 0.78 | 0.14 | 88,88,88,88 | 0 |
| 81 | MG | 6 | 1939 | 1/1 | 0.78 | 0.14 | 104,104,104,104 | 0 |
| 81 | MG | L8 | 301 | 1/1 | 0.79 | 0.25 | 73,73,73,73 | 0 |
| 80 | PAR | 6 | 1906 | 42/42 | 0.79 | 0.27 | 120,120,120,120 | 0 |
| 81 | MG | 5 | 3981 | 1/1 | 0.79 | 0.30 | 79,79,79,79 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 80 | PAR | 2 | 1905 | 42/42 | 0.79 | 0.32 | 80,80,80,80 | 42 |
| 81 | MG | 1 | 3491 | 1/1 | 0.79 | 0.45 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3792 | 1/1 | 0.79 | 0.40 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3946 | 1/1 | 0.79 | 0.50 | 56,56,56,56 | 0 |
| 81 | MG | 4 | 232 | 1/1 | 0.79 | 0.25 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3682 | 1/1 | 0.79 | 0.46 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3985 | 1/1 | 0.79 | 0.61 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 4122 | 1/1 | 0.79 | 0.34 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3902 | 1/1 | 0.79 | 0.36 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 3615 | 1/1 | 0.79 | 0.33 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 3510 | 1/1 | 0.79 | 0.32 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3875 | 1/1 | 0.79 | 0.21 | 64,64,64,64 | 1 |
| 81 | MG | 4 | 203 | 1/1 | 0.79 | 0.30 | 44,44,44,44 | 0 |
| 81 | MG | 4 | 216 | 1/1 | 0.79 | 0.31 | 41,41,41,41 | 0 |
| 81 | MG | 1 | 3935 | 1/1 | 0.79 | 0.27 | 56,56,56,56 | 0 |
| 81 | MG | M4 | 201 | 1/1 | 0.79 | 0.24 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3852 | 1/1 | 0.79 | 0.17 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3535 | 1/1 | 0.79 | 0.53 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3826 | 1/1 | 0.79 | 0.77 | 78,78,78,78 | 0 |
| 81 | MG | 6 | 2055 | 1/1 | 0.79 | 0.20 | 106,106,106,106 | 0 |
| 81 | MG | 4 | 205 | 1/1 | 0.79 | 0.39 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 4164 | 1/1 | 0.79 | 0.27 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 4100 | 1/1 | 0.79 | 0.42 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3872 | 1/1 | 0.79 | 0.34 | 72,72,72,72 | 0 |
| 81 | MG | N6 | 203 | 1/1 | 0.79 | 0.27 | 55,55,55,55 | 0 |
| 81 | MG | 2 | 1968 | 1/1 | 0.79 | 0.15 | 129,129,129,129 | 0 |
| 81 | MG | 5 | 3964 | 1/1 | 0.79 | 0.20 | 67,67,67,67 | 1 |
| 81 | MG | 5 | 3883 | 1/1 | 0.79 | 0.37 | 73,73,73,73 | 0 |
| 81 | MG | 2 | 1910 | 1/1 | 0.79 | 0.32 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3879 | 1/1 | 0.79 | 0.18 | 137,137,137,137 | 0 |
| 81 | MG | 5 | 3774 | 1/1 | 0.79 | 0.38 | 59,59,59,59 | 1 |
| 81 | MG | 5 | 3741 | 1/1 | 0.79 | 0.29 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3946 | 1/1 | 0.79 | 0.29 | 72,72,72,72 | 0 |
| 81 | MG | M6 | 203 | 1/1 | 0.79 | 0.34 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4175 | 1/1 | 0.79 | 0.62 | 69,69,69,69 | 0 |
| 81 | MG | 6 | 1920 | 1/1 | 0.79 | 0.26 | 70,70,70,70 | 1 |
| 81 | MG | 2 | 2003 | 1/1 | 0.79 | 0.51 | 66,66,66,66 | 0 |
| 81 | MG | 7 | 211 | 1/1 | 0.79 | 0.50 | 72,72,72,72 | 0 |
| 81 | MG | 2 | 1924 | 1/1 | 0.80 | 0.23 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 4043 | 1/1 | 0.80 | 0.31 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3791 | 1/1 | 0.80 | 0.28 | 62,62,62,62 | 0 |
| 81 | MG | 2 | 2109 | 1/1 | 0.80 | 0.32 | 103,103,103,103 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3871 | 1/1 | 0.80 | 0.65 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3886 | 1/1 | 0.80 | 0.14 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 4080 | 1/1 | 0.80 | 0.31 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3690 | 1/1 | 0.80 | 0.81 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 4084 | 1/1 | 0.80 | 0.42 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3805 | 1/1 | 0.80 | 0.33 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3585 | 1/1 | 0.80 | 0.27 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3680 | 1/1 | 0.80 | 0.36 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3577 | 1/1 | 0.80 | 0.44 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 4104 | 1/1 | 0.80 | 0.34 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3894 | 1/1 | 0.80 | 0.27 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 3990 | 1/1 | 0.80 | 0.32 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4015 | 1/1 | 0.80 | 0.78 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 4076 | 1/1 | 0.80 | 0.38 | 61,61,61,61 | 0 |
| 81 | MG | 2 | 1917 | 1/1 | 0.80 | 0.49 | 88,88,88,88 | 0 |
| 81 | MG | 5 | 3814 | 1/1 | 0.80 | 0.36 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 4011 | 1/1 | 0.80 | 0.72 | 63,63,63,63 | 0 |
| 81 | MG | M6 | 204 | 1/1 | 0.80 | 0.25 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 3948 | 1/1 | 0.80 | 0.43 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3786 | 1/1 | 0.80 | 0.34 | 67,67,67,67 | 0 |
| 81 | MG | 2 | 2014 | 1/1 | 0.80 | 0.35 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3883 | 1/1 | 0.80 | 0.35 | 67,67,67,67 | 0 |
| 81 | MG | S2 | 301 | 1/1 | 0.80 | 0.32 | 91,91,91,91 | 0 |
| 81 | MG | 1 | 4102 | 1/1 | 0.80 | 0.47 | 66,66,66,66 | 0 |
| 81 | MG | c4 | 201 | 1/1 | 0.80 | 0.14 | 118,118,118,118 | 0 |
| 81 | MG | 1 | 4042 | 1/1 | 0.80 | 0.18 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3586 | 1/1 | 0.80 | 0.35 | 41,41,41,41 | 0 |
| 81 | MG | 6 | 2042 | 1/1 | 0.80 | 0.34 | 98,98,98,98 | 0 |
| 81 | MG | 5 | 4003 | 1/1 | 0.80 | 0.41 | 64,64,64,64 | 0 |
| 81 | MG | n0 | 203 | 1/1 | 0.80 | 0.22 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3922 | 1/1 | 0.80 | 0.16 | 87,87,87,87 | 0 |
| 81 | MG | 1 | 3768 | 1/1 | 0.80 | 0.26 | 77,77,77,77 | 0 |
| 81 | MG | 2 | 1973 | 1/1 | 0.80 | 0.44 | 82,82,82,82 | 0 |
| 81 | MG | 1 | 3508 | 1/1 | 0.80 | 0.11 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 4039 | 1/1 | 0.80 | 0.26 | 72,72,72,72 | 0 |
| 81 | MG | 2 | 1957 | 1/1 | 0.80 | 0.23 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3564 | 1/1 | 0.80 | 0.29 | 48,48,48,48 | 0 |
| 80 | PAR | 5 | 3427 | 42/42 | 0.80 | 0.35 | 94,94,94,94 | 42 |
| 81 | MG | 2 | 2058 | 1/1 | 0.80 | 0.54 | 58,58,58,58 | 0 |
| 81 | MG | 6 | 2049 | 1/1 | 0.81 | 0.25 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 4007 | 1/1 | 0.81 | 0.46 | 46,46,46,46 | 0 |
| 81 | MG | 8 | 210 | 1/1 | 0.81 | 0.28 | 62,62,62,62 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3669 | 1/1 | 0.81 | 0.25 | 48,48,48,48 | 0 |
| 81 | MG | 2 | 2089 | 1/1 | 0.81 | 0.22 | 93,93,93,93 | 0 |
| 81 | MG | 2 | 1980 | 1/1 | 0.81 | 0.39 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3809 | 1/1 | 0.81 | 0.27 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3785 | 1/1 | 0.81 | 0.38 | 53,53,53,53 | 0 |
| 81 | MG | 6 | 1977 | 1/1 | 0.81 | 0.12 | 107,107,107,107 | 0 |
| 81 | MG | 1 | 3698 | 1/1 | 0.81 | 0.52 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4013 | 1/1 | 0.81 | 0.70 | 70,70,70,70 | 0 |
| 81 | MG | D6 | 102 | 1/1 | 0.81 | 0.36 | 79,79,79,79 | 0 |
| 81 | MG | 6 | 2035 | 1/1 | 0.81 | 0.24 | 87,87,87,87 | 0 |
| 81 | MG | N3 | 201 | 1/1 | 0.81 | 0.29 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3941 | 1/1 | 0.81 | 0.26 | 113,113,113,113 | 0 |
| 81 | MG | 5 | 4069 | 1/1 | 0.81 | 0.28 | 69,69,69,69 | 1 |
| 81 | MG | 1 | 3683 | 1/1 | 0.81 | 0.56 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3904 | 1/1 | 0.81 | 0.42 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 4125 | 1/1 | 0.81 | 0.41 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3990 | 1/1 | 0.81 | 0.14 | 91,91,91,91 | 0 |
| 81 | MG | C9 | 202 | 1/1 | 0.81 | 0.11 | 133,133,133,133 | 0 |
| 81 | MG | 1 | 3861 | 1/1 | 0.81 | 0.24 | 44,44,44,44 | 0 |
| 81 | MG | 2 | 2072 | 1/1 | 0.81 | 0.16 | 83,83,83,83 | 0 |
| 81 | MG | 2 | 1907 | 1/1 | 0.81 | 0.14 | 81,81,81,81 | 0 |
| 81 | MG | 2 | 2092 | 1/1 | 0.81 | 0.23 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3560 | 1/1 | 0.81 | 0.09 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 3611 | 1/1 | 0.81 | 0.33 | 67,67,67,67 | 0 |
| 81 | MG | 6 | 2059 | 1/1 | 0.81 | 0.20 | 118,118,118,118 | 0 |
| 81 | MG | 2 | 2028 | 1/1 | 0.81 | 0.37 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 4161 | 1/1 | 0.81 | 0.18 | 61,61,61,61 | 1 |
| 81 | MG | 2 | 2018 | 1/1 | 0.81 | 0.10 | 99,99,99,99 | 0 |
| 81 | MG | 1 | 4029 | 1/1 | 0.81 | 0.42 | 40,40,40,40 | 0 |
| 81 | MG | L3 | 405 | 1/1 | 0.81 | 0.18 | 73,73,73,73 | 0 |
| 81 | MG | c4 | 203 | 1/1 | 0.81 | 0.19 | 118,118,118,118 | 0 |
| 81 | MG | 5 | 3972 | 1/1 | 0.81 | 0.28 | 68,68,68,68 | 0 |
| 80 | PAR | 5 | 3405 | 42/42 | 0.81 | 0.23 | 131,131,131,131 | 0 |
| 81 | MG | q0 | 202 | 1/1 | 0.81 | 0.40 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3525 | 1/1 | 0.81 | 0.45 | 54,54,54,54 | 0 |
| 81 | MG | N7 | 201 | 1/1 | 0.81 | 0.22 | 64,64,64,64 | 0 |
| 81 | MG | 2 | 2001 | 1/1 | 0.81 | 0.17 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3580 | 1/1 | 0.81 | 0.29 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 4024 | 1/1 | 0.81 | 0.37 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3985 | 1/1 | 0.81 | 0.46 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 4105 | 1/1 | 0.81 | 0.23 | 63,63,63,63 | 0 |
| 81 | MG | 2 | 1919 | 1/1 | 0.81 | 0.24 | 73,73,73,73 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3935 | 1/1 | 0.81 | 0.71 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3639 | 1/1 | 0.81 | 0.20 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4112 | 1/1 | 0.81 | 0.82 | 69,69,69,69 | 0 |
| 81 | MG | 2 | 1964 | 1/1 | 0.81 | 0.15 | 102,102,102,102 | 0 |
| 81 | MG | M9 | 201 | 1/1 | 0.81 | 0.43 | 65,65,65,65 | 0 |
| 81 | MG | n8 | 202 | 1/1 | 0.81 | 0.42 | 52,52,52,52 | 1 |
| 81 | MG | 1 | 4048 | 1/1 | 0.81 | 0.22 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3947 | 1/1 | 0.82 | 0.33 | 54,54,54,54 | 0 |
| 81 | MG | 6 | 1962 | 1/1 | 0.82 | 0.37 | 110,110,110,110 | 0 |
| 81 | MG | 5 | 3899 | 1/1 | 0.82 | 0.21 | 73,73,73,73 | 0 |
| 81 | MG | L9 | 203 | 1/1 | 0.82 | 0.19 | 71,71,71,71 | 0 |
| 81 | MG | 2 | 2063 | 1/1 | 0.82 | 0.44 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 4140 | 1/1 | 0.82 | 0.27 | 56,56,56,56 | 1 |
| 81 | MG | 5 | 4097 | 1/1 | 0.82 | 0.43 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3949 | 1/1 | 0.82 | 0.45 | 38,38,38,38 | 1 |
| 81 | MG | 6 | 1995 | 1/1 | 0.82 | 0.36 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3772 | 1/1 | 0.82 | 0.35 | 73,73,73,73 | 0 |
| 81 | MG | 6 | 1997 | 1/1 | 0.82 | 0.38 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3693 | 1/1 | 0.82 | 0.38 | 51,51,51,51 | 0 |
| 80 | PAR | 5 | 3422 | 42/42 | 0.82 | 0.20 | 105,105,105,105 | 0 |
| 81 | MG | 5 | 3620 | 1/1 | 0.82 | 0.54 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 4010 | 1/1 | 0.82 | 0.32 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3880 | 1/1 | 0.82 | 0.58 | 77,77,77,77 | 0 |
| 81 | MG | 1 | 3962 | 1/1 | 0.82 | 0.41 | 44,44,44,44 | 0 |
| 81 | MG | m6 | 201 | 1/1 | 0.82 | 0.35 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 2016 | 1/1 | 0.82 | 0.34 | 95,95,95,95 | 0 |
| 81 | MG | 2 | 2000 | 1/1 | 0.82 | 0.13 | 78,78,78,78 | 0 |
| 81 | MG | l3 | 406 | 1/1 | 0.82 | 0.25 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4002 | 1/1 | 0.82 | 0.56 | 75,75,75,75 | 0 |
| 81 | MG | Q3 | 502 | 1/1 | 0.82 | 0.34 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3862 | 1/1 | 0.82 | 0.25 | 62,62,62,62 | 0 |
| 81 | MG | 6 | 2001 | 1/1 | 0.82 | 0.24 | 105,105,105,105 | 0 |
| 81 | MG | 2 | 2004 | 1/1 | 0.82 | 0.34 | 69,69,69,69 | 0 |
| 81 | MG | M7 | 205 | 1/1 | 0.82 | 0.26 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3592 | 1/1 | 0.82 | 0.71 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3573 | 1/1 | 0.82 | 0.22 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3638 | 1/1 | 0.82 | 0.30 | 68,68,68,68 | 0 |
| 81 | MG | 2 | 2037 | 1/1 | 0.82 | 0.10 | 123,123,123,123 | 0 |
| 81 | MG | 1 | 3821 | 1/1 | 0.82 | 0.26 | 52,52,52,52 | 0 |
| 81 | MG | 2 | 2098 | 1/1 | 0.82 | 0.29 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 3981 | 1/1 | 0.82 | 0.34 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3954 | 1/1 | 0.82 | 0.24 | 65,65,65,65 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 4120 | 1/1 | 0.82 | 0.21 | 58,58,58,58 | 0 |
| 81 | MG | 2 | 2100 | 1/1 | 0.82 | 0.60 | 58,58,58,58 | 0 |
| 80 | PAR | 1 | 3413 | 42/42 | 0.82 | 0.27 | 64,64,64,64 | 42 |
| 81 | MG | 5 | 3734 | 1/1 | 0.82 | 0.73 | 65,65,65,65 | 0 |
| 81 | MG | 2 | 2104 | 1/1 | 0.82 | 0.77 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3837 | 1/1 | 0.82 | 0.30 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3724 | 1/1 | 0.82 | 0.51 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3738 | 1/1 | 0.82 | 0.41 | 54,54,54,54 | 0 |
| 81 | MG | O9 | 101 | 1/1 | 0.82 | 0.45 | 48,48,48,48 | 1 |
| 81 | MG | 6 | 1975 | 1/1 | 0.82 | 0.07 | 104,104,104,104 | 1 |
| 81 | MG | 1 | 3864 | 1/1 | 0.82 | 0.24 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4073 | 1/1 | 0.82 | 0.13 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3639 | 1/1 | 0.82 | 0.39 | 54,54,54,54 | 0 |
| 81 | MG | 2 | 1922 | 1/1 | 0.82 | 0.27 | 60,60,60,60 | 1 |
| 81 | MG | 1 | 4192 | 1/1 | 0.82 | 0.71 | 62,62,62,62 | 0 |
| 81 | MG | 6 | 2039 | 1/1 | 0.82 | 0.33 | 69,69,69,69 | 0 |
| 81 | MG | 6 | 2044 | 1/1 | 0.83 | 0.22 | 87,87,87,87 | 0 |
| 81 | MG | 1 | 4078 | 1/1 | 0.83 | 0.25 | 71,71,71,71 | 0 |
| 81 | MG | 2 | 2095 | 1/1 | 0.83 | 0.42 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4084 | 1/1 | 0.83 | 0.20 | 69,69,69,69 | 0 |
| 80 | PAR | 1 | 3433 | 42/42 | 0.83 | 0.27 | 64,64,64,64 | 42 |
| 81 | MG | 5 | 4035 | 1/1 | 0.83 | 0.17 | 85,85,85,85 | 0 |
| 81 | MG | 5 | 3598 | 1/1 | 0.83 | 0.38 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3892 | 1/1 | 0.83 | 0.25 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3818 | 1/1 | 0.83 | 0.27 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 4014 | 1/1 | 0.83 | 0.90 | 70,70,70,70 | 0 |
| 81 | MG | 4 | 231 | 1/1 | 0.83 | 0.28 | 49,49,49,49 | 0 |
| 81 | MG | 6 | 2036 | 1/1 | 0.83 | 0.43 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3673 | 1/1 | 0.83 | 0.33 | 51,51,51,51 | 0 |
| 81 | MG | M5 | 303 | 1/1 | 0.83 | 0.32 | 44,44,44,44 | 1 |
| 81 | MG | 2 | 2049 | 1/1 | 0.83 | 0.56 | 88,88,88,88 | 0 |
| 81 | MG | 2 | 2031 | 1/1 | 0.83 | 0.13 | 98,98,98,98 | 0 |
| 81 | MG | 1 | 4010 | 1/1 | 0.83 | 0.50 | 53,53,53,53 | 0 |
| 81 | MG | M7 | 202 | 1/1 | 0.83 | 0.47 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3767 | 1/1 | 0.83 | 0.37 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 4097 | 1/1 | 0.83 | 0.25 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 4021 | 1/1 | 0.83 | 0.61 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 4016 | 1/1 | 0.83 | 0.37 | 77,77,77,77 | 0 |
| 81 | MG | M8 | 201 | 1/1 | 0.83 | 0.32 | 63,63,63,63 | 0 |
| 81 | MG | 7 | 212 | 1/1 | 0.83 | 0.22 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 4096 | 1/1 | 0.83 | 0.30 | 62,62,62,62 | 0 |
| 81 | MG | l3 | 407 | 1/1 | 0.83 | 0.40 | 51,51,51,51 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3822 | 1/1 | 0.83 | 0.11 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 3695 | 1/1 | 0.83 | 0.38 | 50,50,50,50 | 1 |
| 81 | MG | 5 | 3986 | 1/1 | 0.83 | 0.61 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3530 | 1/1 | 0.83 | 0.34 | 37,37,37,37 | 0 |
| 81 | MG | 2 | 1979 | 1/1 | 0.83 | 0.30 | 77,77,77,77 | 0 |
| 81 | MG | 5 | 3873 | 1/1 | 0.83 | 0.39 | 66,66,66,66 | 0 |
| 81 | MG | 6 | 2066 | 1/1 | 0.83 | 0.37 | 55,55,55,55 | 0 |
| 81 | MG | M4 | 203 | 1/1 | 0.83 | 0.15 | 64,64,64,64 | 0 |
| 81 | MG | 6 | 2072 | 1/1 | 0.83 | 0.42 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 4171 | 1/1 | 0.83 | 0.36 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3974 | 1/1 | 0.83 | 0.42 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 4027 | 1/1 | 0.83 | 0.41 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3513 | 1/1 | 0.83 | 0.57 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 3483 | 1/1 | 0.83 | 0.33 | 53,53,53,53 | 0 |
| 81 | MG | 2 | 1978 | 1/1 | 0.83 | 0.21 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 3503 | 1/1 | 0.83 | 0.26 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4005 | 1/1 | 0.83 | 0.33 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 4053 | 1/1 | 0.83 | 0.35 | 55,55,55,55 | 0 |
| 81 | MG | n6 | 202 | 1/1 | 0.83 | 0.10 | 69,69,69,69 | 0 |
| 80 | PAR | n3 | 201 | 42/42 | 0.83 | 0.30 | 63,63,63,63 | 42 |
| 81 | MG | 5 | 3861 | 1/1 | 0.83 | 0.38 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 4118 | 1/1 | 0.83 | 0.27 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3697 | 1/1 | 0.83 | 0.69 | 60,60,60,60 | 0 |
| 81 | MG | 6 | 2051 | 1/1 | 0.83 | 0.26 | 110,110,110,110 | 0 |
| 81 | MG | 6 | 1938 | 1/1 | 0.83 | 0.09 | 99,99,99,99 | 0 |
| 81 | MG | 1 | 4000 | 1/1 | 0.83 | 0.24 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3789 | 1/1 | 0.83 | 0.44 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3882 | 1/1 | 0.83 | 0.17 | 74,74,74,74 | 0 |
| 81 | MG | L5 | 303 | 1/1 | 0.83 | 0.20 | 86,86,86,86 | 0 |
| 80 | PAR | o2 | 201 | 42/42 | 0.83 | 0.32 | 51,51,51,51 | 42 |
| 81 | MG | 1 | 3987 | 1/1 | 0.83 | 0.33 | 54,54,54,54 | 0 |
| 81 | MG | L4 | 401 | 1/1 | 0.84 | 0.23 | 49,49,49,49 | 0 |
| 82 | ZN | D7 | 101 | 1/1 | 0.84 | 0.16 | 173,173,173,173 | 0 |
| 81 | MG | 1 | 4030 | 1/1 | 0.84 | 0.37 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3500 | 1/1 | 0.84 | 0.76 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3896 | 1/1 | 0.84 | 0.28 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 4041 | 1/1 | 0.84 | 0.15 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 4001 | 1/1 | 0.84 | 0.22 | 62,62,62,62 | 0 |
| 81 | MG | 3 | 218 | 1/1 | 0.84 | 0.40 | 57,57,57,57 | 0 |
| 80 | PAR | 1 | 3403 | 42/42 | 0.84 | 0.31 | 58,58,58,58 | 42 |
| 81 | MG | 5 | 3713 | 1/1 | 0.84 | 0.48 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3995 | 1/1 | 0.84 | 0.26 | 49,49,49,49 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3549 | 1/1 | 0.84 | 0.34 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3835 | 1/1 | 0.84 | 0.37 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3991 | 1/1 | 0.84 | 0.17 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3984 | 1/1 | 0.84 | 0.36 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 4014 | 1/1 | 0.84 | 0.39 | 71,71,71,71 | 0 |
| 81 | MG | 2 | 2066 | 1/1 | 0.84 | 0.35 | 82,82,82,82 | 0 |
| 81 | MG | 2 | 1936 | 1/1 | 0.84 | 0.54 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 4054 | 1/1 | 0.84 | 0.29 | 75,75,75,75 | 0 |
| 81 | MG | l7 | 303 | 1/1 | 0.84 | 0.25 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3936 | 1/1 | 0.84 | 0.54 | 60,60,60,60 | 1 |
| 81 | MG | 1 | 3855 | 1/1 | 0.84 | 0.23 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 4055 | 1/1 | 0.84 | 0.20 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 3899 | 1/1 | 0.84 | 0.22 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 3469 | 1/1 | 0.84 | 0.36 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3707 | 1/1 | 0.84 | 0.60 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3630 | 1/1 | 0.84 | 0.29 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 4027 | 1/1 | 0.84 | 0.52 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 3868 | 1/1 | 0.84 | 0.32 | 39,39,39,39 | 0 |
| 81 | MG | M4 | 202 | 1/1 | 0.84 | 0.30 | 60,60,60,60 | 0 |
| 81 | MG | o1 | 202 | 1/1 | 0.84 | 0.50 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3852 | 1/1 | 0.84 | 0.41 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 4146 | 1/1 | 0.84 | 0.46 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3889 | 1/1 | 0.84 | 0.32 | 54,54,54,54 | 0 |
| 80 | PAR | 5 | 3404 | 42/42 | 0.84 | 0.23 | 90,90,90,90 | 0 |
| 81 | MG | 6 | 2004 | 1/1 | 0.84 | 0.74 | 77,77,77,77 | 0 |
| 80 | PAR | 1 | 3426 | 42/42 | 0.84 | 0.28 | 82,82,82,82 | 0 |
| 81 | MG | 1 | 3614 | 1/1 | 0.84 | 0.26 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3971 | 1/1 | 0.84 | 0.19 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3667 | 1/1 | 0.84 | 0.37 | 53,53,53,53 | 0 |
| 80 | PAR | 1 | 3401 | 42/42 | 0.84 | 0.22 | 87,87,87,87 | 42 |
| 81 | MG | 5 | 3847 | 1/1 | 0.84 | 0.33 | 96,96,96,96 | 0 |
| 81 | MG | 1 | 4092 | 1/1 | 0.84 | 0.20 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3788 | 1/1 | 0.84 | 0.27 | 68,68,68,68 | 0 |
| 81 | MG | 2 | 1987 | 1/1 | 0.84 | 0.59 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3501 | 1/1 | 0.84 | 0.57 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 4145 | 1/1 | 0.84 | 0.28 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 4116 | 1/1 | 0.84 | 0.31 | 107,107,107,107 | 0 |
| 81 | MG | 5 | 3603 | 1/1 | 0.84 | 0.24 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 3972 | 1/1 | 0.84 | 0.39 | 84,84,84,84 | 0 |
| 81 | MG | 5 | 3764 | 1/1 | 0.84 | 0.34 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3867 | 1/1 | 0.84 | 0.26 | 66,66,66,66 | 0 |
| 81 | MG | s8 | 301 | 1/1 | 0.84 | 0.32 | 70,70,70,70 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3956 | 1/1 | 0.84 | 0.23 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3874 | 1/1 | 0.84 | 0.20 | 67,67,67,67 | 1 |
| 81 | MG | 1 | 3930 | 1/1 | 0.84 | 0.40 | 45,45,45,45 | 0 |
| 81 | MG | 2 | 2080 | 1/1 | 0.84 | 0.17 | 81,81,81,81 | 0 |
| 81 | MG | n0 | 202 | 1/1 | 0.85 | 0.23 | 59,59,59,59 | 0 |
| 81 | MG | l7 | 302 | 1/1 | 0.85 | 0.41 | 57,57,57,57 | 0 |
| 80 | PAR | 2 | 1901 | 42/42 | 0.85 | 0.32 | 82,82,82,82 | 42 |
| 80 | PAR | 1 | 3405 | 42/42 | 0.85 | 0.35 | 44,44,44,44 | 42 |
| 81 | MG | 1 | 3797 | 1/1 | 0.85 | 0.19 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 4103 | 1/1 | 0.85 | 0.49 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 4004 | 1/1 | 0.85 | 0.27 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 3747 | 1/1 | 0.85 | 0.60 | 60,60,60,60 | 0 |
| 80 | PAR | 4 | 201 | 42/42 | 0.85 | 0.31 | 43,43,43,43 | 42 |
| 81 | MG | 6 | 2074 | 1/1 | 0.85 | 0.32 | 81,81,81,81 | 0 |
| 81 | MG | n1 | 202 | 1/1 | 0.85 | 0.50 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3947 | 1/1 | 0.85 | 0.28 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3973 | 1/1 | 0.85 | 0.36 | 71,71,71,71 | 0 |
| 81 | MG | 6 | 1954 | 1/1 | 0.85 | 0.16 | 98,98,98,98 | 0 |
| 80 | PAR | 1 | 3436 | 42/42 | 0.85 | 0.22 | 85,85,85,85 | 0 |
| 81 | MG | 6 | 1959 | 1/1 | 0.85 | 0.29 | 119,119,119,119 | 0 |
| 81 | MG | 5 | 3938 | 1/1 | 0.85 | 0.25 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3597 | 1/1 | 0.85 | 0.32 | 65,65,65,65 | 0 |
| 81 | MG | 2 | 1941 | 1/1 | 0.85 | 0.28 | 75,75,75,75 | 0 |
| 80 | PAR | 8 | 202 | 42/42 | 0.85 | 0.30 | 62,62,62,62 | 42 |
| 81 | MG | 1 | 3538 | 1/1 | 0.85 | 0.38 | 35,35,35,35 | 0 |
| 81 | MG | 8 | 217 | 1/1 | 0.85 | 0.24 | 69,69,69,69 | 0 |
| 81 | MG | 6 | 2017 | 1/1 | 0.85 | 0.20 | 93,93,93,93 | 0 |
| 81 | MG | 2 | 2116 | 1/1 | 0.85 | 0.38 | 93,93,93,93 | 0 |
| 81 | MG | 5 | 3771 | 1/1 | 0.85 | 0.37 | 88,88,88,88 | 0 |
| 81 | MG | 1 | 3511 | 1/1 | 0.85 | 0.11 | 73,73,73,73 | 0 |
| 81 | MG | 5 | 3950 | 1/1 | 0.85 | 0.34 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3521 | 1/1 | 0.85 | 0.28 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3530 | 1/1 | 0.85 | 0.29 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3932 | 1/1 | 0.85 | 0.28 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 4181 | 1/1 | 0.85 | 0.26 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3616 | 1/1 | 0.85 | 0.14 | 81,81,81,81 | 0 |
| 81 | MG | 2 | 1915 | 1/1 | 0.85 | 0.33 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3546 | 1/1 | 0.85 | 0.30 | 59,59,59,59 | 0 |
| 81 | MG | L2 | 306 | 1/1 | 0.85 | 0.37 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3923 | 1/1 | 0.85 | 0.42 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3546 | 1/1 | 0.85 | 0.18 | 43,43,43,43 | 0 |
| 81 | MG | 2 | 2106 | 1/1 | 0.85 | 0.17 | 84,84,84,84 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3541 | 1/1 | 0.85 | 0.47 | 41,41,41,41 | 0 |
| 81 | MG | O7 | 104 | 1/1 | 0.85 | 0.31 | 43,43,43,43 | 0 |
| 81 | MG | 2 | 2041 | 1/1 | 0.85 | 0.11 | 126,126,126,126 | 0 |
| 81 | MG | 1 | 4199 | 1/1 | 0.85 | 0.19 | 47,47,47,47 | 0 |
| 81 | MG | 6 | 2068 | 1/1 | 0.85 | 0.63 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3941 | 1/1 | 0.85 | 0.36 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 4176 | 1/1 | 0.85 | 0.71 | 78,78,78,78 | 0 |
| 81 | MG | M9 | 202 | 1/1 | 0.85 | 0.34 | 61,61,61,61 | 0 |
| 80 | PAR | 1 | 3435 | 42/42 | 0.85 | 0.31 | 40,40,40,40 | 42 |
| 81 | MG | 1 | 4177 | 1/1 | 0.85 | 0.39 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3496 | 1/1 | 0.85 | 0.50 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 1940 | 1/1 | 0.85 | 0.11 | 100,100,100,100 | 0 |
| 81 | MG | 5 | 3876 | 1/1 | 0.85 | 0.28 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3621 | 1/1 | 0.85 | 0.49 | 65,65,65,65 | 0 |
| 80 | PAR | 1 | 3431 | 42/42 | 0.85 | 0.25 | 67,67,67,67 | 42 |
| 80 | PAR | 5 | 3411 | 42/42 | 0.85 | 0.29 | 83,83,83,83 | 0 |
| 81 | MG | M5 | 309 | 1/1 | 0.85 | 0.37 | 43,43,43,43 | 0 |
| 81 | MG | Q1 | 1301 | 1/1 | 0.85 | 0.44 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4147 | 1/1 | 0.85 | 0.32 | 51,51,51,51 | 0 |
| 80 | PAR | 8 | 201 | 42/42 | 0.85 | 0.28 | 79,79,79,79 | 42 |
| 81 | MG | 2 | 1911 | 1/1 | 0.85 | 0.14 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 3499 | 1/1 | 0.85 | 0.51 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3643 | 1/1 | 0.85 | 0.24 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3626 | 1/1 | 0.85 | 0.32 | 60,60,60,60 | 0 |
| 81 | MG | L4 | 403 | 1/1 | 0.85 | 0.36 | 39,39,39,39 | 0 |
| 81 | MG | 5 | 3916 | 1/1 | 0.85 | 0.29 | 96,96,96,96 | 0 |
| 81 | MG | 1 | 4061 | 1/1 | 0.85 | 0.32 | 41,41,41,41 | 1 |
| 81 | MG | 5 | 3777 | 1/1 | 0.85 | 0.42 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 4195 | 1/1 | 0.85 | 0.31 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3898 | 1/1 | 0.85 | 0.24 | 66,66,66,66 | 0 |
| 81 | MG | 2 | 1943 | 1/1 | 0.85 | 0.64 | 82,82,82,82 | 0 |
| 81 | MG | 2 | 1956 | 1/1 | 0.85 | 0.23 | 119,119,119,119 | 0 |
| 81 | MG | 5 | 3743 | 1/1 | 0.85 | 0.29 | 54,54,54,54 | 1 |
| 81 | MG | L9 | 204 | 1/1 | 0.85 | 0.29 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 4109 | 1/1 | 0.85 | 0.87 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 4101 | 1/1 | 0.85 | 0.81 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3848 | 1/1 | 0.85 | 0.58 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3839 | 1/1 | 0.85 | 0.29 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3553 | 1/1 | 0.85 | 0.32 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3807 | 1/1 | 0.86 | 0.23 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 4015 | 1/1 | 0.86 | 0.30 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3623 | 1/1 | 0.86 | 0.19 | 63,63,63,63 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3683 | 1/1 | 0.86 | 0.55 | 53,53,53,53 | 0 |
| 80 | PAR | 6 | 1905 | 42/42 | 0.86 | 0.20 | 112,112,112,112 | 0 |
| 81 | MG | c9 | 202 | 1/1 | 0.86 | 0.15 | 124,124,124,124 | 0 |
| 81 | MG | 2 | 1999 | 1/1 | 0.86 | 0.17 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3996 | 1/1 | 0.86 | 0.49 | 78,78,78,78 | 0 |
| 81 | MG | 2 | 1969 | 1/1 | 0.86 | 0.16 | 114,114,114,114 | 0 |
| 81 | MG | 2 | 1972 | 1/1 | 0.86 | 0.55 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 4104 | 1/1 | 0.86 | 0.42 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3961 | 1/1 | 0.86 | 0.22 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3851 | 1/1 | 0.86 | 0.68 | 61,61,61,61 | 0 |
| 81 | MG | 7 | 208 | 1/1 | 0.86 | 0.11 | 117,117,117,117 | 0 |
| 81 | MG | 2 | 1970 | 1/1 | 0.86 | 0.09 | 118,118,118,118 | 0 |
| 81 | MG | 1 | 3628 | 1/1 | 0.86 | 0.65 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3993 | 1/1 | 0.86 | 0.28 | 64,64,64,64 | 0 |
| 81 | MG | 6 | 1993 | 1/1 | 0.86 | 0.35 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 4095 | 1/1 | 0.86 | 0.29 | 56,56,56,56 | 1 |
| 80 | PAR | 1 | 3406 | 42/42 | 0.86 | 0.38 | 68,68,68,68 | 42 |
| 81 | MG | 6 | 1951 | 1/1 | 0.86 | 0.20 | 78,78,78,78 | 0 |
| 81 | MG | 6 | 1979 | 1/1 | 0.86 | 0.13 | 90,90,90,90 | 0 |
| 81 | MG | 1 | 3781 | 1/1 | 0.86 | 0.33 | 51,51,51,51 | 1 |
| 81 | MG | 2 | 2060 | 1/1 | 0.86 | 0.41 | 103,103,103,103 | 0 |
| 81 | MG | 1 | 3953 | 1/1 | 0.86 | 0.18 | 54,54,54,54 | 0 |
| 81 | MG | 2 | 2112 | 1/1 | 0.86 | 0.51 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 4154 | 1/1 | 0.86 | 0.35 | 38,38,38,38 | 0 |
| 81 | MG | 8 | 204 | 1/1 | 0.86 | 0.69 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 4007 | 1/1 | 0.86 | 0.61 | 76,76,76,76 | 0 |
| 80 | PAR | 1 | 3437 | 42/42 | 0.86 | 0.31 | 64,64,64,64 | 42 |
| 81 | MG | 1 | 3560 | 1/1 | 0.86 | 0.17 | 42,42,42,42 | 0 |
| 81 | MG | m9 | 201 | 1/1 | 0.86 | 0.22 | 63,63,63,63 | 0 |
| 81 | MG | 6 | 2030 | 1/1 | 0.86 | 0.39 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3784 | 1/1 | 0.86 | 0.39 | 56,56,56,56 | 0 |
| 81 | MG | 2 | 2052 | 1/1 | 0.86 | 0.25 | 95,95,95,95 | 0 |
| 81 | MG | 2 | 1958 | 1/1 | 0.86 | 0.18 | 114,114,114,114 | 0 |
| 81 | MG | m7 | 205 | 1/1 | 0.86 | 0.26 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3720 | 1/1 | 0.86 | 0.33 | 65,65,65,65 | 0 |
| 81 | MG | 6 | 1980 | 1/1 | 0.86 | 0.14 | 105,105,105,105 | 0 |
| 81 | MG | M8 | 202 | 1/1 | 0.86 | 0.67 | 52,52,52,52 | 0 |
| 81 | MG | 2 | 2065 | 1/1 | 0.86 | 0.36 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3603 | 1/1 | 0.86 | 0.33 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 2052 | 1/1 | 0.86 | 0.22 | 72,72,72,72 | 0 |
| 80 | PAR | 1 | 3410 | 42/42 | 0.86 | 0.33 | 52,52,52,52 | 42 |
| 81 | MG | 5 | 3723 | 1/1 | 0.86 | 0.32 | 69,69,69,69 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 4072 | 1/1 | 0.86 | 0.19 | 65,65,65,65 | 0 |
| 81 | MG | 4 | 212 | 1/1 | 0.86 | 0.19 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3824 | 1/1 | 0.86 | 0.34 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3954 | 1/1 | 0.86 | 0.45 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3532 | 1/1 | 0.86 | 0.28 | 48,48,48,48 | 0 |
| 81 | MG | O4 | 202 | 1/1 | 0.86 | 0.24 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 4113 | 1/1 | 0.86 | 0.88 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3612 | 1/1 | 0.86 | 0.17 | 74,74,74,74 | 0 |
| 81 | MG | 2 | 1938 | 1/1 | 0.86 | 0.27 | 85,85,85,85 | 0 |
| 80 | PAR | 5 | 3409 | 42/42 | 0.87 | 0.32 | 56,56,56,56 | 42 |
| 81 | MG | 2 | 2086 | 1/1 | 0.87 | 0.33 | 95,95,95,95 | 0 |
| 80 | PAR | 5 | 3402 | 42/42 | 0.87 | 0.23 | 81,81,81,81 | 42 |
| 81 | MG | 1 | 3558 | 1/1 | 0.87 | 0.53 | 36,36,36,36 | 0 |
| 81 | MG | 5 | 3751 | 1/1 | 0.87 | 0.42 | 50,50,50,50 | 0 |
| 81 | MG | m9 | 205 | 1/1 | 0.87 | 0.39 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 4037 | 1/1 | 0.87 | 0.21 | 97,97,97,97 | 0 |
| 80 | PAR | 5 | 3413 | 42/42 | 0.87 | 0.29 | 72,72,72,72 | 42 |
| 81 | MG | 5 | 3979 | 1/1 | 0.87 | 0.31 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3782 | 1/1 | 0.87 | 0.21 | 82,82,82,82 | 0 |
| 81 | MG | 5 | 3857 | 1/1 | 0.87 | 0.23 | 60,60,60,60 | 0 |
| 81 | MG | O1 | 203 | 1/1 | 0.87 | 0.27 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3624 | 1/1 | 0.87 | 0.39 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 3825 | 1/1 | 0.87 | 0.93 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3821 | 1/1 | 0.87 | 0.26 | 62,62,62,62 | 0 |
| 81 | MG | 2 | 1988 | 1/1 | 0.87 | 0.14 | 86,86,86,86 | 0 |
| 81 | MG | 1 | 3665 | 1/1 | 0.87 | 0.32 | 54,54,54,54 | 0 |
| 81 | MG | L3 | 403 | 1/1 | 0.87 | 0.29 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 4071 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3799 | 1/1 | 0.87 | 0.23 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3645 | 1/1 | 0.87 | 0.30 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3678 | 1/1 | 0.87 | 0.25 | 58,58,58,58 | 1 |
| 81 | MG | 1 | 3523 | 1/1 | 0.87 | 0.31 | 50,50,50,50 | 0 |
| 81 | MG | 6 | 2040 | 1/1 | 0.87 | 0.42 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3550 | 1/1 | 0.87 | 0.28 | 55,55,55,55 | 0 |
| 81 | MG | 6 | 1983 | 1/1 | 0.87 | 0.32 | 88,88,88,88 | 0 |
| 81 | MG | 5 | 3644 | 1/1 | 0.87 | 0.48 | 59,59,59,59 | 0 |
| 81 | MG | 2 | 2097 | 1/1 | 0.87 | 0.49 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3895 | 1/1 | 0.87 | 0.24 | 65,65,65,65 | 0 |
| 81 | MG | 3 | 217 | 1/1 | 0.87 | 0.18 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 3642 | 1/1 | 0.87 | 0.17 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3680 | 1/1 | 0.87 | 0.24 | 60,60,60,60 | 0 |
| 80 | PAR | 3 | 203 | 42/42 | 0.87 | 0.26 | 78,78,78,78 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | M3 | 201 | 1/1 | 0.87 | 0.27 | 36,36,36,36 | 0 |
| 81 | MG | n0 | 201 | 1/1 | 0.87 | 0.14 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 4055 | 1/1 | 0.87 | 0.21 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3856 | 1/1 | 0.87 | 0.24 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3631 | 1/1 | 0.87 | 0.34 | 47,47,47,47 | 0 |
| 81 | MG | Q2 | 504 | 1/1 | 0.87 | 0.22 | 42,42,42,42 | 0 |
| 81 | MG | 2 | 2101 | 1/1 | 0.87 | 0.52 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3702 | 1/1 | 0.87 | 0.42 | 42,42,42,42 | 0 |
| 80 | PAR | 5 | 3421 | 42/42 | 0.87 | 0.19 | 102,102,102,102 | 0 |
| 81 | MG | 1 | 3714 | 1/1 | 0.87 | 0.22 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3925 | 1/1 | 0.87 | 0.34 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3961 | 1/1 | 0.87 | 0.20 | 40,40,40,40 | 0 |
| 81 | MG | 1 | 3600 | 1/1 | 0.87 | 0.42 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3838 | 1/1 | 0.87 | 0.25 | 57,57,57,57 | 0 |
| 81 | MG | 6 | 2050 | 1/1 | 0.87 | 0.42 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3726 | 1/1 | 0.87 | 0.62 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 4148 | 1/1 | 0.87 | 0.35 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 4046 | 1/1 | 0.87 | 0.34 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 4008 | 1/1 | 0.87 | 0.47 | 50,50,50,50 | 0 |
| 81 | MG | 6 | 1958 | 1/1 | 0.87 | 0.33 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3451 | 1/1 | 0.87 | 0.33 | 36,36,36,36 | 0 |
| 81 | MG | 1 | 3701 | 1/1 | 0.87 | 0.30 | 46,46,46,46 | 0 |
| 80 | PAR | 1 | 3404 | 42/42 | 0.87 | 0.27 | 53,53,53,53 | 42 |
| 81 | MG | 1 | 3676 | 1/1 | 0.87 | 0.21 | 64,64,64,64 | 0 |
| 81 | MG | l4 | 401 | 1/1 | 0.87 | 0.18 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 4065 | 1/1 | 0.87 | 0.17 | 100,100,100,100 | 0 |
| 81 | MG | 4 | 214 | 1/1 | 0.87 | 0.35 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3818 | 1/1 | 0.87 | 0.33 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 3823 | 1/1 | 0.87 | 0.33 | 78,78,78,78 | 0 |
| 81 | MG | 6 | 1988 | 1/1 | 0.87 | 0.64 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3958 | 1/1 | 0.87 | 0.24 | 61,61,61,61 | 1 |
| 80 | PAR | 5 | 3425 | 42/42 | 0.87 | 0.29 | 75,75,75,75 | 42 |
| 81 | MG | 2 | 1959 | 1/1 | 0.87 | 0.31 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 4006 | 1/1 | 0.88 | 0.61 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3713 | 1/1 | 0.88 | 0.28 | 53,53,53,53 | 0 |
| 81 | MG | o2 | 203 | 1/1 | 0.88 | 0.26 | 49,49,49,49 | 0 |
| 80 | PAR | 7 | 202 | 42/42 | 0.88 | 0.27 | 59,59,59,59 | 42 |
| 81 | MG | 5 | 4121 | 1/1 | 0.88 | 0.17 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3921 | 1/1 | 0.88 | 0.26 | 91,91,91,91 | 0 |
| 81 | MG | 5 | 3773 | 1/1 | 0.88 | 0.32 | 80,80,80,80 | 0 |
| 81 | MG | 2 | 1948 | 1/1 | 0.88 | 0.21 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 3909 | 1/1 | 0.88 | 0.86 | 65,65,65,65 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3709 | 1/1 | 0.88 | 0.36 | 54,54,54,54 | 0 |
| 81 | MG | 2 | 2056 | 1/1 | 0.88 | 0.42 | 80,80,80,80 | 0 |
| 81 | MG | M5 | 304 | 1/1 | 0.88 | 0.28 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3756 | 1/1 | 0.88 | 0.21 | 47,47,47,47 | 0 |
| 81 | MG | 6 | 2002 | 1/1 | 0.88 | 0.60 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 3913 | 1/1 | 0.88 | 0.39 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3915 | 1/1 | 0.88 | 0.40 | 69,69,69,69 | 0 |
| 81 | MG | 2 | 1935 | 1/1 | 0.88 | 0.35 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3984 | 1/1 | 0.88 | 0.56 | 85,85,85,85 | 0 |
| 81 | MG | 5 | 3547 | 1/1 | 0.88 | 0.25 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3539 | 1/1 | 0.88 | 0.21 | 30,30,30,30 | 0 |
| 81 | MG | 1 | 4046 | 1/1 | 0.88 | 0.23 | 49,49,49,49 | 0 |
| 81 | MG | 6 | 2046 | 1/1 | 0.88 | 0.33 | 118,118,118,118 | 0 |
| 80 | PAR | 1 | 3432 | 42/42 | 0.88 | 0.30 | 51,51,51,51 | 42 |
| 81 | MG | 1 | 3841 | 1/1 | 0.88 | 0.31 | 60,60,60,60 | 0 |
| 81 | MG | 2 | 2036 | 1/1 | 0.88 | 0.12 | 127,127,127,127 | 0 |
| 81 | MG | 4 | 233 | 1/1 | 0.88 | 0.36 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 4142 | 1/1 | 0.88 | 0.20 | 83,83,83,83 | 0 |
| 81 | MG | 1 | 3783 | 1/1 | 0.88 | 0.22 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 4022 | 1/1 | 0.88 | 0.26 | 47,47,47,47 | 1 |
| 81 | MG | 5 | 3770 | 1/1 | 0.88 | 0.48 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3813 | 1/1 | 0.88 | 1.07 | 70,70,70,70 | 0 |
| 81 | MG | 1 | 3881 | 1/1 | 0.88 | 0.22 | 72,72,72,72 | 0 |
| 81 | MG | N6 | 205 | 1/1 | 0.88 | 0.36 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3635 | 1/1 | 0.88 | 0.31 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3958 | 1/1 | 0.88 | 0.26 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3897 | 1/1 | 0.88 | 0.19 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3945 | 1/1 | 0.88 | 0.18 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3769 | 1/1 | 0.88 | 0.25 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 4162 | 1/1 | 0.88 | 0.24 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3881 | 1/1 | 0.88 | 0.23 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3596 | 1/1 | 0.88 | 0.18 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 4126 | 1/1 | 0.88 | 0.34 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 3527 | 1/1 | 0.88 | 0.25 | 32,32,32,32 | 0 |
| 81 | MG | l3 | 402 | 1/1 | 0.88 | 0.13 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3531 | 1/1 | 0.88 | 0.48 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4069 | 1/1 | 0.88 | 0.21 | 74,74,74,74 | 0 |
| 81 | MG | 2 | 2034 | 1/1 | 0.88 | 0.09 | 113,113,113,113 | 0 |
| 81 | MG | 2 | 1967 | 1/1 | 0.88 | 0.32 | 100,100,100,100 | 0 |
| 81 | MG | 5 | 4017 | 1/1 | 0.88 | 0.88 | 67,67,67,67 | 0 |
| 81 | MG | 2 | 2075 | 1/1 | 0.88 | 0.14 | 95,95,95,95 | 0 |
| 80 | PAR | 5 | 3426 | 42/42 | 0.88 | 0.26 | 56,56,56,56 | 42 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 2 | 1981 | 1/1 | 0.88 | 0.29 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 4094 | 1/1 | 0.88 | 0.24 | 84,84,84,84 | 0 |
| 81 | MG | 1 | 4024 | 1/1 | 0.88 | 0.66 | 61,61,61,61 | 0 |
| 81 | MG | O6 | 201 | 1/1 | 0.88 | 0.37 | 56,56,56,56 | 0 |
| 81 | MG | 2 | 2117 | 1/1 | 0.88 | 0.30 | 90,90,90,90 | 0 |
| 80 | PAR | 1 | 3434 | 42/42 | 0.88 | 0.20 | 85,85,85,85 | 42 |
| 81 | MG | 8 | 214 | 1/1 | 0.88 | 0.17 | 61,61,61,61 | 0 |
| 81 | MG | N3 | 204 | 1/1 | 0.88 | 0.34 | 53,53,53,53 | 0 |
| 81 | MG | 2 | 1984 | 1/1 | 0.88 | 0.74 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3565 | 1/1 | 0.88 | 0.22 | 80,80,80,80 | 0 |
| 80 | PAR | 1 | 3417 | 42/42 | 0.88 | 0.31 | 66,66,66,66 | 42 |
| 81 | MG | 1 | 3731 | 1/1 | 0.88 | 0.52 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3663 | 1/1 | 0.88 | 0.34 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3467 | 1/1 | 0.88 | 0.49 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4044 | 1/1 | 0.88 | 0.25 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3613 | 1/1 | 0.88 | 0.23 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 3917 | 1/1 | 0.88 | 0.31 | 69,69,69,69 | 0 |
| 81 | MG | O7 | 102 | 1/1 | 0.88 | 0.25 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 4060 | 1/1 | 0.88 | 0.24 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4047 | 1/1 | 0.88 | 0.20 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3617 | 1/1 | 0.88 | 0.20 | 75,75,75,75 | 0 |
| 81 | MG | 2 | 1996 | 1/1 | 0.88 | 0.21 | 80,80,80,80 | 0 |
| 81 | MG | 2 | 1951 | 1/1 | 0.88 | 0.09 | 134,134,134,134 | 0 |
| 81 | MG | 1 | 3519 | 1/1 | 0.88 | 0.31 | 43,43,43,43 | 0 |
| 81 | MG | 2 | 2082 | 1/1 | 0.88 | 0.26 | 119,119,119,119 | 0 |
| 81 | MG | 6 | 1984 | 1/1 | 0.88 | 0.17 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 3520 | 1/1 | 0.88 | 0.40 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3653 | 1/1 | 0.88 | 0.32 | 51,51,51,51 | 0 |
| 80 | PAR | 3 | 202 | 42/42 | 0.88 | 0.31 | 55,55,55,55 | 42 |
| 81 | MG | 3 | 211 | 1/1 | 0.88 | 0.24 | 86,86,86,86 | 0 |
| 81 | MG | 1 | 3610 | 1/1 | 0.88 | 0.20 | 58,58,58,58 | 0 |
| 81 | MG | 2 | 2046 | 1/1 | 0.88 | 0.29 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 4114 | 1/1 | 0.88 | 0.29 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3517 | 1/1 | 0.88 | 0.30 | 57,57,57,57 | 0 |
| 81 | MG | 2 | 2042 | 1/1 | 0.88 | 0.12 | 126,126,126,126 | 0 |
| 81 | MG | M6 | 205 | 1/1 | 0.88 | 0.37 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3788 | 1/1 | 0.88 | 0.24 | 68,68,68,68 | 0 |
| 81 | MG | 6 | 1974 | 1/1 | 0.88 | 0.12 | 110,110,110,110 | 0 |
| 81 | MG | 5 | 3640 | 1/1 | 0.88 | 0.26 | 49,49,49,49 | 0 |
| 81 | MG | 6 | 2006 | 1/1 | 0.89 | 0.48 | 76,76,76,76 | 0 |
| 81 | MG | 2 | 2105 | 1/1 | 0.89 | 0.27 | 62,62,62,62 | 0 |
| 81 | MG | 6 | 1971 | 1/1 | 0.89 | 0.16 | 89,89,89,89 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 4159 | 1/1 | 0.89 | 0.16 | 55,55,55,55 | 1 |
| 81 | MG | 5 | 3610 | 1/1 | 0.89 | 0.20 | 81,81,81,81 | 0 |
| 81 | MG | o4 | 202 | 1/1 | 0.89 | 0.16 | 89,89,89,89 | 0 |
| 81 | MG | 5 | 3978 | 1/1 | 0.89 | 0.27 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 3809 | 1/1 | 0.89 | 0.34 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3997 | 1/1 | 0.89 | 0.38 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 3481 | 1/1 | 0.89 | 0.24 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3550 | 1/1 | 0.89 | 0.24 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3506 | 1/1 | 0.89 | 0.25 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3969 | 1/1 | 0.89 | 0.28 | 55,55,55,55 | 0 |
| 81 | MG | O7 | 105 | 1/1 | 0.89 | 0.28 | 41,41,41,41 | 0 |
| 81 | MG | 1 | 3727 | 1/1 | 0.89 | 0.51 | 39,39,39,39 | 1 |
| 81 | MG | 5 | 3648 | 1/1 | 0.89 | 0.24 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 4120 | 1/1 | 0.89 | 0.28 | 81,81,81,81 | 0 |
| 81 | MG | L2 | 305 | 1/1 | 0.89 | 0.35 | 47,47,47,47 | 0 |
| 81 | MG | S9 | 201 | 1/1 | 0.89 | 0.24 | 126,126,126,126 | 0 |
| 81 | MG | 6 | 2023 | 1/1 | 0.89 | 0.29 | 90,90,90,90 | 0 |
| 81 | MG | 5 | 3868 | 1/1 | 0.89 | 0.16 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 4080 | 1/1 | 0.89 | 0.16 | 64,64,64,64 | 0 |
| 81 | MG | 2 | 1971 | 1/1 | 0.89 | 0.43 | 73,73,73,73 | 0 |
| 81 | MG | 6 | 1987 | 1/1 | 0.89 | 0.21 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3854 | 1/1 | 0.89 | 0.27 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3641 | 1/1 | 0.89 | 0.20 | 57,57,57,57 | 0 |
| 81 | MG | 6 | 1976 | 1/1 | 0.89 | 0.37 | 89,89,89,89 | 0 |
| 81 | MG | 5 | 3558 | 1/1 | 0.89 | 0.31 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 2067 | 1/1 | 0.89 | 0.25 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3870 | 1/1 | 0.89 | 0.23 | 36,36,36,36 | 1 |
| 81 | MG | 1 | 3498 | 1/1 | 0.89 | 0.49 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3970 | 1/1 | 0.89 | 0.28 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 4032 | 1/1 | 0.89 | 0.34 | 41,41,41,41 | 0 |
| 81 | MG | 1 | 4106 | 1/1 | 0.89 | 0.57 | 68,68,68,68 | 0 |
| 81 | MG | 2 | 2039 | 1/1 | 0.89 | 0.23 | 113,113,113,113 | 0 |
| 81 | MG | 2 | 2076 | 1/1 | 0.89 | 0.46 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 3740 | 1/1 | 0.89 | 0.44 | 68,68,68,68 | 0 |
| 81 | MG | m7 | 206 | 1/1 | 0.89 | 0.28 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 4063 | 1/1 | 0.89 | 0.36 | 80,80,80,80 | 0 |
| 80 | PAR | 1 | 3414 | 42/42 | 0.89 | 0.24 | 63,63,63,63 | 42 |
| 81 | MG | N1 | 203 | 1/1 | 0.89 | 0.21 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3893 | 1/1 | 0.89 | 0.24 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3656 | 1/1 | 0.89 | 0.35 | 40,40,40,40 | 0 |
| 81 | MG | 1 | 3994 | 1/1 | 0.89 | 0.49 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3815 | 1/1 | 0.89 | 0.34 | 55,55,55,55 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 4049 | 1/1 | 0.89 | 0.18 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3568 | 1/1 | 0.89 | 0.26 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3992 | 1/1 | 0.89 | 0.37 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3888 | 1/1 | 0.89 | 0.30 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3587 | 1/1 | 0.89 | 0.50 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 4018 | 1/1 | 0.89 | 0.56 | 95,95,95,95 | 0 |
| 81 | MG | 1 | 4122 | 1/1 | 0.89 | 0.24 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 4102 | 1/1 | 0.89 | 0.24 | 48,48,48,48 | 1 |
| 81 | MG | n3 | 204 | 1/1 | 0.89 | 0.35 | 50,50,50,50 | 0 |
| 80 | PAR | 1 | 3427 | 42/42 | 0.89 | 0.26 | 65,65,65,65 | 42 |
| 81 | MG | 1 | 4157 | 1/1 | 0.89 | 0.35 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3975 | 1/1 | 0.89 | 0.33 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3952 | 1/1 | 0.89 | 0.19 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3504 | 1/1 | 0.89 | 0.36 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4158 | 1/1 | 0.89 | 0.20 | 55,55,55,55 | 0 |
| 80 | PAR | 5 | 3415 | 42/42 | 0.89 | 0.23 | 83,83,83,83 | 0 |
| 81 | MG | 4 | 206 | 1/1 | 0.89 | 0.31 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3730 | 1/1 | 0.89 | 0.70 | 47,47,47,47 | 0 |
| 80 | PAR | 2 | 1904 | 42/42 | 0.89 | 0.18 | 107,107,107,107 | 0 |
| 81 | MG | 1 | 3729 | 1/1 | 0.89 | 0.47 | 44,44,44,44 | 0 |
| 81 | MG | 2 | 2053 | 1/1 | 0.89 | 0.20 | 100,100,100,100 | 0 |
| 81 | MG | 8 | 224 | 1/1 | 0.89 | 0.60 | 59,59,59,59 | 0 |
| 81 | MG | 6 | 2025 | 1/1 | 0.89 | 0.23 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 3858 | 1/1 | 0.89 | 0.17 | 106,106,106,106 | 0 |
| 81 | MG | 5 | 4008 | 1/1 | 0.89 | 0.70 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3991 | 1/1 | 0.89 | 0.30 | 41,41,41,41 | 1 |
| 81 | MG | 5 | 3689 | 1/1 | 0.89 | 0.31 | 59,59,59,59 | 0 |
| 80 | PAR | 6 | 1901 | 42/42 | 0.89 | 0.27 | 90,90,90,90 | 0 |
| 81 | MG | M5 | 307 | 1/1 | 0.89 | 0.37 | 43,43,43,43 | 0 |
| 81 | MG | 6 | 1927 | 1/1 | 0.89 | 0.43 | 73,73,73,73 | 0 |
| 81 | MG | 5 | 3754 | 1/1 | 0.89 | 0.18 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3537 | 1/1 | 0.89 | 0.37 | 31,31,31,31 | 0 |
| 81 | MG | 1 | 4067 | 1/1 | 0.89 | 0.16 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3940 | 1/1 | 0.89 | 0.41 | 37,37,37,37 | 0 |
| 81 | MG | 5 | 4083 | 1/1 | 0.89 | 0.29 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3837 | 1/1 | 0.89 | 0.35 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3744 | 1/1 | 0.89 | 0.31 | 39,39,39,39 | 0 |
| 81 | MG | o7 | 503 | 1/1 | 0.89 | 0.28 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3752 | 1/1 | 0.89 | 0.12 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 3670 | 1/1 | 0.89 | 0.27 | 57,57,57,57 | 1 |
| 81 | MG | 1 | 3927 | 1/1 | 0.89 | 0.18 | 53,53,53,53 | 0 |
| 81 | MG | m6 | 203 | 1/1 | 0.89 | 0.27 | 55,55,55,55 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3493 | 1/1 | 0.89 | 0.18 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3745 | 1/1 | 0.89 | 0.69 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3939 | 1/1 | 0.89 | 0.29 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3806 | 1/1 | 0.89 | 0.24 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 3465 | 1/1 | 0.89 | 0.26 | 34,34,34,34 | 0 |
| 81 | MG | 6 | 2038 | 1/1 | 0.89 | 0.25 | 105,105,105,105 | 0 |
| 80 | PAR | 5 | 3401 | 42/42 | 0.89 | 0.20 | 78,78,78,78 | 42 |
| 81 | MG | n0 | 205 | 1/1 | 0.89 | 0.12 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3748 | 1/1 | 0.89 | 0.24 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 4074 | 1/1 | 0.90 | 0.13 | 71,71,71,71 | 0 |
| 81 | MG | o2 | 202 | 1/1 | 0.90 | 0.47 | 53,53,53,53 | 0 |
| 81 | MG | Q2 | 502 | 1/1 | 0.90 | 0.28 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 4134 | 1/1 | 0.90 | 0.36 | 69,69,69,69 | 0 |
| 81 | MG | 2 | 2002 | 1/1 | 0.90 | 0.16 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 4029 | 1/1 | 0.90 | 0.35 | 57,57,57,57 | 0 |
| 81 | MG | 2 | 2073 | 1/1 | 0.90 | 0.16 | 99,99,99,99 | 0 |
| 81 | MG | 1 | 4124 | 1/1 | 0.90 | 0.40 | 69,69,69,69 | 0 |
| 80 | PAR | 1 | 3407 | 42/42 | 0.90 | 0.33 | 69,69,69,69 | 42 |
| 81 | MG | 5 | 3653 | 1/1 | 0.90 | 0.57 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 4048 | 1/1 | 0.90 | 0.27 | 66,66,66,66 | 0 |
| 81 | MG | 6 | 2032 | 1/1 | 0.90 | 0.23 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3569 | 1/1 | 0.90 | 0.17 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3750 | 1/1 | 0.90 | 0.37 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3820 | 1/1 | 0.90 | 0.21 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 4103 | 1/1 | 0.90 | 0.47 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3976 | 1/1 | 0.90 | 0.34 | 58,58,58,58 | 0 |
| 80 | PAR | 5 | 3424 | 42/42 | 0.90 | 0.28 | 65,65,65,65 | 42 |
| 81 | MG | 1 | 3825 | 1/1 | 0.90 | 0.21 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 3891 | 1/1 | 0.90 | 0.23 | 59,59,59,59 | 0 |
| 81 | MG | 6 | 1934 | 1/1 | 0.90 | 0.41 | 83,83,83,83 | 0 |
| 81 | MG | 4 | 224 | 1/1 | 0.90 | 0.34 | 55,55,55,55 | 0 |
| 80 | PAR | 5 | 3414 | 42/42 | 0.90 | 0.22 | 67,67,67,67 | 42 |
| 81 | MG | 4 | 220 | 1/1 | 0.90 | 0.30 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 4128 | 1/1 | 0.90 | 0.33 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4017 | 1/1 | 0.90 | 0.35 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 4052 | 1/1 | 0.90 | 0.21 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3773 | 1/1 | 0.90 | 0.38 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3490 | 1/1 | 0.90 | 0.35 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3602 | 1/1 | 0.90 | 0.14 | 87,87,87,87 | 0 |
| 81 | MG | 5 | 3504 | 1/1 | 0.90 | 0.23 | 53,53,53,53 | 0 |
| 81 | MG | d2 | 201 | 1/1 | 0.90 | 0.43 | 84,84,84,84 | 0 |
| 81 | MG | 2 | 2079 | 1/1 | 0.90 | 0.29 | 75,75,75,75 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 8 | 206 | 1/1 | 0.90 | 0.20 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3684 | 1/1 | 0.90 | 0.57 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3736 | 1/1 | 0.90 | 0.37 | 46,46,46,46 | 0 |
| 81 | MG | 6 | 1969 | 1/1 | 0.90 | 0.31 | 101,101,101,101 | 0 |
| 81 | MG | 1 | 3983 | 1/1 | 0.90 | 0.30 | 51,51,51,51 | 1 |
| 81 | MG | 5 | 3859 | 1/1 | 0.90 | 0.41 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 4096 | 1/1 | 0.90 | 0.25 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3742 | 1/1 | 0.90 | 0.25 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3674 | 1/1 | 0.90 | 0.31 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3834 | 1/1 | 0.90 | 0.12 | 77,77,77,77 | 0 |
| 81 | MG | 5 | 4002 | 1/1 | 0.90 | 0.32 | 66,66,66,66 | 0 |
| 81 | MG | O2 | 203 | 1/1 | 0.90 | 0.16 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 4068 | 1/1 | 0.90 | 0.33 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3944 | 1/1 | 0.90 | 0.44 | 48,48,48,48 | 0 |
| 81 | MG | 6 | 2021 | 1/1 | 0.90 | 0.46 | 85,85,85,85 | 0 |
| 81 | MG | 5 | 3781 | 1/1 | 0.90 | 0.40 | 49,49,49,49 | 0 |
| 80 | PAR | 1 | 3422 | 42/42 | 0.90 | 0.27 | 51,51,51,51 | 42 |
| 81 | MG | 1 | 4130 | 1/1 | 0.90 | 0.26 | 38,38,38,38 | 1 |
| 81 | MG | 2 | 2012 | 1/1 | 0.90 | 0.10 | 104,104,104,104 | 0 |
| 81 | MG | 5 | 3836 | 1/1 | 0.90 | 0.28 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3535 | 1/1 | 0.90 | 0.42 | 36,36,36,36 | 1 |
| 81 | MG | 5 | 3651 | 1/1 | 0.90 | 0.17 | 63,63,63,63 | 1 |
| 81 | MG | 2 | 1983 | 1/1 | 0.90 | 0.74 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3714 | 1/1 | 0.90 | 0.28 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3533 | 1/1 | 0.90 | 0.24 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3740 | 1/1 | 0.90 | 0.36 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3892 | 1/1 | 0.90 | 0.14 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 4110 | 1/1 | 0.90 | 0.77 | 82,82,82,82 | 0 |
| 81 | MG | 1 | 3607 | 1/1 | 0.90 | 0.71 | 57,57,57,57 | 1 |
| 81 | MG | 5 | 4081 | 1/1 | 0.90 | 0.28 | 102,102,102,102 | 0 |
| 81 | MG | 5 | 3884 | 1/1 | 0.90 | 0.15 | 67,67,67,67 | 0 |
| 81 | MG | 1 | 3649 | 1/1 | 0.90 | 0.51 | 37,37,37,37 | 0 |
| 81 | MG | 6 | 1916 | 1/1 | 0.90 | 0.21 | 79,79,79,79 | 0 |
| 81 | MG | M0 | 301 | 1/1 | 0.90 | 0.21 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3763 | 1/1 | 0.90 | 0.36 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3931 | 1/1 | 0.90 | 0.46 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3949 | 1/1 | 0.90 | 0.15 | 58,58,58,58 | 1 |
| 81 | MG | 1 | 3739 | 1/1 | 0.90 | 0.27 | 43,43,43,43 | 0 |
| 81 | MG | 4 | 204 | 1/1 | 0.90 | 0.53 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3542 | 1/1 | 0.90 | 0.24 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 4088 | 1/1 | 0.90 | 0.69 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 3933 | 1/1 | 0.90 | 0.60 | 42,42,42,42 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3930 | 1/1 | 0.90 | 0.34 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3662 | 1/1 | 0.90 | 0.41 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4190 | 1/1 | 0.90 | 0.21 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3775 | 1/1 | 0.90 | 0.35 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4011 | 1/1 | 0.90 | 0.77 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3795 | 1/1 | 0.90 | 0.12 | 106,106,106,106 | 0 |
| 81 | MG | 2 | 2040 | 1/1 | 0.90 | 0.30 | 123,123,123,123 | 0 |
| 80 | PAR | 5 | 3419 | 42/42 | 0.90 | 0.27 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 4059 | 1/1 | 0.90 | 0.33 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3919 | 1/1 | 0.90 | 0.32 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3804 | 1/1 | 0.90 | 0.26 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 4005 | 1/1 | 0.90 | 0.25 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 3563 | 1/1 | 0.90 | 0.10 | 55,55,55,55 | 0 |
| 81 | MG | 2 | 1945 | 1/1 | 0.90 | 0.17 | 88,88,88,88 | 0 |
| 80 | PAR | 6 | 1904 | 42/42 | 0.90 | 0.28 | 72,72,72,72 | 0 |
| 81 | MG | Q3 | 503 | 1/1 | 0.90 | 0.28 | 54,54,54,54 | 0 |
| 80 | PAR | 5 | 3418 | 42/42 | 0.90 | 0.24 | 98,98,98,98 | 0 |
| 81 | MG | 1 | 3583 | 1/1 | 0.90 | 0.25 | 49,49,49,49 | 0 |
| 80 | PAR | 1 | 3418 | 42/42 | 0.90 | 0.21 | 69,69,69,69 | 42 |
| 81 | MG | 1 | 3681 | 1/1 | 0.90 | 0.37 | 53,53,53,53 | 0 |
| 80 | PAR | 1 | 3420 | 42/42 | 0.90 | 0.21 | 65,65,65,65 | 42 |
| 81 | MG | 1 | 3921 | 1/1 | 0.90 | 0.28 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3595 | 1/1 | 0.90 | 0.15 | 83,83,83,83 | 0 |
| 81 | MG | 2 | 1975 | 1/1 | 0.90 | 0.31 | 94,94,94,94 | 0 |
| 81 | MG | 6 | 1950 | 1/1 | 0.90 | 0.23 | 83,83,83,83 | 0 |
| 81 | MG | 1 | 3970 | 1/1 | 0.90 | 0.20 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3933 | 1/1 | 0.91 | 0.15 | 65,65,65,65 | 1 |
| 81 | MG | 1 | 3810 | 1/1 | 0.91 | 0.36 | 96,96,96,96 | 0 |
| 81 | MG | 5 | 3891 | 1/1 | 0.91 | 0.17 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 4009 | 1/1 | 0.91 | 0.42 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3885 | 1/1 | 0.91 | 0.17 | 67,67,67,67 | 0 |
| 80 | PAR | 6 | 1903 | 42/42 | 0.91 | 0.26 | 74,74,74,74 | 0 |
| 80 | PAR | 1 | 3402 | 42/42 | 0.91 | 0.19 | 62,62,62,62 | 42 |
| 81 | MG | 5 | 3889 | 1/1 | 0.91 | 0.36 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3604 | 1/1 | 0.91 | 0.23 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4063 | 1/1 | 0.91 | 0.38 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3625 | 1/1 | 0.91 | 0.23 | 36,36,36,36 | 1 |
| 81 | MG | 2 | 2055 | 1/1 | 0.91 | 0.35 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3666 | 1/1 | 0.91 | 0.18 | 44,44,44,44 | 0 |
| 81 | MG | 8 | 207 | 1/1 | 0.91 | 0.12 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 3555 | 1/1 | 0.91 | 0.46 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3905 | 1/1 | 0.91 | 0.21 | 121,121,121,121 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 4081 | 1/1 | 0.91 | 0.23 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3492 | 1/1 | 0.91 | 0.36 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3910 | 1/1 | 0.91 | 0.54 | 48,48,48,48 | 0 |
| 81 | MG | 6 | 1933 | 1/1 | 0.91 | 0.70 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 3965 | 1/1 | 0.91 | 0.36 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3649 | 1/1 | 0.91 | 0.35 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3548 | 1/1 | 0.91 | 0.38 | 52,52,52,52 | 0 |
| 81 | MG | N6 | 202 | 1/1 | 0.91 | 0.30 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3973 | 1/1 | 0.91 | 0.32 | 47,47,47,47 | 1 |
| 81 | MG | 1 | 3570 | 1/1 | 0.91 | 0.34 | 60,60,60,60 | 0 |
| 80 | PAR | 1 | 3415 | 42/42 | 0.91 | 0.27 | 46,46,46,46 | 42 |
| 81 | MG | 5 | 3858 | 1/1 | 0.91 | 0.28 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4087 | 1/1 | 0.91 | 0.49 | 67,67,67,67 | 0 |
| 80 | PAR | 7 | 201 | 42/42 | 0.91 | 0.21 | 85,85,85,85 | 0 |
| 81 | MG | M5 | 305 | 1/1 | 0.91 | 0.28 | 52,52,52,52 | 0 |
| 81 | MG | m0 | 302 | 1/1 | 0.91 | 0.20 | 66,66,66,66 | 0 |
| 81 | MG | 2 | 2033 | 1/1 | 0.91 | 0.23 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 4194 | 1/1 | 0.91 | 0.25 | 50,50,50,50 | 0 |
| 81 | MG | 6 | 1908 | 1/1 | 0.91 | 0.23 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3867 | 1/1 | 0.91 | 0.53 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3760 | 1/1 | 0.91 | 0.13 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 4051 | 1/1 | 0.91 | 0.33 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3803 | 1/1 | 0.91 | 0.27 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 4170 | 1/1 | 0.91 | 0.43 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3790 | 1/1 | 0.91 | 0.15 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3481 | 1/1 | 0.91 | 0.24 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3854 | 1/1 | 0.91 | 0.21 | 65,65,65,65 | 0 |
| 81 | MG | 2 | 1909 | 1/1 | 0.91 | 0.20 | 88,88,88,88 | 0 |
| 81 | MG | 5 | 3820 | 1/1 | 0.91 | 0.19 | 59,59,59,59 | 0 |
| 81 | MG | 2 | 2006 | 1/1 | 0.91 | 0.14 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3622 | 1/1 | 0.91 | 0.43 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3768 | 1/1 | 0.91 | 0.26 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3500 | 1/1 | 0.91 | 0.52 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4074 | 1/1 | 0.91 | 0.49 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3607 | 1/1 | 0.91 | 0.24 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3719 | 1/1 | 0.91 | 0.16 | 42,42,42,42 | 0 |
| 81 | MG | l2 | 303 | 1/1 | 0.91 | 0.43 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3888 | 1/1 | 0.91 | 0.21 | 42,42,42,42 | 0 |
| 80 | PAR | 2 | 1902 | 42/42 | 0.91 | 0.27 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3811 | 1/1 | 0.91 | 0.07 | 64,64,64,64 | 0 |
| 81 | MG | d4 | 201 | 1/1 | 0.91 | 0.22 | 91,91,91,91 | 0 |
| 81 | MG | 6 | 2000 | 1/1 | 0.91 | 0.09 | 107,107,107,107 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3627 | 1/1 | 0.91 | 0.27 | 59,59,59,59 | 0 |
| 81 | MG | 8 | 208 | 1/1 | 0.91 | 0.21 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3917 | 1/1 | 0.91 | 0.47 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 3588 | 1/1 | 0.91 | 0.20 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3650 | 1/1 | 0.91 | 0.40 | 46,46,46,46 | 0 |
| 81 | MG | 2 | 2099 | 1/1 | 0.91 | 0.35 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3929 | 1/1 | 0.91 | 0.32 | 47,47,47,47 | 1 |
| 81 | MG | 1 | 3943 | 1/1 | 0.91 | 0.32 | 40,40,40,40 | 0 |
| 81 | MG | 1 | 3551 | 1/1 | 0.91 | 0.36 | 46,46,46,46 | 0 |
| 81 | MG | 6 | 1968 | 1/1 | 0.91 | 0.23 | 77,77,77,77 | 0 |
| 81 | MG | 1 | 3918 | 1/1 | 0.91 | 0.20 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 1977 | 1/1 | 0.91 | 0.10 | 96,96,96,96 | 0 |
| 81 | MG | 5 | 3635 | 1/1 | 0.91 | 0.16 | 59,59,59,59 | 0 |
| 81 | MG | 4 | 228 | 1/1 | 0.91 | 0.17 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4143 | 1/1 | 0.91 | 0.47 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3638 | 1/1 | 0.91 | 0.25 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3976 | 1/1 | 0.91 | 0.22 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3920 | 1/1 | 0.91 | 0.40 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 4020 | 1/1 | 0.91 | 0.41 | 100,100,100,100 | 0 |
| 81 | MG | 5 | 3779 | 1/1 | 0.91 | 0.38 | 52,52,52,52 | 0 |
| 81 | MG | 2 | 1993 | 1/1 | 0.91 | 0.26 | 83,83,83,83 | 0 |
| 81 | MG | 1 | 4196 | 1/1 | 0.91 | 0.24 | 46,46,46,46 | 1 |
| 81 | MG | L7 | 301 | 1/1 | 0.91 | 0.24 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3753 | 1/1 | 0.91 | 0.31 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 4188 | 1/1 | 0.91 | 0.20 | 57,57,57,57 | 0 |
| 81 | MG | 6 | 1910 | 1/1 | 0.91 | 0.19 | 78,78,78,78 | 0 |
| 81 | MG | N8 | 202 | 1/1 | 0.91 | 0.15 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3671 | 1/1 | 0.91 | 0.45 | 56,56,56,56 | 0 |
| 80 | PAR | 1 | 3419 | 42/42 | 0.91 | 0.24 | 59,59,59,59 | 0 |
| 81 | MG | m9 | 202 | 1/1 | 0.91 | 0.21 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 3850 | 1/1 | 0.91 | 0.14 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 4051 | 1/1 | 0.91 | 0.31 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3447 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3918 | 1/1 | 0.91 | 0.44 | 60,60,60,60 | 0 |
| 81 | MG | 2 | 1942 | 1/1 | 0.91 | 0.20 | 77,77,77,77 | 0 |
| 81 | MG | 5 | 3934 | 1/1 | 0.91 | 0.46 | 58,58,58,58 | 0 |
| 80 | PAR | 1 | 3430 | 42/42 | 0.91 | 0.20 | 65,65,65,65 | 42 |
| 81 | MG | 4 | 213 | 1/1 | 0.91 | 0.13 | 41,41,41,41 | 0 |
| 81 | MG | 6 | 2043 | 1/1 | 0.91 | 0.18 | 97,97,97,97 | 0 |
| 81 | MG | 4 | 217 | 1/1 | 0.91 | 0.32 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 4086 | 1/1 | 0.91 | 0.16 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 3907 | 1/1 | 0.91 | 0.28 | 81,81,81,81 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3544 | 1/1 | 0.91 | 0.41 | 55,55,55,55 | 0 |
| 80 | PAR | 1 | 3412 | 42/42 | 0.91 | 0.25 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3542 | 1/1 | 0.91 | 0.62 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3885 | 1/1 | 0.91 | 0.19 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 4094 | 1/1 | 0.91 | 0.28 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3911 | 1/1 | 0.91 | 0.35 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3926 | 1/1 | 0.91 | 0.31 | 53,53,53,53 | 0 |
| 81 | MG | n2 | 201 | 1/1 | 0.91 | 0.15 | 97,97,97,97 | 0 |
| 81 | MG | 2 | 1997 | 1/1 | 0.91 | 0.16 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3522 | 1/1 | 0.91 | 0.31 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3895 | 1/1 | 0.91 | 0.19 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3978 | 1/1 | 0.91 | 0.20 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 4049 | 1/1 | 0.91 | 0.26 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 3688 | 1/1 | 0.91 | 0.31 | 59,59,59,59 | 0 |
| 81 | MG | 5 | 3468 | 1/1 | 0.91 | 0.32 | 44,44,44,44 | 0 |
| 81 | MG | s2 | 301 | 1/1 | 0.91 | 0.12 | 95,95,95,95 | 0 |
| 81 | MG | S6 | 301 | 1/1 | 0.91 | 0.33 | 118,118,118,118 | 0 |
| 81 | MG | 5 | 3737 | 1/1 | 0.91 | 0.36 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3540 | 1/1 | 0.91 | 0.34 | 33,33,33,33 | 0 |
| 81 | MG | 1 | 3908 | 1/1 | 0.92 | 0.65 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3652 | 1/1 | 0.92 | 0.41 | 49,49,49,49 | 0 |
| 80 | PAR | 1 | 3425 | 42/42 | 0.92 | 0.23 | 48,48,48,48 | 42 |
| 81 | MG | 1 | 3652 | 1/1 | 0.92 | 0.35 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 3912 | 1/1 | 0.92 | 0.20 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3810 | 1/1 | 0.92 | 0.21 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3563 | 1/1 | 0.92 | 0.26 | 85,85,85,85 | 0 |
| 81 | MG | 5 | 3732 | 1/1 | 0.92 | 0.50 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3869 | 1/1 | 0.92 | 0.14 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 3869 | 1/1 | 0.92 | 0.28 | 44,44,44,44 | 0 |
| 80 | PAR | 5 | 3420 | 42/42 | 0.92 | 0.29 | 77,77,77,77 | 0 |
| 81 | MG | 1 | 3643 | 1/1 | 0.92 | 0.32 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3581 | 1/1 | 0.92 | 0.34 | 42,42,42,42 | 0 |
| 80 | PAR | 4 | 202 | 42/42 | 0.92 | 0.24 | 49,49,49,49 | 42 |
| 81 | MG | 1 | 4101 | 1/1 | 0.92 | 0.23 | 113,113,113,113 | 0 |
| 81 | MG | 1 | 3959 | 1/1 | 0.92 | 0.29 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3494 | 1/1 | 0.92 | 0.41 | 44,44,44,44 | 0 |
| 81 | MG | L9 | 202 | 1/1 | 0.92 | 0.29 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3678 | 1/1 | 0.92 | 0.23 | 50,50,50,50 | 0 |
| 81 | MG | 2 | 1952 | 1/1 | 0.92 | 0.20 | 132,132,132,132 | 0 |
| 81 | MG | M6 | 201 | 1/1 | 0.92 | 0.30 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3940 | 1/1 | 0.92 | 0.16 | 73,73,73,73 | 0 |
| 81 | MG | 2 | 2029 | 1/1 | 0.92 | 0.34 | 81,81,81,81 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 4193 | 1/1 | 0.92 | 0.34 | 66,66,66,66 | 0 |
| 81 | MG | 5 | 3692 | 1/1 | 0.92 | 0.38 | 56,56,56,56 | 0 |
| 81 | MG | 2 | 2088 | 1/1 | 0.92 | 0.35 | 64,64,64,64 | 0 |
| 81 | MG | 2 | 2050 | 1/1 | 0.92 | 0.44 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3696 | 1/1 | 0.92 | 0.29 | 59,59,59,59 | 0 |
| 81 | MG | 2 | 2022 | 1/1 | 0.92 | 0.22 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 3509 | 1/1 | 0.92 | 0.10 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 4152 | 1/1 | 0.92 | 0.17 | 47,47,47,47 | 1 |
| 80 | PAR | 5 | 3412 | 42/42 | 0.92 | 0.21 | 47,47,47,47 | 42 |
| 81 | MG | 1 | 4153 | 1/1 | 0.92 | 0.81 | 50,50,50,50 | 0 |
| 81 | MG | o3 | 201 | 1/1 | 0.92 | 0.36 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3578 | 1/1 | 0.92 | 0.24 | 41,41,41,41 | 0 |
| 81 | MG | 6 | 1999 | 1/1 | 0.92 | 0.30 | 82,82,82,82 | 0 |
| 81 | MG | 1 | 3776 | 1/1 | 0.92 | 0.46 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3570 | 1/1 | 0.92 | 0.21 | 110,110,110,110 | 0 |
| 81 | MG | 5 | 3819 | 1/1 | 0.92 | 0.21 | 60,60,60,60 | 0 |
| 81 | MG | 2 | 2057 | 1/1 | 0.92 | 0.29 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 4028 | 1/1 | 0.92 | 0.28 | 45,45,45,45 | 0 |
| 81 | MG | 2 | 2077 | 1/1 | 0.92 | 0.06 | 121,121,121,121 | 0 |
| 81 | MG | 1 | 3672 | 1/1 | 0.92 | 0.29 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 4124 | 1/1 | 0.92 | 0.40 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3928 | 1/1 | 0.92 | 0.21 | 46,46,46,46 | 0 |
| 81 | MG | d6 | 102 | 1/1 | 0.92 | 0.26 | 85,85,85,85 | 0 |
| 81 | MG | 4 | 219 | 1/1 | 0.92 | 0.27 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3567 | 1/1 | 0.92 | 0.18 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3659 | 1/1 | 0.92 | 0.16 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3939 | 1/1 | 0.92 | 0.30 | 49,49,49,49 | 1 |
| 81 | MG | 1 | 3467 | 1/1 | 0.92 | 0.28 | 31,31,31,31 | 0 |
| 81 | MG | 5 | 3540 | 1/1 | 0.92 | 0.24 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3470 | 1/1 | 0.92 | 0.26 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3894 | 1/1 | 0.92 | 0.15 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3556 | 1/1 | 0.92 | 0.28 | 36,36,36,36 | 0 |
| 81 | MG | 5 | 4039 | 1/1 | 0.92 | 0.64 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3826 | 1/1 | 0.92 | 0.23 | 37,37,37,37 | 1 |
| 81 | MG | 1 | 3812 | 1/1 | 0.92 | 0.21 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3886 | 1/1 | 0.92 | 0.34 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3897 | 1/1 | 0.92 | 0.31 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 4023 | 1/1 | 0.92 | 0.43 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 3986 | 1/1 | 0.92 | 0.30 | 51,51,51,51 | 0 |
| 81 | MG | 2 | 2038 | 1/1 | 0.92 | 0.13 | 109,109,109,109 | 0 |
| 81 | MG | 5 | 3843 | 1/1 | 0.92 | 0.64 | 86,86,86,86 | 0 |
| 81 | MG | l7 | 301 | 1/1 | 0.92 | 0.19 | 58,58,58,58 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 4151 | 1/1 | 0.92 | 0.24 | 40,40,40,40 | 0 |
| 80 | PAR | 5 | 3416 | 42/42 | 0.92 | 0.23 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3605 | 1/1 | 0.92 | 0.12 | 71,71,71,71 | 0 |
| 81 | MG | s6 | 302 | 1/1 | 0.92 | 0.33 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3693 | 1/1 | 0.92 | 0.31 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3722 | 1/1 | 0.92 | 0.29 | 50,50,50,50 | 0 |
| 81 | MG | L5 | 302 | 1/1 | 0.92 | 0.23 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3612 | 1/1 | 0.92 | 0.14 | 70,70,70,70 | 0 |
| 81 | MG | 6 | 1907 | 1/1 | 0.92 | 0.28 | 93,93,93,93 | 0 |
| 81 | MG | 5 | 3782 | 1/1 | 0.92 | 0.26 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3545 | 1/1 | 0.92 | 0.28 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 4169 | 1/1 | 0.92 | 0.28 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3698 | 1/1 | 0.92 | 0.28 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3730 | 1/1 | 0.92 | 0.47 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3948 | 1/1 | 0.92 | 0.27 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3744 | 1/1 | 0.92 | 0.79 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4052 | 1/1 | 0.92 | 0.22 | 50,50,50,50 | 0 |
| 81 | MG | l4 | 403 | 1/1 | 0.92 | 0.31 | 80,80,80,80 | 0 |
| 80 | PAR | 1 | 3429 | 42/42 | 0.92 | 0.24 | 58,58,58,58 | 42 |
| 81 | MG | 1 | 3863 | 1/1 | 0.92 | 0.17 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3687 | 1/1 | 0.92 | 0.24 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3706 | 1/1 | 0.92 | 0.39 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3431 | 1/1 | 0.92 | 0.25 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3916 | 1/1 | 0.92 | 0.28 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3838 | 1/1 | 0.92 | 0.27 | 53,53,53,53 | 0 |
| 81 | MG | 6 | 1923 | 1/1 | 0.92 | 0.41 | 65,65,65,65 | 0 |
| 81 | MG | N6 | 201 | 1/1 | 0.92 | 0.11 | 57,57,57,57 | 1 |
| 81 | MG | 6 | 2008 | 1/1 | 0.92 | 0.59 | 98,98,98,98 | 0 |
| 81 | MG | 5 | 3659 | 1/1 | 0.92 | 0.34 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3746 | 1/1 | 0.92 | 0.30 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3617 | 1/1 | 0.92 | 0.20 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 3633 | 1/1 | 0.92 | 0.41 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3486 | 1/1 | 0.92 | 0.20 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 4090 | 1/1 | 0.92 | 0.38 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3646 | 1/1 | 0.92 | 0.19 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3932 | 1/1 | 0.92 | 0.35 | 54,54,54,54 | 1 |
| 81 | MG | 5 | 3437 | 1/1 | 0.92 | 0.22 | 43,43,43,43 | 0 |
| 81 | MG | L2 | 304 | 1/1 | 0.92 | 0.29 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3848 | 1/1 | 0.92 | 0.27 | 95,95,95,95 | 0 |
| 81 | MG | 1 | 3616 | 1/1 | 0.92 | 0.24 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3544 | 1/1 | 0.92 | 0.28 | 32,32,32,32 | 0 |
| 81 | MG | 1 | 3505 | 1/1 | 0.92 | 0.22 | 64,64,64,64 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3588 | 1/1 | 0.92 | 0.35 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3757 | 1/1 | 0.92 | 0.22 | 57,57,57,57 | 0 |
| 81 | MG | 2 | 2051 | 1/1 | 0.92 | 0.21 | 96,96,96,96 | 0 |
| 81 | MG | 1 | 3898 | 1/1 | 0.92 | 0.09 | 70,70,70,70 | 0 |
| 81 | MG | 6 | 1917 | 1/1 | 0.92 | 0.35 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 4072 | 1/1 | 0.92 | 0.23 | 80,80,80,80 | 0 |
| 81 | MG | c4 | 202 | 1/1 | 0.92 | 0.22 | 119,119,119,119 | 0 |
| 81 | MG | 1 | 4138 | 1/1 | 0.92 | 0.27 | 55,55,55,55 | 0 |
| 81 | MG | 2 | 1928 | 1/1 | 0.92 | 0.22 | 75,75,75,75 | 0 |
| 81 | MG | 6 | 2056 | 1/1 | 0.92 | 0.08 | 126,126,126,126 | 0 |
| 81 | MG | 1 | 3762 | 1/1 | 0.92 | 0.17 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 4075 | 1/1 | 0.92 | 0.34 | 55,55,55,55 | 0 |
| 81 | MG | 6 | 1936 | 1/1 | 0.93 | 0.23 | 84,84,84,84 | 0 |
| 81 | MG | 2 | 1925 | 1/1 | 0.93 | 0.33 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3791 | 1/1 | 0.93 | 0.16 | 70,70,70,70 | 0 |
| 81 | MG | 5 | 3775 | 1/1 | 0.93 | 0.59 | 60,60,60,60 | 0 |
| 81 | MG | 5 | 4107 | 1/1 | 0.93 | 0.28 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 2031 | 1/1 | 0.93 | 0.75 | 64,64,64,64 | 0 |
| 81 | MG | 7 | 205 | 1/1 | 0.93 | 0.12 | 93,93,93,93 | 0 |
| 81 | MG | 6 | 2005 | 1/1 | 0.93 | 0.67 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3804 | 1/1 | 0.93 | 0.28 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 4041 | 1/1 | 0.93 | 0.18 | 70,70,70,70 | 0 |
| 80 | PAR | 5 | 3407 | 42/42 | 0.93 | 0.23 | 51,51,51,51 | 42 |
| 81 | MG | 1 | 4006 | 1/1 | 0.93 | 0.25 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3568 | 1/1 | 0.93 | 0.11 | 74,74,74,74 | 0 |
| 81 | MG | 6 | 1960 | 1/1 | 0.93 | 0.24 | 110,110,110,110 | 0 |
| 81 | MG | 5 | 3929 | 1/1 | 0.93 | 0.52 | 55,55,55,55 | 0 |
| 81 | MG | 7 | 206 | 1/1 | 0.93 | 0.20 | 116,116,116,116 | 0 |
| 81 | MG | 2 | 2021 | 1/1 | 0.93 | 0.28 | 73,73,73,73 | 0 |
| 81 | MG | 6 | 1989 | 1/1 | 0.93 | 0.22 | 75,75,75,75 | 0 |
| 81 | MG | 2 | 1974 | 1/1 | 0.93 | 0.19 | 101,101,101,101 | 0 |
| 81 | MG | 5 | 3725 | 1/1 | 0.93 | 0.31 | 63,63,63,63 | 0 |
| 81 | MG | 2 | 2087 | 1/1 | 0.93 | 0.27 | 70,70,70,70 | 0 |
| 81 | MG | n0 | 204 | 1/1 | 0.93 | 0.20 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3518 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3702 | 1/1 | 0.93 | 0.56 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3906 | 1/1 | 0.93 | 0.31 | 38,38,38,38 | 0 |
| 80 | PAR | 1 | 3416 | 42/42 | 0.93 | 0.23 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 4064 | 1/1 | 0.93 | 0.17 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3728 | 1/1 | 0.93 | 0.29 | 61,61,61,61 | 1 |
| 81 | MG | 5 | 4093 | 1/1 | 0.93 | 0.31 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 4012 | 1/1 | 0.93 | 0.40 | 56,56,56,56 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 4 | 209 | 1/1 | 0.93 | 0.18 | 36,36,36,36 | 0 |
| 80 | PAR | 1 | 3428 | 42/42 | 0.93 | 0.21 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4150 | 1/1 | 0.93 | 0.25 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3637 | 1/1 | 0.93 | 0.49 | 45,45,45,45 | 0 |
| 81 | MG | 8 | 211 | 1/1 | 0.93 | 0.24 | 66,66,66,66 | 0 |
| 81 | MG | 8 | 203 | 1/1 | 0.93 | 0.18 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3807 | 1/1 | 0.93 | 0.20 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3675 | 1/1 | 0.93 | 0.32 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3456 | 1/1 | 0.93 | 0.28 | 43,43,43,43 | 0 |
| 81 | MG | 2 | 2047 | 1/1 | 0.93 | 0.38 | 94,94,94,94 | 0 |
| 81 | MG | 5 | 3797 | 1/1 | 0.93 | 0.36 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3441 | 1/1 | 0.93 | 0.28 | 30,30,30,30 | 0 |
| 81 | MG | 5 | 3628 | 1/1 | 0.93 | 0.20 | 59,59,59,59 | 0 |
| 81 | MG | 2 | 1955 | 1/1 | 0.93 | 0.09 | 133,133,133,133 | 0 |
| 81 | MG | 1 | 3787 | 1/1 | 0.93 | 0.11 | 97,97,97,97 | 0 |
| 81 | MG | 5 | 3956 | 1/1 | 0.93 | 0.51 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3980 | 1/1 | 0.93 | 0.21 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3772 | 1/1 | 0.93 | 0.37 | 49,49,49,49 | 0 |
| 81 | MG | 2 | 2017 | 1/1 | 0.93 | 0.23 | 93,93,93,93 | 0 |
| 81 | MG | 5 | 3833 | 1/1 | 0.93 | 0.30 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3780 | 1/1 | 0.93 | 0.32 | 42,42,42,42 | 0 |
| 81 | MG | 2 | 1965 | 1/1 | 0.93 | 0.19 | 95,95,95,95 | 0 |
| 81 | MG | 1 | 3524 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 81 | MG | n1 | 201 | 1/1 | 0.93 | 0.24 | 70,70,70,70 | 0 |
| 81 | MG | 6 | 2069 | 1/1 | 0.93 | 0.28 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3943 | 1/1 | 0.93 | 0.25 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3480 | 1/1 | 0.93 | 0.28 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3755 | 1/1 | 0.93 | 0.18 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 4163 | 1/1 | 0.93 | 0.33 | 39,39,39,39 | 1 |
| 80 | PAR | 1 | 3408 | 42/42 | 0.93 | 0.24 | 44,44,44,44 | 42 |
| 81 | MG | 1 | 3573 | 1/1 | 0.93 | 0.30 | 45,45,45,45 | 0 |
| 81 | MG | 2 | 1953 | 1/1 | 0.93 | 0.15 | 131,131,131,131 | 0 |
| 81 | MG | 1 | 3704 | 1/1 | 0.93 | 0.19 | 42,42,42,42 | 0 |
| 81 | MG | 4 | 221 | 1/1 | 0.93 | 0.15 | 46,46,46,46 | 1 |
| 81 | MG | 5 | 3600 | 1/1 | 0.93 | 0.15 | 93,93,93,93 | 0 |
| 81 | MG | 5 | 3676 | 1/1 | 0.93 | 0.28 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3578 | 1/1 | 0.93 | 0.26 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3971 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3800 | 1/1 | 0.93 | 0.39 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 4144 | 1/1 | 0.93 | 0.34 | 40,40,40,40 | 1 |
| 81 | MG | 5 | 3501 | 1/1 | 0.93 | 0.22 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4040 | 1/1 | 0.93 | 0.22 | 59,59,59,59 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3582 | 1/1 | 0.93 | 0.57 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3923 | 1/1 | 0.93 | 0.11 | 112,112,112,112 | 0 |
| 81 | MG | d3 | 201 | 1/1 | 0.93 | 0.33 | 68,68,68,68 | 0 |
| 81 | MG | 2 | 1990 | 1/1 | 0.93 | 0.28 | 88,88,88,88 | 0 |
| 81 | MG | 1 | 4167 | 1/1 | 0.93 | 0.20 | 65,65,65,65 | 0 |
| 81 | MG | N5 | 201 | 1/1 | 0.93 | 0.19 | 61,61,61,61 | 0 |
| 81 | MG | 6 | 2061 | 1/1 | 0.93 | 0.29 | 110,110,110,110 | 0 |
| 81 | MG | 1 | 3536 | 1/1 | 0.93 | 0.31 | 37,37,37,37 | 0 |
| 81 | MG | 2 | 2009 | 1/1 | 0.93 | 0.29 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 1906 | 1/1 | 0.93 | 0.25 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 4117 | 1/1 | 0.93 | 0.24 | 62,62,62,62 | 0 |
| 81 | MG | C8 | 201 | 1/1 | 0.93 | 0.18 | 137,137,137,137 | 0 |
| 81 | MG | 1 | 3988 | 1/1 | 0.93 | 0.22 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 4023 | 1/1 | 0.93 | 0.30 | 49,49,49,49 | 0 |
| 81 | MG | N0 | 201 | 1/1 | 0.93 | 0.46 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 4172 | 1/1 | 0.93 | 0.27 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 3434 | 1/1 | 0.93 | 0.34 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3657 | 1/1 | 0.93 | 0.26 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3462 | 1/1 | 0.93 | 0.40 | 30,30,30,30 | 0 |
| 81 | MG | 5 | 3562 | 1/1 | 0.93 | 0.12 | 94,94,94,94 | 0 |
| 81 | MG | 5 | 3780 | 1/1 | 0.93 | 0.32 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3736 | 1/1 | 0.93 | 0.24 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4165 | 1/1 | 0.93 | 0.33 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3624 | 1/1 | 0.93 | 0.22 | 34,34,34,34 | 0 |
| 80 | PAR | 5 | 3406 | 42/42 | 0.93 | 0.22 | 51,51,51,51 | 42 |
| 81 | MG | 1 | 4003 | 1/1 | 0.93 | 0.27 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 4088 | 1/1 | 0.93 | 0.17 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 1916 | 1/1 | 0.93 | 0.26 | 86,86,86,86 | 0 |
| 81 | MG | 1 | 4025 | 1/1 | 0.93 | 0.20 | 41,41,41,41 | 0 |
| 81 | MG | 1 | 3602 | 1/1 | 0.93 | 0.22 | 55,55,55,55 | 0 |
| 80 | PAR | 5 | 3408 | 42/42 | 0.93 | 0.22 | 58,58,58,58 | 42 |
| 81 | MG | 5 | 3790 | 1/1 | 0.93 | 0.11 | 76,76,76,76 | 0 |
| 81 | MG | m6 | 204 | 1/1 | 0.93 | 0.38 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3672 | 1/1 | 0.93 | 0.23 | 40,40,40,40 | 0 |
| 80 | PAR | 5 | 3410 | 42/42 | 0.93 | 0.23 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3856 | 1/1 | 0.93 | 0.18 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4019 | 1/1 | 0.93 | 0.38 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3908 | 1/1 | 0.93 | 0.12 | 86,86,86,86 | 0 |
| 80 | PAR | 1 | 3424 | 42/42 | 0.93 | 0.28 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 3492 | 1/1 | 0.93 | 0.33 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3722 | 1/1 | 0.93 | 0.16 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3576 | 1/1 | 0.93 | 0.20 | 39,39,39,39 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 4189 | 1/1 | 0.93 | 0.30 | 77,77,77,77 | 0 |
| 81 | MG | 6 | 1955 | 1/1 | 0.93 | 0.30 | 91,91,91,91 | 0 |
| 81 | MG | 5 | 3566 | 1/1 | 0.93 | 0.42 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 4191 | 1/1 | 0.93 | 0.32 | 48,48,48,48 | 0 |
| 81 | MG | O7 | 103 | 1/1 | 0.93 | 0.31 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 3724 | 1/1 | 0.93 | 0.37 | 31,31,31,31 | 0 |
| 81 | MG | 5 | 3811 | 1/1 | 0.93 | 0.49 | 54,54,54,54 | 0 |
| 81 | MG | 4 | 227 | 1/1 | 0.93 | 0.08 | 76,76,76,76 | 0 |
| 81 | MG | 2 | 1921 | 1/1 | 0.93 | 0.27 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 4040 | 1/1 | 0.93 | 0.24 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3770 | 1/1 | 0.93 | 0.38 | 45,45,45,45 | 1 |
| 81 | MG | 1 | 3936 | 1/1 | 0.93 | 0.14 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3519 | 1/1 | 0.93 | 0.30 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3613 | 1/1 | 0.93 | 0.19 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3703 | 1/1 | 0.93 | 0.55 | 58,58,58,58 | 0 |
| 81 | MG | 6 | 1991 | 1/1 | 0.93 | 0.40 | 62,62,62,62 | 0 |
| 81 | MG | 1 | 3912 | 1/1 | 0.93 | 0.39 | 44,44,44,44 | 0 |
| 81 | MG | 8 | 205 | 1/1 | 0.93 | 0.27 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3466 | 1/1 | 0.93 | 0.31 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3787 | 1/1 | 0.93 | 0.30 | 59,59,59,59 | 0 |
| 81 | MG | 4 | 218 | 1/1 | 0.93 | 0.15 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3650 | 1/1 | 0.93 | 0.50 | 31,31,31,31 | 0 |
| 81 | MG | 1 | 3733 | 1/1 | 0.94 | 0.29 | 41,41,41,41 | 0 |
| 81 | MG | 6 | 2018 | 1/1 | 0.94 | 0.23 | 89,89,89,89 | 0 |
| 81 | MG | 1 | 3589 | 1/1 | 0.94 | 0.63 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3920 | 1/1 | 0.94 | 0.34 | 50,50,50,50 | 0 |
| 81 | MG | 6 | 1996 | 1/1 | 0.94 | 0.09 | 96,96,96,96 | 0 |
| 81 | MG | 1 | 3865 | 1/1 | 0.94 | 0.21 | 46,46,46,46 | 1 |
| 81 | MG | 2 | 2114 | 1/1 | 0.94 | 0.22 | 104,104,104,104 | 0 |
| 81 | MG | O4 | 203 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3746 | 1/1 | 0.94 | 0.40 | 36,36,36,36 | 0 |
| 81 | MG | 6 | 1994 | 1/1 | 0.94 | 0.29 | 79,79,79,79 | 0 |
| 81 | MG | 1 | 3566 | 1/1 | 0.94 | 0.23 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3673 | 1/1 | 0.94 | 0.28 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3569 | 1/1 | 0.94 | 0.26 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3658 | 1/1 | 0.94 | 0.23 | 41,41,41,41 | 0 |
| 81 | MG | 2 | 2068 | 1/1 | 0.94 | 0.21 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 4106 | 1/1 | 0.94 | 0.37 | 73,73,73,73 | 0 |
| 81 | MG | 2 | 1926 | 1/1 | 0.94 | 0.36 | 62,62,62,62 | 0 |
| 81 | MG | m0 | 301 | 1/1 | 0.94 | 0.09 | 58,58,58,58 | 0 |
| 81 | MG | n8 | 204 | 1/1 | 0.94 | 0.22 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3606 | 1/1 | 0.94 | 0.24 | 74,74,74,74 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3827 | 1/1 | 0.94 | 0.30 | 35,35,35,35 | 0 |
| 80 | PAR | 1 | 3409 | 42/42 | 0.94 | 0.22 | 38,38,38,38 | 42 |
| 81 | MG | 1 | 3721 | 1/1 | 0.94 | 0.26 | 47,47,47,47 | 1 |
| 81 | MG | 1 | 3934 | 1/1 | 0.94 | 0.19 | 57,57,57,57 | 0 |
| 81 | MG | n3 | 202 | 1/1 | 0.94 | 0.31 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3547 | 1/1 | 0.94 | 0.17 | 65,65,65,65 | 0 |
| 80 | PAR | 2 | 1903 | 42/42 | 0.94 | 0.24 | 69,69,69,69 | 0 |
| 81 | MG | 6 | 2048 | 1/1 | 0.94 | 0.29 | 88,88,88,88 | 0 |
| 81 | MG | 7 | 207 | 1/1 | 0.94 | 0.18 | 118,118,118,118 | 0 |
| 81 | MG | 1 | 3887 | 1/1 | 0.94 | 0.13 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3776 | 1/1 | 0.94 | 0.49 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3552 | 1/1 | 0.94 | 0.36 | 61,61,61,61 | 0 |
| 81 | MG | 6 | 1961 | 1/1 | 0.94 | 0.20 | 98,98,98,98 | 0 |
| 81 | MG | 5 | 3803 | 1/1 | 0.94 | 0.18 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3691 | 1/1 | 0.94 | 0.28 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3668 | 1/1 | 0.94 | 0.25 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3488 | 1/1 | 0.94 | 0.23 | 43,43,43,43 | 0 |
| 81 | MG | 2 | 1913 | 1/1 | 0.94 | 0.23 | 87,87,87,87 | 0 |
| 81 | MG | 5 | 3534 | 1/1 | 0.94 | 0.30 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3515 | 1/1 | 0.94 | 0.17 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3835 | 1/1 | 0.94 | 0.36 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 4178 | 1/1 | 0.94 | 0.32 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 4197 | 1/1 | 0.94 | 0.33 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3878 | 1/1 | 0.94 | 0.38 | 54,54,54,54 | 1 |
| 81 | MG | 4 | 208 | 1/1 | 0.94 | 0.27 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3938 | 1/1 | 0.94 | 0.38 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3877 | 1/1 | 0.94 | 0.42 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3509 | 1/1 | 0.94 | 0.13 | 72,72,72,72 | 0 |
| 81 | MG | 5 | 3721 | 1/1 | 0.94 | 0.28 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3882 | 1/1 | 0.94 | 0.38 | 55,55,55,55 | 0 |
| 81 | MG | 6 | 1930 | 1/1 | 0.94 | 0.25 | 86,86,86,86 | 0 |
| 81 | MG | 6 | 1913 | 1/1 | 0.94 | 0.14 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 3960 | 1/1 | 0.94 | 0.25 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3661 | 1/1 | 0.94 | 0.26 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3831 | 1/1 | 0.94 | 0.24 | 37,37,37,37 | 0 |
| 81 | MG | 6 | 2073 | 1/1 | 0.94 | 0.46 | 94,94,94,94 | 0 |
| 81 | MG | N1 | 201 | 1/1 | 0.94 | 0.16 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3779 | 1/1 | 0.94 | 0.30 | 41,41,41,41 | 0 |
| 81 | MG | M5 | 308 | 1/1 | 0.94 | 0.39 | 58,58,58,58 | 0 |
| 81 | MG | 4 | 207 | 1/1 | 0.94 | 0.16 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3801 | 1/1 | 0.94 | 0.30 | 47,47,47,47 | 0 |
| 80 | PAR | 5 | 3417 | 42/42 | 0.94 | 0.19 | 76,76,76,76 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 2 | 1966 | 1/1 | 0.94 | 0.18 | 99,99,99,99 | 0 |
| 81 | MG | M7 | 204 | 1/1 | 0.94 | 0.22 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 4071 | 1/1 | 0.94 | 0.18 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3793 | 1/1 | 0.94 | 0.27 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 4042 | 1/1 | 0.94 | 0.27 | 69,69,69,69 | 0 |
| 81 | MG | 2 | 1962 | 1/1 | 0.94 | 0.12 | 106,106,106,106 | 0 |
| 81 | MG | 5 | 3592 | 1/1 | 0.94 | 0.26 | 61,61,61,61 | 1 |
| 81 | MG | o7 | 502 | 1/1 | 0.94 | 0.34 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 4089 | 1/1 | 0.94 | 0.30 | 69,69,69,69 | 0 |
| 81 | MG | 2 | 1908 | 1/1 | 0.94 | 0.24 | 104,104,104,104 | 0 |
| 81 | MG | 5 | 3668 | 1/1 | 0.94 | 0.31 | 47,47,47,47 | 1 |
| 81 | MG | 5 | 4077 | 1/1 | 0.94 | 0.28 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3629 | 1/1 | 0.94 | 0.58 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 4045 | 1/1 | 0.94 | 0.30 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3757 | 1/1 | 0.94 | 0.31 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3866 | 1/1 | 0.94 | 0.19 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3489 | 1/1 | 0.94 | 0.26 | 46,46,46,46 | 0 |
| 81 | MG | 4 | 211 | 1/1 | 0.94 | 0.18 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3480 | 1/1 | 0.94 | 0.22 | 39,39,39,39 | 0 |
| 81 | MG | 6 | 1914 | 1/1 | 0.94 | 0.17 | 81,81,81,81 | 0 |
| 81 | MG | 5 | 3435 | 1/1 | 0.94 | 0.25 | 44,44,44,44 | 0 |
| 81 | MG | O3 | 202 | 1/1 | 0.94 | 0.20 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 4078 | 1/1 | 0.94 | 0.28 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3626 | 1/1 | 0.94 | 0.39 | 36,36,36,36 | 0 |
| 81 | MG | o0 | 201 | 1/1 | 0.94 | 0.25 | 89,89,89,89 | 0 |
| 81 | MG | m7 | 208 | 1/1 | 0.94 | 0.30 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3832 | 1/1 | 0.94 | 0.55 | 52,52,52,52 | 0 |
| 81 | MG | n8 | 203 | 1/1 | 0.94 | 0.84 | 51,51,51,51 | 1 |
| 81 | MG | 5 | 3865 | 1/1 | 0.94 | 0.13 | 58,58,58,58 | 0 |
| 80 | PAR | 1 | 3411 | 42/42 | 0.94 | 0.24 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 4026 | 1/1 | 0.94 | 0.50 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 3712 | 1/1 | 0.94 | 0.33 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3792 | 1/1 | 0.94 | 0.22 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3996 | 1/1 | 0.94 | 0.33 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3452 | 1/1 | 0.94 | 0.35 | 30,30,30,30 | 0 |
| 81 | MG | 2 | 2027 | 1/1 | 0.94 | 0.20 | 69,69,69,69 | 0 |
| 81 | MG | L3 | 404 | 1/1 | 0.94 | 0.29 | 43,43,43,43 | 0 |
| 81 | MG | n5 | 201 | 1/1 | 0.94 | 0.35 | 60,60,60,60 | 0 |
| 81 | MG | 4 | 215 | 1/1 | 0.94 | 0.24 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3618 | 1/1 | 0.94 | 0.19 | 68,68,68,68 | 0 |
| 80 | PAR | 1 | 3421 | 42/42 | 0.94 | 0.24 | 43,43,43,43 | 42 |
| 81 | MG | 5 | 3571 | 1/1 | 0.94 | 0.15 | 92,92,92,92 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 6 | 1929 | 1/1 | 0.94 | 0.25 | 80,80,80,80 | 0 |
| 81 | MG | 1 | 4135 | 1/1 | 0.94 | 0.31 | 37,37,37,37 | 1 |
| 81 | MG | 1 | 4086 | 1/1 | 0.94 | 0.47 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3684 | 1/1 | 0.94 | 0.35 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3707 | 1/1 | 0.94 | 0.36 | 40,40,40,40 | 0 |
| 81 | MG | 1 | 3662 | 1/1 | 0.94 | 0.34 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 4036 | 1/1 | 0.94 | 0.51 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3661 | 1/1 | 0.94 | 0.35 | 47,47,47,47 | 0 |
| 81 | MG | n3 | 203 | 1/1 | 0.94 | 0.27 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3925 | 1/1 | 0.94 | 0.20 | 52,52,52,52 | 1 |
| 81 | MG | 1 | 4077 | 1/1 | 0.94 | 0.28 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 4056 | 1/1 | 0.94 | 0.22 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3808 | 1/1 | 0.94 | 0.18 | 54,54,54,54 | 1 |
| 81 | MG | n6 | 203 | 1/1 | 0.94 | 0.23 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3666 | 1/1 | 0.94 | 0.30 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3484 | 1/1 | 0.94 | 0.27 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3747 | 1/1 | 0.94 | 0.28 | 36,36,36,36 | 0 |
| 81 | MG | 5 | 3463 | 1/1 | 0.94 | 0.43 | 44,44,44,44 | 0 |
| 81 | MG | 6 | 2019 | 1/1 | 0.94 | 0.19 | 107,107,107,107 | 0 |
| 81 | MG | 1 | 4168 | 1/1 | 0.94 | 0.13 | 64,64,64,64 | 0 |
| 80 | PAR | 1 | 3423 | 42/42 | 0.94 | 0.23 | 54,54,54,54 | 0 |
| 81 | MG | 2 | 2110 | 1/1 | 0.94 | 0.46 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3470 | 1/1 | 0.94 | 0.26 | 45,45,45,45 | 0 |
| 81 | MG | 6 | 1931 | 1/1 | 0.94 | 0.20 | 94,94,94,94 | 0 |
| 81 | MG | 1 | 3655 | 1/1 | 0.94 | 0.29 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3609 | 1/1 | 0.94 | 0.29 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3450 | 1/1 | 0.94 | 0.28 | 29,29,29,29 | 0 |
| 81 | MG | L2 | 303 | 1/1 | 0.94 | 0.24 | 38,38,38,38 | 0 |
| 81 | MG | s4 | 301 | 1/1 | 0.94 | 0.10 | 96,96,96,96 | 0 |
| 81 | MG | 1 | 3688 | 1/1 | 0.94 | 0.29 | 39,39,39,39 | 0 |
| 81 | MG | 6 | 1945 | 1/1 | 0.94 | 0.31 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3453 | 1/1 | 0.94 | 0.24 | 45,45,45,45 | 0 |
| 81 | MG | L2 | 301 | 1/1 | 0.94 | 0.31 | 31,31,31,31 | 0 |
| 81 | MG | m7 | 209 | 1/1 | 0.94 | 0.29 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3697 | 1/1 | 0.94 | 0.69 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3494 | 1/1 | 0.94 | 0.17 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 3562 | 1/1 | 0.94 | 0.40 | 44,44,44,44 | 0 |
| 81 | MG | 2 | 2015 | 1/1 | 0.94 | 0.09 | 140,140,140,140 | 0 |
| 81 | MG | 6 | 1942 | 1/1 | 0.94 | 0.19 | 105,105,105,105 | 0 |
| 81 | MG | 1 | 3796 | 1/1 | 0.94 | 0.29 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3816 | 1/1 | 0.94 | 0.18 | 58,58,58,58 | 0 |
| 81 | MG | 2 | 2005 | 1/1 | 0.94 | 0.22 | 58,58,58,58 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3794 | 1/1 | 0.94 | 0.23 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3587 | 1/1 | 0.94 | 0.20 | 66,66,66,66 | 0 |
| 81 | MG | 6 | 1918 | 1/1 | 0.94 | 0.31 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3830 | 1/1 | 0.94 | 0.27 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3735 | 1/1 | 0.94 | 0.55 | 62,62,62,62 | 0 |
| 81 | MG | M5 | 301 | 1/1 | 0.94 | 0.22 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 4137 | 1/1 | 0.94 | 0.21 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3741 | 1/1 | 0.94 | 0.28 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 3765 | 1/1 | 0.94 | 0.18 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3549 | 1/1 | 0.94 | 0.49 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 4156 | 1/1 | 0.94 | 0.21 | 44,44,44,44 | 1 |
| 81 | MG | 1 | 3510 | 1/1 | 0.94 | 0.11 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3758 | 1/1 | 0.95 | 0.33 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3432 | 1/1 | 0.95 | 0.37 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 4053 | 1/1 | 0.95 | 0.18 | 59,59,59,59 | 0 |
| 81 | MG | l3 | 403 | 1/1 | 0.95 | 0.28 | 43,43,43,43 | 1 |
| 81 | MG | 5 | 3760 | 1/1 | 0.95 | 0.23 | 50,50,50,50 | 0 |
| 81 | MG | 8 | 221 | 1/1 | 0.95 | 0.11 | 86,86,86,86 | 0 |
| 81 | MG | 1 | 3674 | 1/1 | 0.95 | 0.37 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3514 | 1/1 | 0.95 | 0.26 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3430 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 81 | MG | 6 | 1911 | 1/1 | 0.95 | 0.26 | 73,73,73,73 | 0 |
| 81 | MG | 6 | 2057 | 1/1 | 0.95 | 0.09 | 126,126,126,126 | 0 |
| 81 | MG | 8 | 218 | 1/1 | 0.95 | 0.22 | 73,73,73,73 | 0 |
| 81 | MG | 5 | 3849 | 1/1 | 0.95 | 0.57 | 88,88,88,88 | 0 |
| 81 | MG | 1 | 3594 | 1/1 | 0.95 | 0.38 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3555 | 1/1 | 0.95 | 0.26 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3584 | 1/1 | 0.95 | 0.31 | 67,67,67,67 | 0 |
| 81 | MG | C9 | 201 | 1/1 | 0.95 | 0.16 | 121,121,121,121 | 0 |
| 81 | MG | 1 | 3438 | 1/1 | 0.95 | 0.33 | 36,36,36,36 | 0 |
| 81 | MG | 6 | 1963 | 1/1 | 0.95 | 0.39 | 97,97,97,97 | 0 |
| 81 | MG | 1 | 3866 | 1/1 | 0.95 | 0.31 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3482 | 1/1 | 0.95 | 0.45 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3525 | 1/1 | 0.95 | 0.32 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3644 | 1/1 | 0.95 | 0.35 | 46,46,46,46 | 0 |
| 81 | MG | 2 | 1946 | 1/1 | 0.95 | 0.24 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 4032 | 1/1 | 0.95 | 0.16 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 4022 | 1/1 | 0.95 | 0.87 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 4179 | 1/1 | 0.95 | 0.24 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3665 | 1/1 | 0.95 | 0.24 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3487 | 1/1 | 0.95 | 0.32 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3473 | 1/1 | 0.95 | 0.32 | 51,51,51,51 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3699 | 1/1 | 0.95 | 0.24 | 48,48,48,48 | 0 |
| 81 | MG | N3 | 202 | 1/1 | 0.95 | 0.43 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3477 | 1/1 | 0.95 | 0.23 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3444 | 1/1 | 0.95 | 0.18 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3712 | 1/1 | 0.95 | 0.39 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3488 | 1/1 | 0.95 | 0.21 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3814 | 1/1 | 0.95 | 0.27 | 47,47,47,47 | 0 |
| 81 | MG | 2 | 2035 | 1/1 | 0.95 | 0.11 | 116,116,116,116 | 0 |
| 81 | MG | 1 | 3572 | 1/1 | 0.95 | 0.31 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 3863 | 1/1 | 0.95 | 0.31 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3834 | 1/1 | 0.95 | 0.29 | 31,31,31,31 | 0 |
| 81 | MG | 1 | 3942 | 1/1 | 0.95 | 0.16 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3629 | 1/1 | 0.95 | 0.10 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3686 | 1/1 | 0.95 | 0.20 | 45,45,45,45 | 0 |
| 81 | MG | 6 | 2033 | 1/1 | 0.95 | 0.34 | 70,70,70,70 | 0 |
| 81 | MG | 2 | 2064 | 1/1 | 0.95 | 0.12 | 111,111,111,111 | 0 |
| 81 | MG | 5 | 3454 | 1/1 | 0.95 | 0.24 | 40,40,40,40 | 0 |
| 81 | MG | m7 | 202 | 1/1 | 0.95 | 0.23 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 4028 | 1/1 | 0.95 | 0.20 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3778 | 1/1 | 0.95 | 0.29 | 50,50,50,50 | 1 |
| 81 | MG | 1 | 3696 | 1/1 | 0.95 | 0.47 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3808 | 1/1 | 0.95 | 0.23 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 3593 | 1/1 | 0.95 | 0.32 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3691 | 1/1 | 0.95 | 0.55 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3611 | 1/1 | 0.95 | 0.13 | 60,60,60,60 | 0 |
| 81 | MG | 1 | 3802 | 1/1 | 0.95 | 0.14 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3591 | 1/1 | 0.95 | 0.28 | 58,58,58,58 | 0 |
| 81 | MG | 6 | 1926 | 1/1 | 0.95 | 0.31 | 70,70,70,70 | 0 |
| 81 | MG | 1 | 3620 | 1/1 | 0.95 | 0.22 | 68,68,68,68 | 0 |
| 81 | MG | s6 | 301 | 1/1 | 0.95 | 0.09 | 121,121,121,121 | 0 |
| 81 | MG | 1 | 3754 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 2007 | 1/1 | 0.95 | 0.48 | 90,90,90,90 | 0 |
| 81 | MG | 1 | 3598 | 1/1 | 0.95 | 0.29 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 3575 | 1/1 | 0.95 | 0.24 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3765 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 1 |
| 81 | MG | O4 | 204 | 1/1 | 0.95 | 0.24 | 63,63,63,63 | 0 |
| 81 | MG | M7 | 203 | 1/1 | 0.95 | 0.28 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3479 | 1/1 | 0.95 | 0.35 | 37,37,37,37 | 0 |
| 81 | MG | 4 | 237 | 1/1 | 0.95 | 0.39 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3872 | 1/1 | 0.95 | 0.27 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3732 | 1/1 | 0.95 | 0.37 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 4132 | 1/1 | 0.95 | 0.25 | 37,37,37,37 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3709 | 1/1 | 0.95 | 0.24 | 32,32,32,32 | 0 |
| 81 | MG | S7 | 201 | 1/1 | 0.95 | 0.13 | 89,89,89,89 | 0 |
| 81 | MG | 6 | 2022 | 1/1 | 0.95 | 0.41 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3551 | 1/1 | 0.95 | 0.43 | 54,54,54,54 | 1 |
| 81 | MG | 1 | 3737 | 1/1 | 0.95 | 0.33 | 61,61,61,61 | 0 |
| 81 | MG | 5 | 3582 | 1/1 | 0.95 | 0.31 | 54,54,54,54 | 0 |
| 81 | MG | 4 | 222 | 1/1 | 0.95 | 0.18 | 49,49,49,49 | 0 |
| 81 | MG | 2 | 1985 | 1/1 | 0.95 | 0.36 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3443 | 1/1 | 0.95 | 0.24 | 42,42,42,42 | 0 |
| 81 | MG | 6 | 1990 | 1/1 | 0.95 | 0.27 | 69,69,69,69 | 0 |
| 81 | MG | 5 | 3545 | 1/1 | 0.95 | 0.24 | 55,55,55,55 | 0 |
| 81 | MG | 6 | 1967 | 1/1 | 0.95 | 0.31 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3735 | 1/1 | 0.95 | 0.27 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4021 | 1/1 | 0.95 | 0.38 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3734 | 1/1 | 0.95 | 0.35 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3608 | 1/1 | 0.95 | 0.25 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3879 | 1/1 | 0.95 | 0.33 | 61,61,61,61 | 0 |
| 81 | MG | 7 | 210 | 1/1 | 0.95 | 0.24 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3831 | 1/1 | 0.95 | 0.32 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3571 | 1/1 | 0.95 | 0.27 | 40,40,40,40 | 0 |
| 81 | MG | 1 | 3671 | 1/1 | 0.95 | 0.43 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3761 | 1/1 | 0.95 | 0.33 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3664 | 1/1 | 0.95 | 0.37 | 50,50,50,50 | 0 |
| 81 | MG | 2 | 1944 | 1/1 | 0.95 | 0.23 | 84,84,84,84 | 0 |
| 81 | MG | 5 | 3641 | 1/1 | 0.95 | 0.18 | 45,45,45,45 | 0 |
| 81 | MG | 6 | 2047 | 1/1 | 0.95 | 0.19 | 109,109,109,109 | 0 |
| 81 | MG | 1 | 3506 | 1/1 | 0.95 | 0.12 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 3589 | 1/1 | 0.95 | 0.22 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3823 | 1/1 | 0.95 | 0.25 | 42,42,42,42 | 0 |
| 81 | MG | 3 | 204 | 1/1 | 0.95 | 0.16 | 84,84,84,84 | 0 |
| 81 | MG | 1 | 4185 | 1/1 | 0.95 | 0.09 | 56,56,56,56 | 0 |
| 81 | MG | 2 | 2008 | 1/1 | 0.95 | 0.30 | 76,76,76,76 | 0 |
| 81 | MG | 6 | 1964 | 1/1 | 0.95 | 0.18 | 108,108,108,108 | 0 |
| 81 | MG | 1 | 3531 | 1/1 | 0.95 | 0.31 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 4001 | 1/1 | 0.95 | 0.24 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3663 | 1/1 | 0.95 | 0.24 | 57,57,57,57 | 0 |
| 81 | MG | o0 | 202 | 1/1 | 0.95 | 0.46 | 88,88,88,88 | 0 |
| 81 | MG | 5 | 3817 | 1/1 | 0.95 | 0.32 | 57,57,57,57 | 0 |
| 81 | MG | Q2 | 503 | 1/1 | 0.95 | 0.28 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3634 | 1/1 | 0.95 | 0.14 | 55,55,55,55 | 0 |
| 81 | MG | m7 | 203 | 1/1 | 0.95 | 0.20 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3802 | 1/1 | 0.95 | 0.23 | 48,48,48,48 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3645 | 1/1 | 0.95 | 0.20 | 44,44,44,44 | 0 |
| 81 | MG | 2 | 2096 | 1/1 | 0.95 | 0.18 | 76,76,76,76 | 0 |
| 81 | MG | 2 | 1920 | 1/1 | 0.95 | 0.35 | 68,68,68,68 | 0 |
| 81 | MG | 1 | 3992 | 1/1 | 0.95 | 0.24 | 47,47,47,47 | 1 |
| 81 | MG | 5 | 3718 | 1/1 | 0.95 | 0.29 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3478 | 1/1 | 0.95 | 0.31 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 3824 | 1/1 | 0.95 | 0.32 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 4082 | 1/1 | 0.95 | 0.24 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3564 | 1/1 | 0.95 | 0.16 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 3705 | 1/1 | 0.95 | 0.38 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3843 | 1/1 | 0.95 | 0.14 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3609 | 1/1 | 0.95 | 0.15 | 56,56,56,56 | 0 |
| 81 | MG | 4 | 225 | 1/1 | 0.95 | 0.10 | 62,62,62,62 | 1 |
| 81 | MG | m6 | 202 | 1/1 | 0.95 | 0.22 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3842 | 1/1 | 0.95 | 0.22 | 43,43,43,43 | 1 |
| 81 | MG | 1 | 3763 | 1/1 | 0.95 | 0.10 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3516 | 1/1 | 0.95 | 0.18 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4016 | 1/1 | 0.95 | 0.47 | 57,57,57,57 | 0 |
| 81 | MG | q2 | 502 | 1/1 | 0.95 | 0.23 | 70,70,70,70 | 0 |
| 81 | MG | 6 | 1932 | 1/1 | 0.95 | 0.41 | 87,87,87,87 | 0 |
| 81 | MG | 2 | 1927 | 1/1 | 0.95 | 0.14 | 75,75,75,75 | 0 |
| 82 | ZN | o4 | 201 | 1/1 | 0.96 | 0.10 | 102,102,102,102 | 0 |
| 81 | MG | 1 | 3561 | 1/1 | 0.96 | 0.18 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3870 | 1/1 | 0.96 | 0.19 | 63,63,63,63 | 0 |
| 81 | MG | 4 | 235 | 1/1 | 0.96 | 0.37 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3543 | 1/1 | 0.96 | 0.20 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3745 | 1/1 | 0.96 | 0.43 | 33,33,33,33 | 0 |
| 81 | MG | 5 | 3583 | 1/1 | 0.96 | 0.26 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 4075 | 1/1 | 0.96 | 0.16 | 66,66,66,66 | 0 |
| 81 | MG | 1 | 3977 | 1/1 | 0.96 | 0.30 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3682 | 1/1 | 0.96 | 0.32 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3522 | 1/1 | 0.96 | 0.21 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3599 | 1/1 | 0.96 | 0.20 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3664 | 1/1 | 0.96 | 0.26 | 50,50,50,50 | 0 |
| 81 | MG | 3 | 212 | 1/1 | 0.96 | 0.19 | 85,85,85,85 | 0 |
| 81 | MG | 1 | 3685 | 1/1 | 0.96 | 0.31 | 41,41,41,41 | 0 |
| 81 | MG | 1 | 3902 | 1/1 | 0.96 | 0.21 | 61,61,61,61 | 0 |
| 81 | MG | 3 | 205 | 1/1 | 0.96 | 0.17 | 73,73,73,73 | 0 |
| 81 | MG | 1 | 3457 | 1/1 | 0.96 | 0.30 | 36,36,36,36 | 0 |
| 81 | MG | 1 | 3766 | 1/1 | 0.96 | 0.15 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3458 | 1/1 | 0.96 | 0.30 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3997 | 1/1 | 0.96 | 0.55 | 51,51,51,51 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | m5 | 301 | 1/1 | 0.96 | 0.26 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 3999 | 1/1 | 0.96 | 0.31 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3758 | 1/1 | 0.96 | 0.23 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3433 | 1/1 | 0.96 | 0.36 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3859 | 1/1 | 0.96 | 0.16 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3584 | 1/1 | 0.96 | 0.37 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3479 | 1/1 | 0.96 | 0.15 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3699 | 1/1 | 0.96 | 0.61 | 51,51,51,51 | 0 |
| 81 | MG | 6 | 1970 | 1/1 | 0.96 | 0.23 | 86,86,86,86 | 0 |
| 81 | MG | l3 | 401 | 1/1 | 0.96 | 0.22 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3485 | 1/1 | 0.96 | 0.26 | 47,47,47,47 | 0 |
| 81 | MG | l4 | 402 | 1/1 | 0.96 | 0.45 | 57,57,57,57 | 0 |
| 81 | MG | 1 | 3517 | 1/1 | 0.96 | 0.23 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3995 | 1/1 | 0.96 | 0.22 | 47,47,47,47 | 0 |
| 81 | MG | d3 | 203 | 1/1 | 0.96 | 0.15 | 80,80,80,80 | 0 |
| 81 | MG | 5 | 3511 | 1/1 | 0.96 | 0.17 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3438 | 1/1 | 0.96 | 0.25 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3449 | 1/1 | 0.96 | 0.18 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3750 | 1/1 | 0.96 | 0.23 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 4083 | 1/1 | 0.96 | 0.34 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3499 | 1/1 | 0.96 | 0.14 | 56,56,56,56 | 0 |
| 81 | MG | 6 | 2015 | 1/1 | 0.96 | 0.30 | 91,91,91,91 | 0 |
| 81 | MG | 5 | 3686 | 1/1 | 0.96 | 0.21 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3690 | 1/1 | 0.96 | 0.21 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3515 | 1/1 | 0.96 | 0.26 | 44,44,44,44 | 0 |
| 81 | MG | 6 | 2012 | 1/1 | 0.96 | 0.42 | 65,65,65,65 | 0 |
| 82 | ZN | D9 | 101 | 1/1 | 0.96 | 0.12 | 112,112,112,112 | 0 |
| 81 | MG | 1 | 3656 | 1/1 | 0.96 | 0.29 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3931 | 1/1 | 0.96 | 0.16 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3520 | 1/1 | 0.96 | 0.42 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 4149 | 1/1 | 0.96 | 0.22 | 44,44,44,44 | 0 |
| 81 | MG | D3 | 201 | 1/1 | 0.96 | 0.14 | 75,75,75,75 | 0 |
| 81 | MG | 1 | 3580 | 1/1 | 0.96 | 0.20 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 3951 | 1/1 | 0.96 | 0.17 | 60,60,60,60 | 0 |
| 81 | MG | 6 | 1948 | 1/1 | 0.96 | 0.21 | 111,111,111,111 | 0 |
| 81 | MG | 1 | 3679 | 1/1 | 0.96 | 0.25 | 70,70,70,70 | 0 |
| 81 | MG | 6 | 1978 | 1/1 | 0.96 | 0.10 | 111,111,111,111 | 0 |
| 81 | MG | 1 | 3828 | 1/1 | 0.96 | 0.42 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3708 | 1/1 | 0.96 | 0.28 | 39,39,39,39 | 0 |
| 81 | MG | 5 | 3636 | 1/1 | 0.96 | 0.21 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3456 | 1/1 | 0.96 | 0.28 | 36,36,36,36 | 0 |
| 81 | MG | m7 | 207 | 1/1 | 0.96 | 0.26 | 50,50,50,50 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3799 | 1/1 | 0.96 | 0.30 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 3836 | 1/1 | 0.96 | 0.22 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3717 | 1/1 | 0.96 | 0.24 | 55,55,55,55 | 1 |
| 81 | MG | 5 | 3475 | 1/1 | 0.96 | 0.29 | 39,39,39,39 | 0 |
| 81 | MG | O2 | 201 | 1/1 | 0.96 | 0.22 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3832 | 1/1 | 0.96 | 0.27 | 45,45,45,45 | 0 |
| 81 | MG | 2 | 1914 | 1/1 | 0.96 | 0.11 | 92,92,92,92 | 0 |
| 81 | MG | 5 | 3516 | 1/1 | 0.96 | 0.21 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3496 | 1/1 | 0.96 | 0.21 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3486 | 1/1 | 0.96 | 0.55 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3749 | 1/1 | 0.96 | 0.26 | 36,36,36,36 | 0 |
| 81 | MG | M5 | 306 | 1/1 | 0.96 | 0.23 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 4064 | 1/1 | 0.96 | 0.47 | 99,99,99,99 | 0 |
| 81 | MG | 6 | 2027 | 1/1 | 0.96 | 0.08 | 131,131,131,131 | 0 |
| 81 | MG | 5 | 3554 | 1/1 | 0.96 | 0.21 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3528 | 1/1 | 0.96 | 0.33 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3446 | 1/1 | 0.96 | 0.27 | 43,43,43,43 | 0 |
| 81 | MG | M7 | 206 | 1/1 | 0.96 | 0.17 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3651 | 1/1 | 0.96 | 0.31 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 3771 | 1/1 | 0.96 | 0.32 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3762 | 1/1 | 0.96 | 0.41 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3710 | 1/1 | 0.96 | 0.23 | 33,33,33,33 | 0 |
| 81 | MG | 1 | 3529 | 1/1 | 0.96 | 0.44 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3623 | 1/1 | 0.96 | 0.25 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3463 | 1/1 | 0.96 | 0.39 | 39,39,39,39 | 0 |
| 81 | MG | 5 | 3957 | 1/1 | 0.96 | 0.21 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3512 | 1/1 | 0.96 | 0.42 | 61,61,61,61 | 0 |
| 81 | MG | 1 | 3907 | 1/1 | 0.96 | 0.27 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3574 | 1/1 | 0.96 | 0.21 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3798 | 1/1 | 0.96 | 0.18 | 56,56,56,56 | 0 |
| 81 | MG | L2 | 302 | 1/1 | 0.96 | 0.28 | 46,46,46,46 | 0 |
| 81 | MG | 6 | 1935 | 1/1 | 0.96 | 0.32 | 78,78,78,78 | 0 |
| 81 | MG | 1 | 3725 | 1/1 | 0.96 | 0.27 | 40,40,40,40 | 1 |
| 81 | MG | 1 | 3482 | 1/1 | 0.96 | 0.20 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 4060 | 1/1 | 0.96 | 0.22 | 72,72,72,72 | 0 |
| 81 | MG | 1 | 3458 | 1/1 | 0.96 | 0.24 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3442 | 1/1 | 0.96 | 0.21 | 40,40,40,40 | 0 |
| 81 | MG | 1 | 3677 | 1/1 | 0.96 | 0.36 | 48,48,48,48 | 0 |
| 81 | MG | 2 | 2030 | 1/1 | 0.96 | 0.15 | 74,74,74,74 | 0 |
| 81 | MG | 1 | 3694 | 1/1 | 0.96 | 0.15 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 3532 | 1/1 | 0.96 | 0.40 | 46,46,46,46 | 0 |
| 81 | MG | 6 | 1928 | 1/1 | 0.96 | 0.36 | 72,72,72,72 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3491 | 1/1 | 0.96 | 0.28 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3453 | 1/1 | 0.96 | 0.28 | 40,40,40,40 | 0 |
| 81 | MG | 6 | 1982 | 1/1 | 0.96 | 0.19 | 86,86,86,86 | 0 |
| 81 | MG | 5 | 3579 | 1/1 | 0.96 | 0.28 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4129 | 1/1 | 0.96 | 0.28 | 56,56,56,56 | 0 |
| 81 | MG | 6 | 1925 | 1/1 | 0.96 | 0.29 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 3655 | 1/1 | 0.96 | 0.25 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3461 | 1/1 | 0.96 | 0.26 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 3966 | 1/1 | 0.96 | 0.62 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3901 | 1/1 | 0.96 | 0.20 | 32,32,32,32 | 0 |
| 81 | MG | 5 | 3860 | 1/1 | 0.96 | 0.14 | 68,68,68,68 | 0 |
| 81 | MG | O3 | 201 | 1/1 | 0.96 | 0.39 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3524 | 1/1 | 0.96 | 0.12 | 54,54,54,54 | 1 |
| 81 | MG | 1 | 3487 | 1/1 | 0.96 | 0.38 | 37,37,37,37 | 0 |
| 81 | MG | 7 | 209 | 1/1 | 0.96 | 0.11 | 96,96,96,96 | 0 |
| 81 | MG | 5 | 3526 | 1/1 | 0.96 | 0.41 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3801 | 1/1 | 0.96 | 0.21 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3597 | 1/1 | 0.96 | 0.50 | 43,43,43,43 | 0 |
| 81 | MG | 5 | 3695 | 1/1 | 0.96 | 0.31 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3963 | 1/1 | 0.96 | 0.14 | 58,58,58,58 | 0 |
| 81 | MG | 2 | 1995 | 1/1 | 0.96 | 0.14 | 81,81,81,81 | 0 |
| 81 | MG | 1 | 3937 | 1/1 | 0.96 | 0.10 | 59,59,59,59 | 0 |
| 81 | MG | l2 | 302 | 1/1 | 0.96 | 0.23 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3630 | 1/1 | 0.96 | 0.12 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3534 | 1/1 | 0.96 | 0.28 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3450 | 1/1 | 0.96 | 0.36 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3829 | 1/1 | 0.96 | 0.30 | 76,76,76,76 | 0 |
| 81 | MG | 1 | 3601 | 1/1 | 0.96 | 0.31 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 4182 | 1/1 | 0.96 | 0.12 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 3556 | 1/1 | 0.96 | 0.30 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3523 | 1/1 | 0.96 | 0.28 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3749 | 1/1 | 0.96 | 0.26 | 45,45,45,45 | 0 |
| 81 | MG | l2 | 301 | 1/1 | 0.96 | 0.13 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3541 | 1/1 | 0.96 | 0.47 | 29,29,29,29 | 0 |
| 81 | MG | 6 | 1957 | 1/1 | 0.96 | 0.22 | 102,102,102,102 | 0 |
| 81 | MG | 2 | 1933 | 1/1 | 0.97 | 0.21 | 78,78,78,78 | 0 |
| 81 | MG | 2 | 2023 | 1/1 | 0.97 | 0.21 | 81,81,81,81 | 0 |
| 81 | MG | 5 | 3601 | 1/1 | 0.97 | 0.25 | 93,93,93,93 | 0 |
| 81 | MG | 2 | 1998 | 1/1 | 0.97 | 0.24 | 79,79,79,79 | 0 |
| 81 | MG | O0 | 201 | 1/1 | 0.97 | 0.12 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 4110 | 1/1 | 0.97 | 0.33 | 63,63,63,63 | 0 |
| 81 | MG | 5 | 3755 | 1/1 | 0.97 | 0.29 | 59,59,59,59 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3575 | 1/1 | 0.97 | 0.33 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3440 | 1/1 | 0.97 | 0.27 | 47,47,47,47 | 0 |
| 81 | MG | 6 | 1912 | 1/1 | 0.97 | 0.21 | 76,76,76,76 | 0 |
| 81 | MG | 5 | 3538 | 1/1 | 0.97 | 0.38 | 46,46,46,46 | 0 |
| 82 | ZN | q3 | 501 | 1/1 | 0.97 | 0.19 | 96,96,96,96 | 0 |
| 81 | MG | 5 | 3778 | 1/1 | 0.97 | 0.34 | 44,44,44,44 | 0 |
| 81 | MG | 7 | 203 | 1/1 | 0.97 | 0.27 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3485 | 1/1 | 0.97 | 0.26 | 32,32,32,32 | 0 |
| 81 | MG | 5 | 3455 | 1/1 | 0.97 | 0.23 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3777 | 1/1 | 0.97 | 0.20 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3579 | 1/1 | 0.97 | 0.16 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 3476 | 1/1 | 0.97 | 0.23 | 44,44,44,44 | 0 |
| 81 | MG | 2 | 1949 | 1/1 | 0.97 | 0.15 | 102,102,102,102 | 0 |
| 81 | MG | 1 | 3753 | 1/1 | 0.97 | 0.23 | 47,47,47,47 | 0 |
| 81 | MG | l3 | 409 | 1/1 | 0.97 | 0.21 | 55,55,55,55 | 1 |
| 81 | MG | 2 | 2102 | 1/1 | 0.97 | 0.19 | 78,78,78,78 | 0 |
| 81 | MG | M5 | 302 | 1/1 | 0.97 | 0.25 | 35,35,35,35 | 0 |
| 81 | MG | 5 | 3508 | 1/1 | 0.97 | 0.25 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3922 | 1/1 | 0.97 | 0.25 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3700 | 1/1 | 0.97 | 0.29 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3727 | 1/1 | 0.97 | 0.43 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3819 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3767 | 1/1 | 0.97 | 0.07 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3460 | 1/1 | 0.97 | 0.23 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3783 | 1/1 | 0.97 | 0.14 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3715 | 1/1 | 0.97 | 0.38 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3900 | 1/1 | 0.97 | 0.41 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3694 | 1/1 | 0.97 | 0.40 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 1973 | 1/1 | 0.97 | 0.10 | 113,113,113,113 | 0 |
| 81 | MG | 1 | 3748 | 1/1 | 0.97 | 0.33 | 31,31,31,31 | 0 |
| 81 | MG | 3 | 207 | 1/1 | 0.97 | 0.19 | 83,83,83,83 | 0 |
| 81 | MG | 5 | 3798 | 1/1 | 0.97 | 0.31 | 50,50,50,50 | 1 |
| 81 | MG | 1 | 3455 | 1/1 | 0.97 | 0.32 | 45,45,45,45 | 0 |
| 81 | MG | 5 | 3919 | 1/1 | 0.97 | 0.59 | 58,58,58,58 | 0 |
| 81 | MG | 5 | 3439 | 1/1 | 0.97 | 0.26 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3497 | 1/1 | 0.97 | 0.24 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3439 | 1/1 | 0.97 | 0.29 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 3454 | 1/1 | 0.97 | 0.21 | 40,40,40,40 | 0 |
| 81 | MG | M7 | 201 | 1/1 | 0.97 | 0.34 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 4054 | 1/1 | 0.97 | 0.40 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3445 | 1/1 | 0.97 | 0.42 | 28,28,28,28 | 0 |
| 81 | MG | 2 | 2032 | 1/1 | 0.97 | 0.22 | 90,90,90,90 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3606 | 1/1 | 0.97 | 0.16 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3451 | 1/1 | 0.97 | 0.24 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3449 | 1/1 | 0.97 | 0.29 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 3689 | 1/1 | 0.97 | 0.35 | 48,48,48,48 | 1 |
| 81 | MG | 5 | 3474 | 1/1 | 0.97 | 0.29 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3577 | 1/1 | 0.97 | 0.21 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3478 | 1/1 | 0.97 | 0.28 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3489 | 1/1 | 0.97 | 0.30 | 37,37,37,37 | 0 |
| 81 | MG | 1 | 3667 | 1/1 | 0.97 | 0.21 | 52,52,52,52 | 0 |
| 81 | MG | 5 | 3497 | 1/1 | 0.97 | 0.30 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3594 | 1/1 | 0.97 | 0.23 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3552 | 1/1 | 0.97 | 0.15 | 56,56,56,56 | 1 |
| 81 | MG | 6 | 2003 | 1/1 | 0.97 | 0.60 | 71,71,71,71 | 0 |
| 81 | MG | 2 | 1918 | 1/1 | 0.97 | 0.28 | 69,69,69,69 | 0 |
| 81 | MG | 1 | 3738 | 1/1 | 0.97 | 0.22 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3459 | 1/1 | 0.97 | 0.36 | 34,34,34,34 | 0 |
| 81 | MG | 5 | 3637 | 1/1 | 0.97 | 0.39 | 53,53,53,53 | 0 |
| 81 | MG | 5 | 3784 | 1/1 | 0.97 | 0.16 | 50,50,50,50 | 0 |
| 81 | MG | 1 | 3533 | 1/1 | 0.97 | 0.29 | 33,33,33,33 | 0 |
| 81 | MG | 1 | 3726 | 1/1 | 0.97 | 0.18 | 39,39,39,39 | 1 |
| 81 | MG | 5 | 3471 | 1/1 | 0.97 | 0.32 | 47,47,47,47 | 0 |
| 81 | MG | 5 | 3493 | 1/1 | 0.97 | 0.25 | 66,66,66,66 | 0 |
| 81 | MG | 2 | 2045 | 1/1 | 0.97 | 0.26 | 74,74,74,74 | 0 |
| 81 | MG | 5 | 3596 | 1/1 | 0.97 | 0.25 | 71,71,71,71 | 0 |
| 81 | MG | 5 | 3436 | 1/1 | 0.97 | 0.32 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3604 | 1/1 | 0.97 | 0.18 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3704 | 1/1 | 0.97 | 0.24 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3817 | 1/1 | 0.97 | 0.31 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3720 | 1/1 | 0.97 | 0.28 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3472 | 1/1 | 0.97 | 0.32 | 52,52,52,52 | 0 |
| 81 | MG | 6 | 1985 | 1/1 | 0.97 | 0.28 | 85,85,85,85 | 0 |
| 81 | MG | 5 | 3459 | 1/1 | 0.97 | 0.32 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 4066 | 1/1 | 0.97 | 0.26 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3490 | 1/1 | 0.97 | 0.29 | 49,49,49,49 | 0 |
| 81 | MG | 1 | 3443 | 1/1 | 0.97 | 0.26 | 32,32,32,32 | 0 |
| 81 | MG | 1 | 3833 | 1/1 | 0.97 | 0.29 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3716 | 1/1 | 0.97 | 0.19 | 44,44,44,44 | 0 |
| 81 | MG | l9 | 201 | 1/1 | 0.97 | 0.26 | 56,56,56,56 | 0 |
| 81 | MG | 5 | 3632 | 1/1 | 0.97 | 0.27 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3880 | 1/1 | 0.97 | 0.32 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 4050 | 1/1 | 0.97 | 0.18 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3543 | 1/1 | 0.97 | 0.40 | 34,34,34,34 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | l7 | 306 | 1/1 | 0.97 | 0.33 | 65,65,65,65 | 0 |
| 81 | MG | 5 | 4047 | 1/1 | 0.97 | 0.40 | 68,68,68,68 | 0 |
| 81 | MG | 5 | 3608 | 1/1 | 0.97 | 0.34 | 52,52,52,52 | 0 |
| 81 | MG | 1 | 3554 | 1/1 | 0.97 | 0.29 | 34,34,34,34 | 0 |
| 81 | MG | 3 | 208 | 1/1 | 0.97 | 0.32 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3743 | 1/1 | 0.97 | 0.37 | 35,35,35,35 | 0 |
| 81 | MG | 6 | 2010 | 1/1 | 0.97 | 0.09 | 124,124,124,124 | 0 |
| 81 | MG | 1 | 3595 | 1/1 | 0.97 | 0.27 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3475 | 1/1 | 0.97 | 0.30 | 32,32,32,32 | 0 |
| 81 | MG | 4 | 229 | 1/1 | 0.97 | 0.11 | 57,57,57,57 | 0 |
| 81 | MG | 5 | 3926 | 1/1 | 0.97 | 0.12 | 78,78,78,78 | 0 |
| 81 | MG | 5 | 3557 | 1/1 | 0.97 | 0.22 | 67,67,67,67 | 0 |
| 81 | MG | 5 | 3539 | 1/1 | 0.97 | 0.42 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3731 | 1/1 | 0.97 | 0.44 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3829 | 1/1 | 0.97 | 0.29 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3642 | 1/1 | 0.98 | 0.15 | 56,56,56,56 | 0 |
| 81 | MG | 1 | 3585 | 1/1 | 0.98 | 0.15 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3464 | 1/1 | 0.98 | 0.51 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3864 | 1/1 | 0.98 | 0.34 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3574 | 1/1 | 0.98 | 0.28 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 3440 | 1/1 | 0.98 | 0.11 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3448 | 1/1 | 0.98 | 0.23 | 35,35,35,35 | 0 |
| 82 | ZN | Q3 | 501 | 1/1 | 0.98 | 0.17 | 64,64,64,64 | 0 |
| 81 | MG | 5 | 3786 | 1/1 | 0.98 | 0.32 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3813 | 1/1 | 0.98 | 0.23 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3527 | 1/1 | 0.98 | 0.44 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3675 | 1/1 | 0.98 | 0.19 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3462 | 1/1 | 0.98 | 0.36 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3514 | 1/1 | 0.98 | 0.16 | 63,63,63,63 | 1 |
| 81 | MG | 4 | 234 | 1/1 | 0.98 | 0.26 | 46,46,46,46 | 0 |
| 81 | MG | 2 | 1934 | 1/1 | 0.98 | 0.12 | 75,75,75,75 | 0 |
| 81 | MG | 5 | 3618 | 1/1 | 0.98 | 0.16 | 87,87,87,87 | 0 |
| 81 | MG | 5 | 3968 | 1/1 | 0.98 | 0.38 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3751 | 1/1 | 0.98 | 0.26 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3468 | 1/1 | 0.98 | 0.40 | 33,33,33,33 | 0 |
| 81 | MG | 2 | 2107 | 1/1 | 0.98 | 0.12 | 120,120,120,120 | 0 |
| 81 | MG | 5 | 3505 | 1/1 | 0.98 | 0.27 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3447 | 1/1 | 0.98 | 0.25 | 39,39,39,39 | 0 |
| 81 | MG | 5 | 3502 | 1/1 | 0.98 | 0.33 | 52,52,52,52 | 0 |
| 81 | MG | 2 | 1960 | 1/1 | 0.98 | 0.17 | 90,90,90,90 | 0 |
| 81 | MG | 5 | 3654 | 1/1 | 0.98 | 0.33 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3518 | 1/1 | 0.98 | 0.22 | 46,46,46,46 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3460 | 1/1 | 0.98 | 0.41 | 33,33,33,33 | 0 |
| 82 | ZN | q2 | 501 | 1/1 | 0.98 | 0.08 | 113,113,113,113 | 0 |
| 82 | ZN | o7 | 501 | 1/1 | 0.98 | 0.16 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3477 | 1/1 | 0.98 | 0.22 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 3567 | 1/1 | 0.98 | 0.29 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3761 | 1/1 | 0.98 | 0.24 | 51,51,51,51 | 0 |
| 81 | MG | 5 | 3452 | 1/1 | 0.98 | 0.27 | 47,47,47,47 | 0 |
| 81 | MG | 1 | 3484 | 1/1 | 0.98 | 0.30 | 35,35,35,35 | 0 |
| 81 | MG | 5 | 3977 | 1/1 | 0.98 | 0.18 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3495 | 1/1 | 0.98 | 0.27 | 41,41,41,41 | 0 |
| 81 | MG | 2 | 1994 | 1/1 | 0.98 | 0.19 | 79,79,79,79 | 0 |
| 81 | MG | 5 | 3507 | 1/1 | 0.98 | 0.25 | 64,64,64,64 | 0 |
| 81 | MG | 1 | 3627 | 1/1 | 0.98 | 0.19 | 34,34,34,34 | 0 |
| 81 | MG | 1 | 3717 | 1/1 | 0.98 | 0.25 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 3759 | 1/1 | 0.98 | 0.30 | 38,38,38,38 | 0 |
| 81 | MG | 1 | 3718 | 1/1 | 0.98 | 0.28 | 34,34,34,34 | 0 |
| 81 | MG | 1 | 3815 | 1/1 | 0.98 | 0.25 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3710 | 1/1 | 0.98 | 0.28 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3461 | 1/1 | 0.98 | 0.38 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3471 | 1/1 | 0.98 | 0.46 | 37,37,37,37 | 0 |
| 81 | MG | 5 | 3465 | 1/1 | 0.98 | 0.31 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3687 | 1/1 | 0.98 | 0.25 | 45,45,45,45 | 0 |
| 81 | MG | 1 | 3816 | 1/1 | 0.98 | 0.33 | 43,43,43,43 | 0 |
| 81 | MG | 1 | 3483 | 1/1 | 0.98 | 0.17 | 41,41,41,41 | 0 |
| 81 | MG | 5 | 3766 | 1/1 | 0.98 | 0.33 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3850 | 1/1 | 0.98 | 0.19 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3822 | 1/1 | 0.98 | 0.21 | 50,50,50,50 | 0 |
| 81 | MG | 2 | 2013 | 1/1 | 0.98 | 0.11 | 86,86,86,86 | 0 |
| 81 | MG | 5 | 3599 | 1/1 | 0.98 | 0.21 | 84,84,84,84 | 0 |
| 81 | MG | 1 | 3657 | 1/1 | 0.98 | 0.18 | 49,49,49,49 | 0 |
| 81 | MG | m7 | 204 | 1/1 | 0.98 | 0.41 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3647 | 1/1 | 0.98 | 0.21 | 39,39,39,39 | 0 |
| 81 | MG | 5 | 3719 | 1/1 | 0.98 | 0.43 | 63,63,63,63 | 0 |
| 81 | MG | 1 | 3442 | 1/1 | 0.98 | 0.30 | 35,35,35,35 | 0 |
| 81 | MG | 1 | 4141 | 1/1 | 0.98 | 0.15 | 51,51,51,51 | 0 |
| 81 | MG | 4 | 210 | 1/1 | 0.98 | 0.17 | 47,47,47,47 | 0 |
| 81 | MG | N3 | 203 | 1/1 | 0.98 | 0.33 | 45,45,45,45 | 0 |
| 81 | MG | 2 | 1989 | 1/1 | 0.98 | 0.18 | 88,88,88,88 | 0 |
| 81 | MG | 5 | 3759 | 1/1 | 0.98 | 0.28 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3648 | 1/1 | 0.98 | 0.42 | 40,40,40,40 | 0 |
| 81 | MG | 5 | 3503 | 1/1 | 0.98 | 0.53 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3703 | 1/1 | 0.98 | 0.26 | 40,40,40,40 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 5 | 3670 | 1/1 | 0.98 | 0.19 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3711 | 1/1 | 0.98 | 0.34 | 54,54,54,54 | 0 |
| 81 | MG | 5 | 3716 | 1/1 | 0.98 | 0.23 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3950 | 1/1 | 0.98 | 0.17 | 53,53,53,53 | 1 |
| 81 | MG | 2 | 1939 | 1/1 | 0.98 | 0.40 | 84,84,84,84 | 0 |
| 81 | MG | 1 | 3845 | 1/1 | 0.98 | 0.28 | 38,38,38,38 | 0 |
| 81 | MG | 5 | 3862 | 1/1 | 0.98 | 0.10 | 65,65,65,65 | 0 |
| 81 | MG | 1 | 4127 | 1/1 | 0.98 | 0.16 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 4058 | 1/1 | 0.98 | 0.42 | 73,73,73,73 | 0 |
| 81 | MG | L3 | 401 | 1/1 | 0.98 | 0.26 | 46,46,46,46 | 0 |
| 81 | MG | 5 | 3739 | 1/1 | 0.98 | 0.18 | 50,50,50,50 | 0 |
| 82 | ZN | D6 | 101 | 1/1 | 0.98 | 0.17 | 84,84,84,84 | 0 |
| 81 | MG | 1 | 3464 | 1/1 | 0.98 | 0.39 | 34,34,34,34 | 0 |
| 81 | MG | 1 | 3636 | 1/1 | 0.98 | 0.43 | 48,48,48,48 | 0 |
| 81 | MG | 5 | 3448 | 1/1 | 0.98 | 0.23 | 49,49,49,49 | 0 |
| 81 | MG | 5 | 3429 | 1/1 | 0.98 | 0.29 | 42,42,42,42 | 0 |
| 81 | MG | 1 | 3446 | 1/1 | 0.98 | 0.21 | 35,35,35,35 | 0 |
| 81 | MG | 2 | 1930 | 1/1 | 0.98 | 0.35 | 70,70,70,70 | 0 |
| 81 | MG | 1 | 3742 | 1/1 | 0.98 | 0.38 | 32,32,32,32 | 0 |
| 81 | MG | 1 | 3472 | 1/1 | 0.98 | 0.28 | 39,39,39,39 | 0 |
| 81 | MG | 1 | 3846 | 1/1 | 0.98 | 0.22 | 42,42,42,42 | 0 |
| 81 | MG | 5 | 3445 | 1/1 | 0.98 | 0.28 | 48,48,48,48 | 0 |
| 81 | MG | 1 | 3444 | 1/1 | 0.98 | 0.30 | 32,32,32,32 | 0 |
| 81 | MG | 1 | 3844 | 1/1 | 0.98 | 0.20 | 44,44,44,44 | 1 |
| 81 | MG | 5 | 3590 | 1/1 | 0.98 | 0.33 | 62,62,62,62 | 0 |
| 81 | MG | 5 | 3457 | 1/1 | 0.99 | 0.26 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3498 | 1/1 | 0.99 | 0.10 | 53,53,53,53 | 0 |
| 81 | MG | 1 | 3512 | 1/1 | 0.99 | 0.15 | 59,59,59,59 | 0 |
| 81 | MG | 1 | 3800 | 1/1 | 0.99 | 0.32 | 35,35,35,35 | 0 |
| 82 | ZN | d9 | 101 | 1/1 | 0.99 | 0.11 | 123,123,123,123 | 0 |
| 81 | MG | 1 | 3474 | 1/1 | 0.99 | 0.27 | 43,43,43,43 | 0 |
| 81 | MG | m7 | 201 | 1/1 | 0.99 | 0.32 | 44,44,44,44 | 0 |
| 81 | MG | 5 | 3495 | 1/1 | 0.99 | 0.29 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3764 | 1/1 | 0.99 | 0.18 | 55,55,55,55 | 0 |
| 81 | MG | 5 | 3576 | 1/1 | 0.99 | 0.14 | 56,56,56,56 | 0 |
| 82 | ZN | O7 | 101 | 1/1 | 0.99 | 0.19 | 50,50,50,50 | 0 |
| 81 | MG | 5 | 3441 | 1/1 | 0.99 | 0.21 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3469 | 1/1 | 0.99 | 0.25 | 30,30,30,30 | 0 |
| 81 | MG | 1 | 3528 | 1/1 | 0.99 | 0.38 | 33,33,33,33 | 0 |
| 82 | ZN | q0 | 201 | 1/1 | 0.99 | 0.16 | 58,58,58,58 | 0 |
| 81 | MG | 1 | 3565 | 1/1 | 0.99 | 0.21 | 46,46,46,46 | 0 |
| 81 | MG | 1 | 3619 | 1/1 | 0.99 | 0.30 | 58,58,58,58 | 0 |

*Continued on next page...*

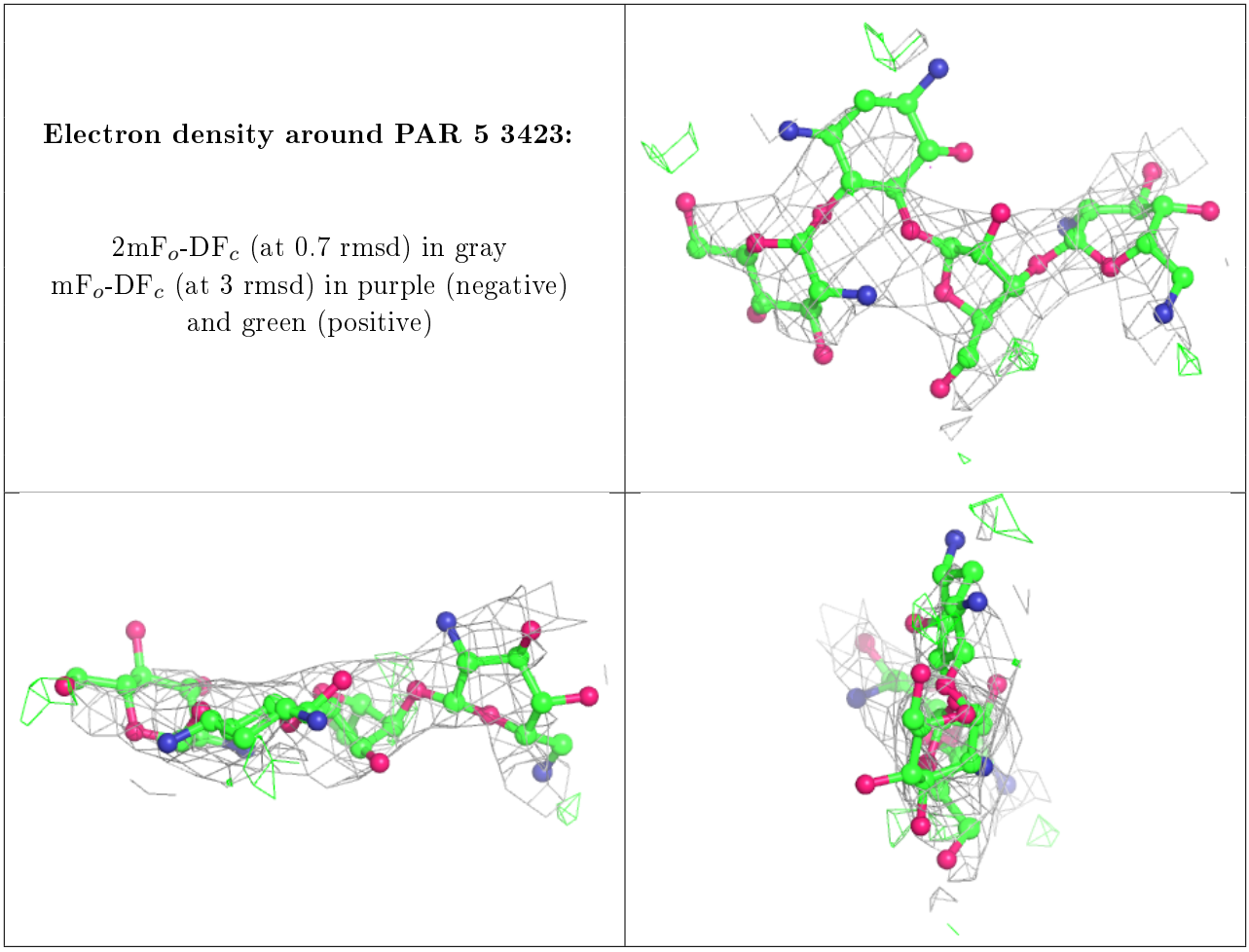
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 81 | MG | 1 | 3473 | 1/1 | 0.99 | 0.42 | 38,38,38,38 | 0 |
| 82 | ZN | O4 | 201 | 1/1 | 0.99 | 0.10 | 63,63,63,63 | 0 |
| 81 | MG | 2 | 2090 | 1/1 | 0.99 | 0.07 | 102,102,102,102 | 0 |
| 82 | ZN | d6 | 101 | 1/1 | 0.99 | 0.14 | 91,91,91,91 | 0 |
| 81 | MG | 1 | 3723 | 1/1 | 0.99 | 0.38 | 34,34,34,34 | 0 |
| 81 | MG | 1 | 3706 | 1/1 | 0.99 | 0.27 | 44,44,44,44 | 0 |
| 81 | MG | 1 | 3476 | 1/1 | 0.99 | 0.27 | 34,34,34,34 | 0 |
| 82 | ZN | Q2 | 501 | 1/1 | 0.99 | 0.10 | 90,90,90,90 | 0 |
| 81 | MG | 1 | 3466 | 1/1 | 0.99 | 0.21 | 39,39,39,39 | 0 |
| 81 | MG | 5 | 3733 | 1/1 | 0.99 | 0.33 | 55,55,55,55 | 0 |
| 81 | MG | 1 | 3805 | 1/1 | 0.99 | 0.12 | 51,51,51,51 | 0 |
| 81 | MG | 1 | 3774 | 1/1 | 0.99 | 0.29 | 41,41,41,41 | 0 |
| 81 | MG | 6 | 1909 | 1/1 | 0.99 | 0.22 | 71,71,71,71 | 0 |
| 81 | MG | 1 | 3553 | 1/1 | 0.99 | 0.21 | 37,37,37,37 | 0 |
| 81 | MG | 5 | 3705 | 1/1 | 0.99 | 0.29 | 54,54,54,54 | 0 |
| 81 | MG | 1 | 3557 | 1/1 | 0.99 | 0.26 | 34,34,34,34 | 0 |
| 81 | MG | N8 | 201 | 1/1 | 0.99 | 0.17 | 41,41,41,41 | 0 |
| 81 | MG | 1 | 3692 | 1/1 | 0.99 | 0.35 | 33,33,33,33 | 0 |
| 82 | ZN | Q0 | 500 | 1/1 | 1.00 | 0.15 | 67,67,67,67 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

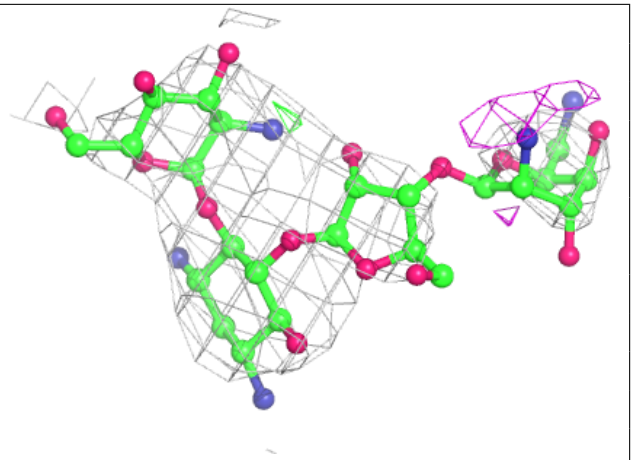
**Electron density around PAR 5 3423:**

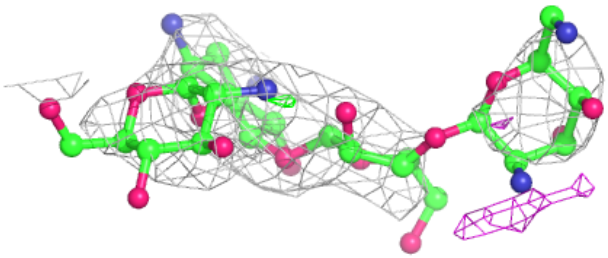
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

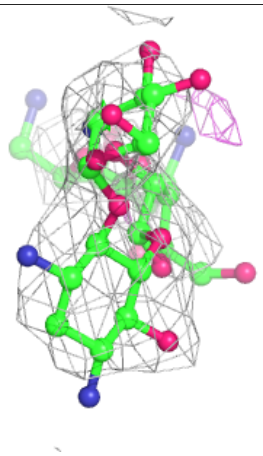


**Electron density around PAR 6 1902:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

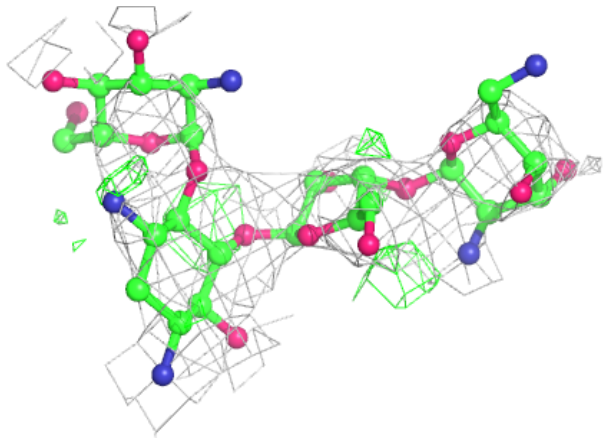


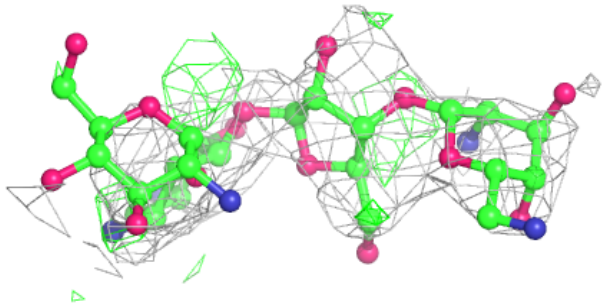


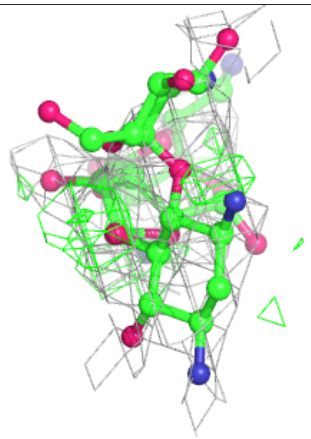


**Electron density around PAR 5 3403:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

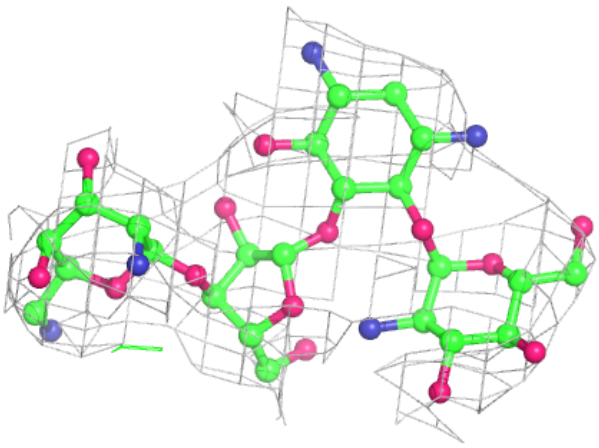


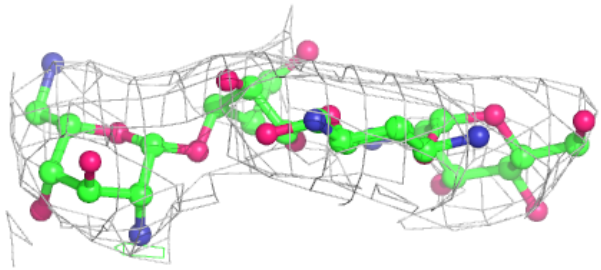


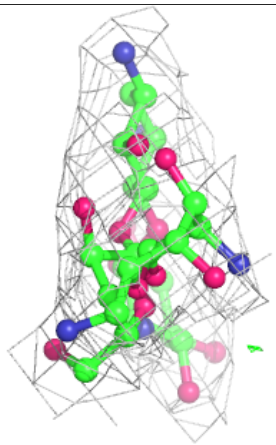


**Electron density around PAR 5 3428:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

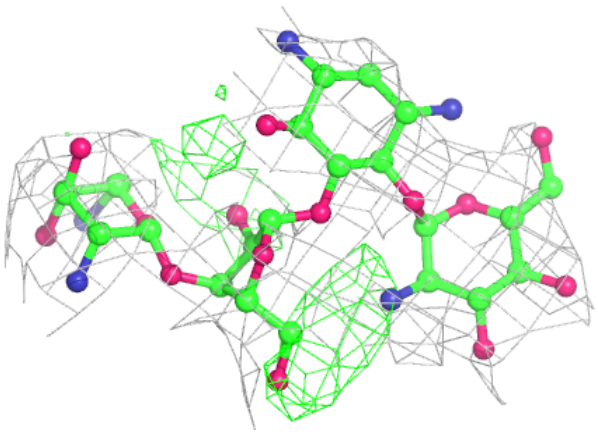


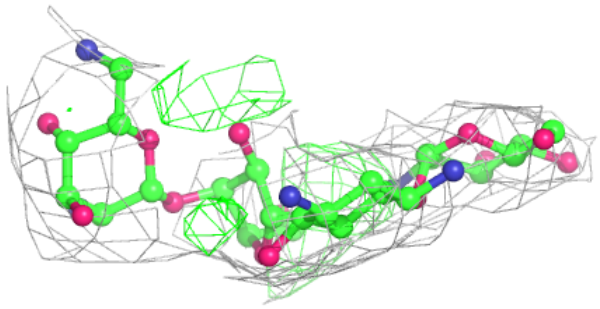


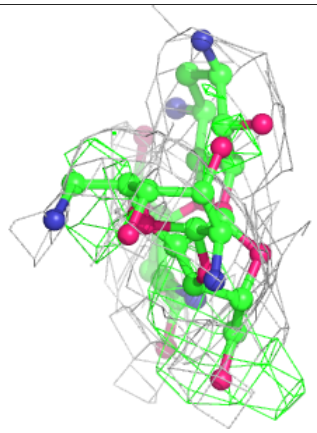


**Electron density around PAR 3 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

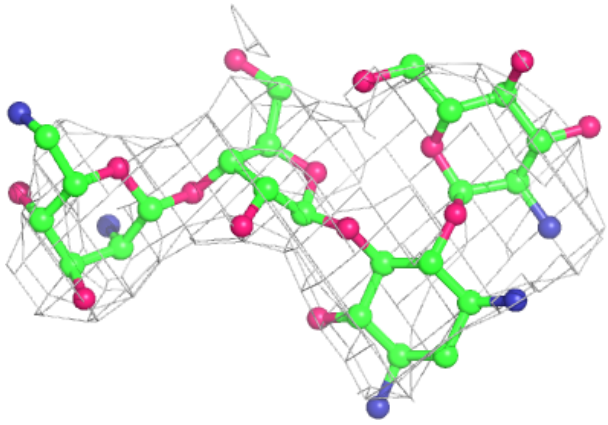


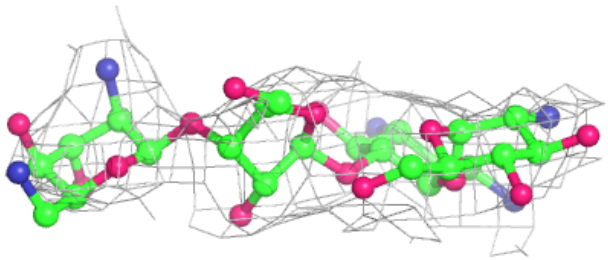


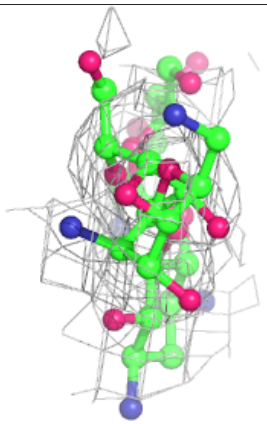


**Electron density around PAR 6 1906:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

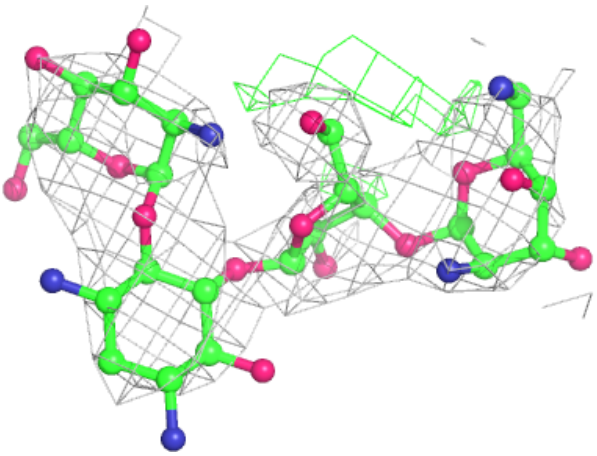


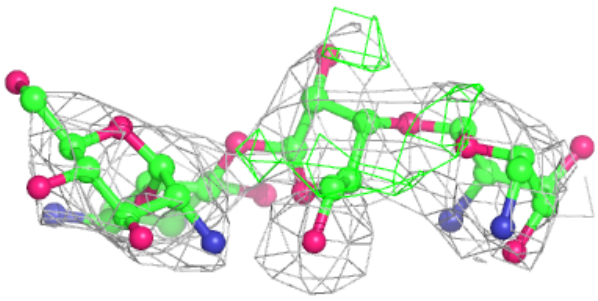


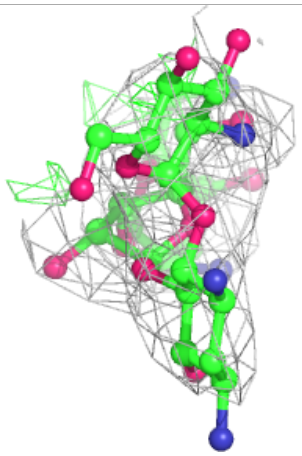


**Electron density around PAR 2 1905:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

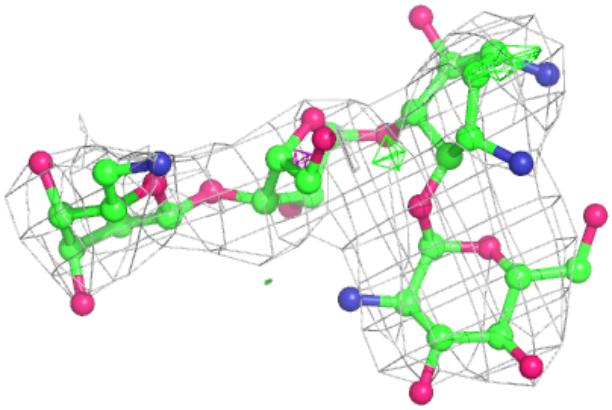


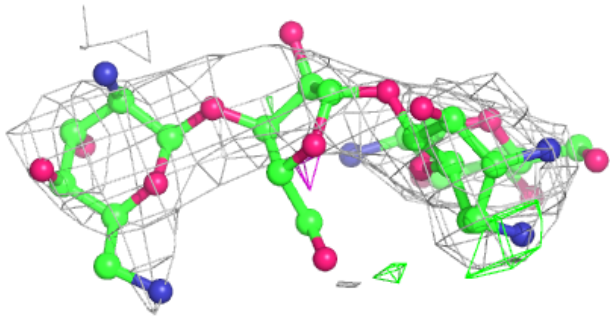


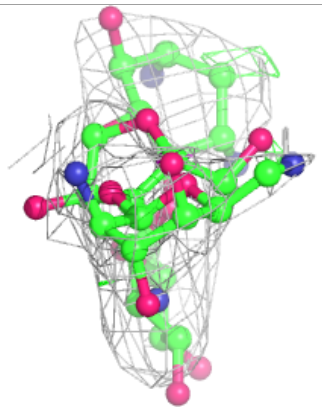


**Electron density around PAR 5 3427:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

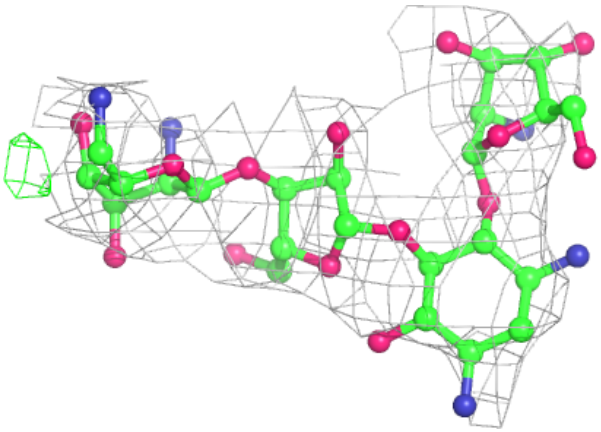


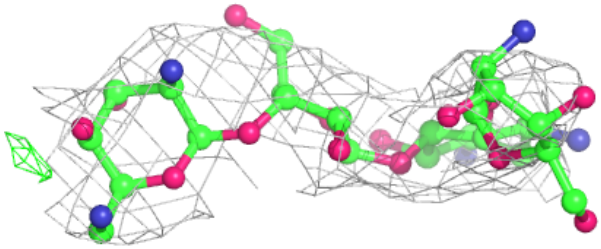


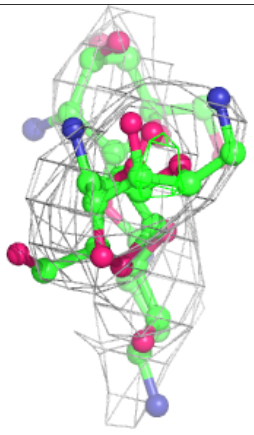


**Electron density around PAR 5 3405:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

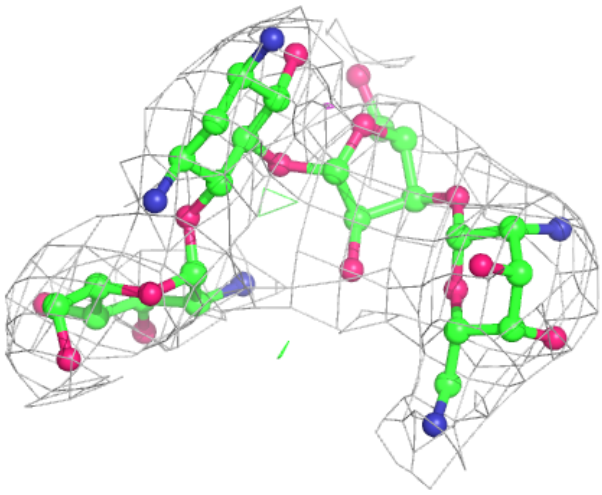


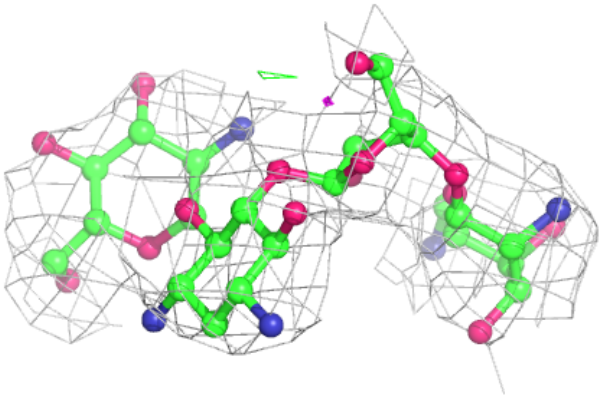


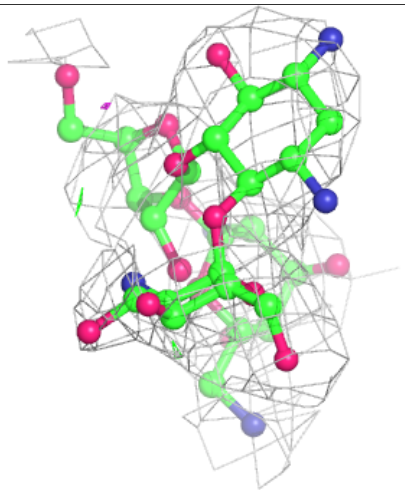


**Electron density around PAR 5 3422:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

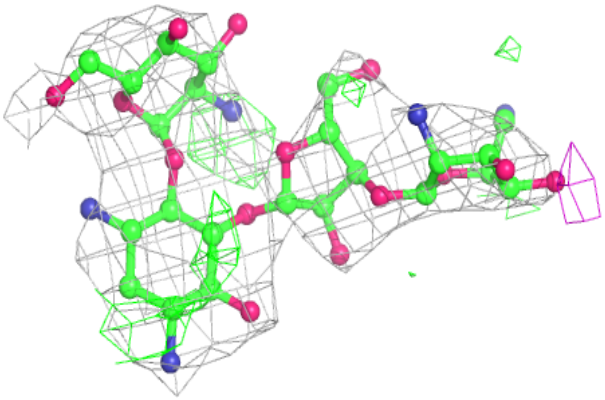


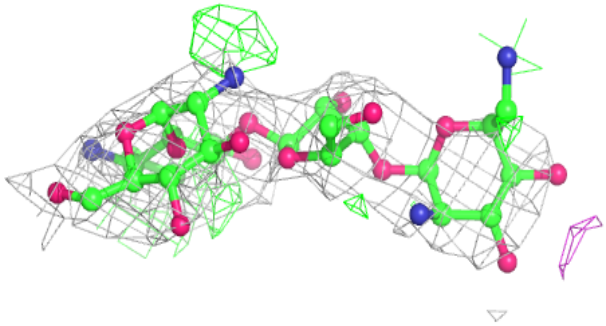


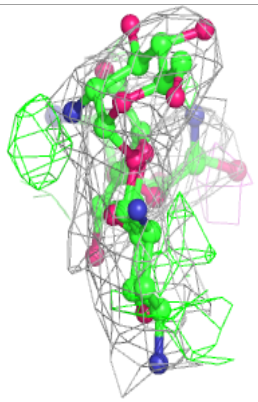


**Electron density around PAR 1 3413:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

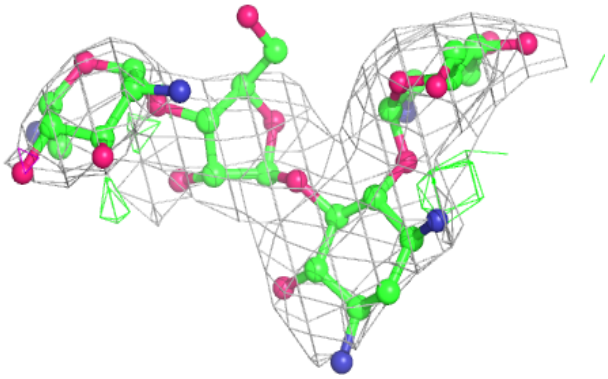


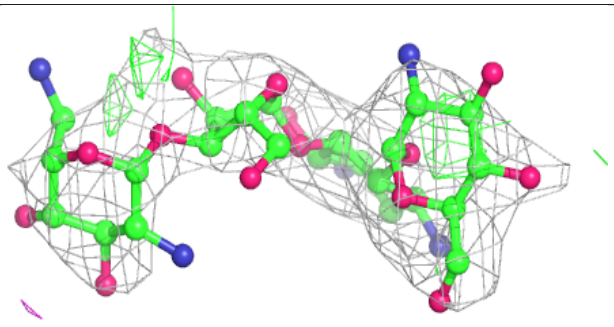


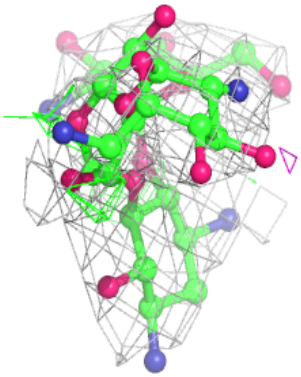


**Electron density around PAR 1 3433:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

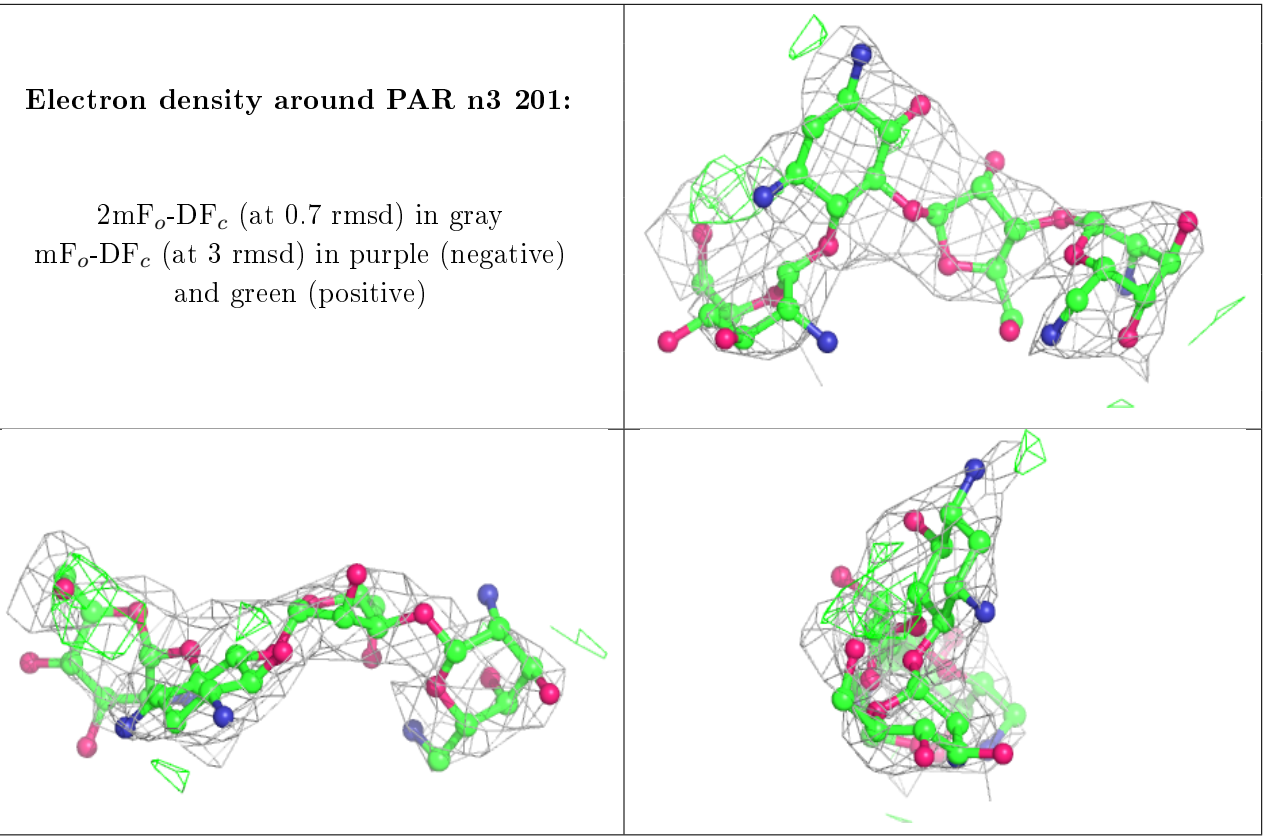






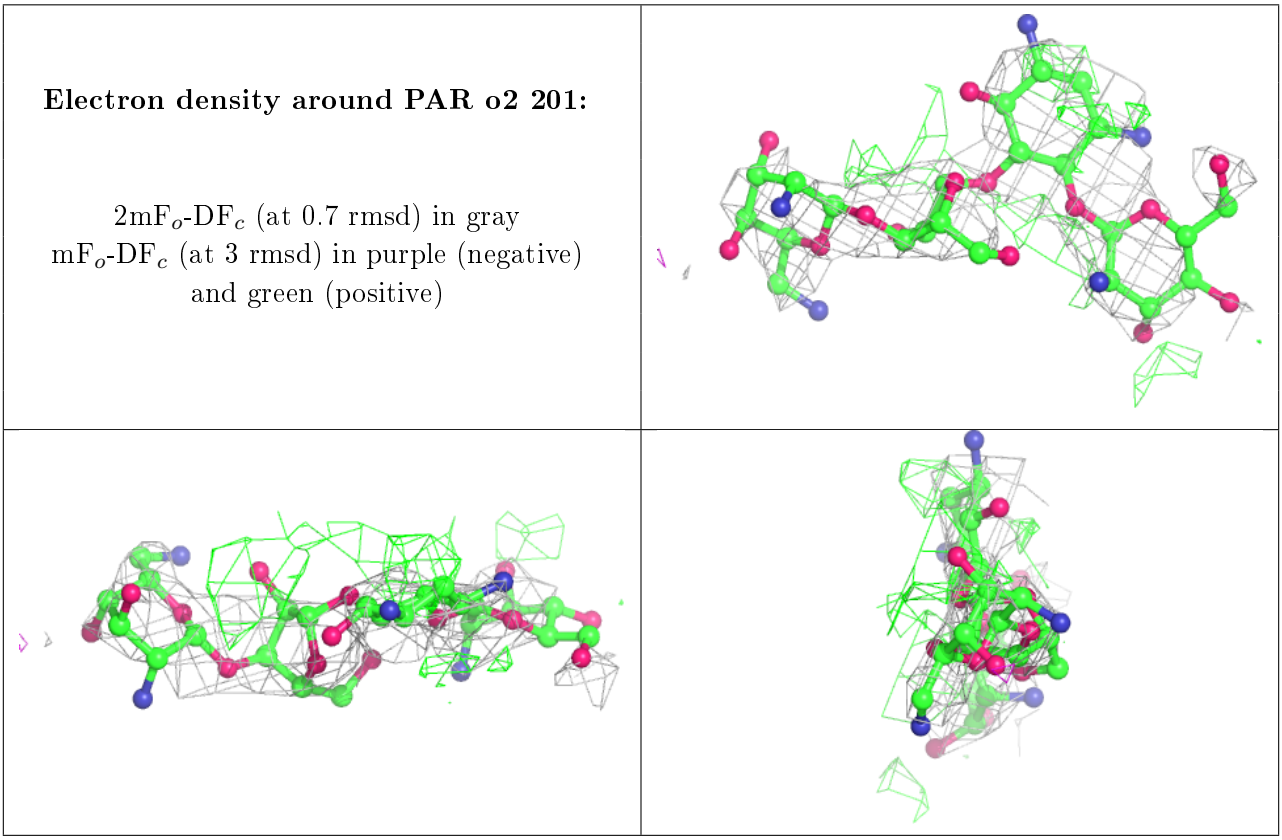
**Electron density around PAR n3 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



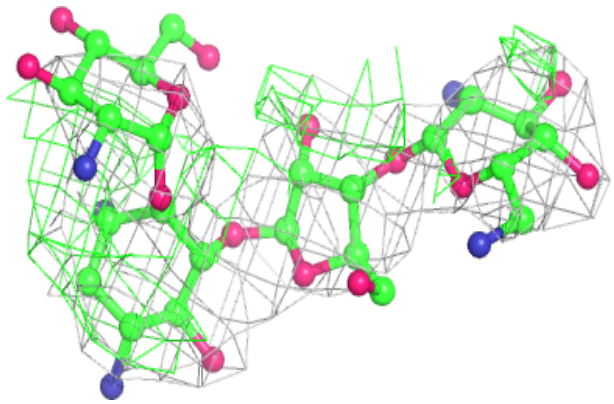
**Electron density around PAR o2 201:**

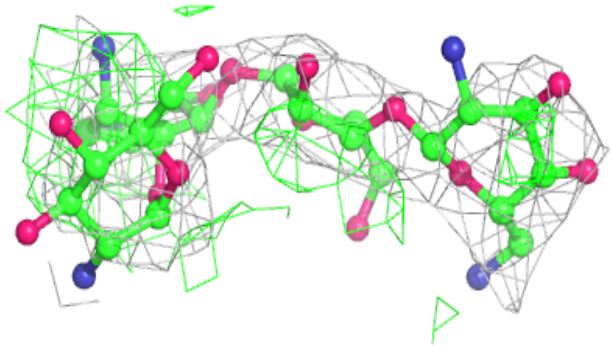
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

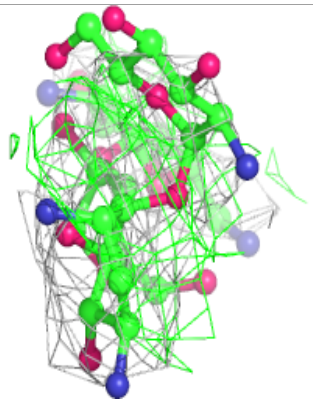


**Electron density around PAR 1 3403:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

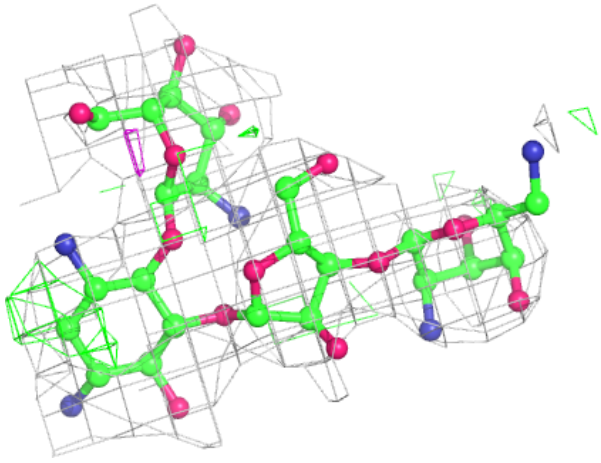


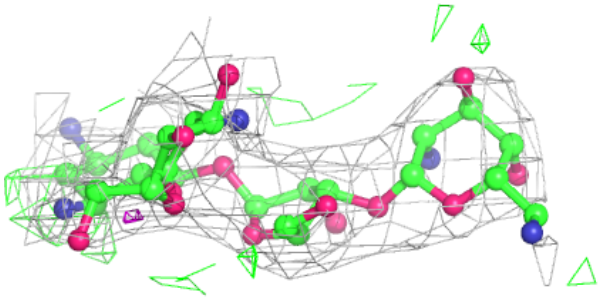


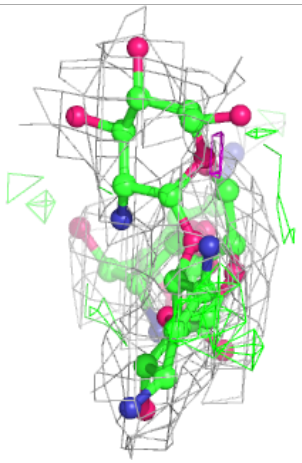


**Electron density around PAR 5 3404:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

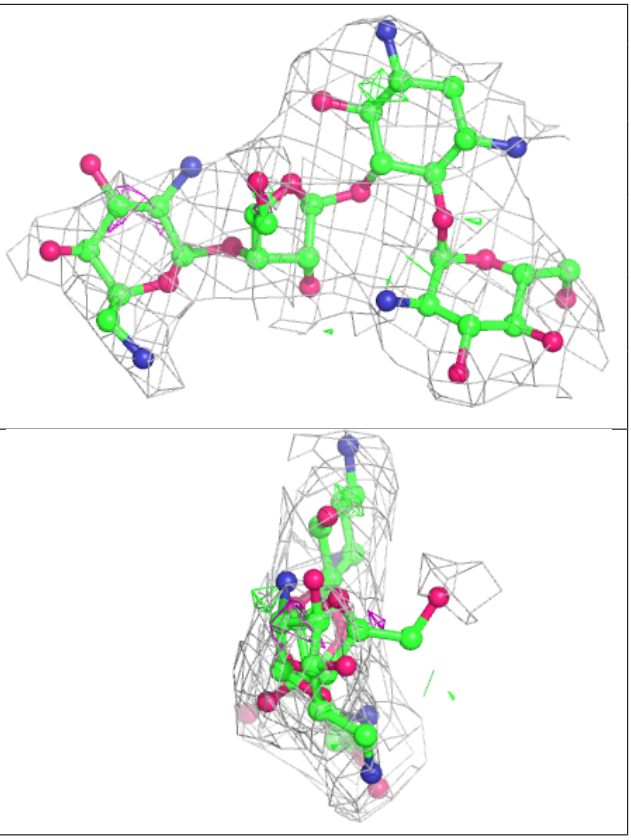






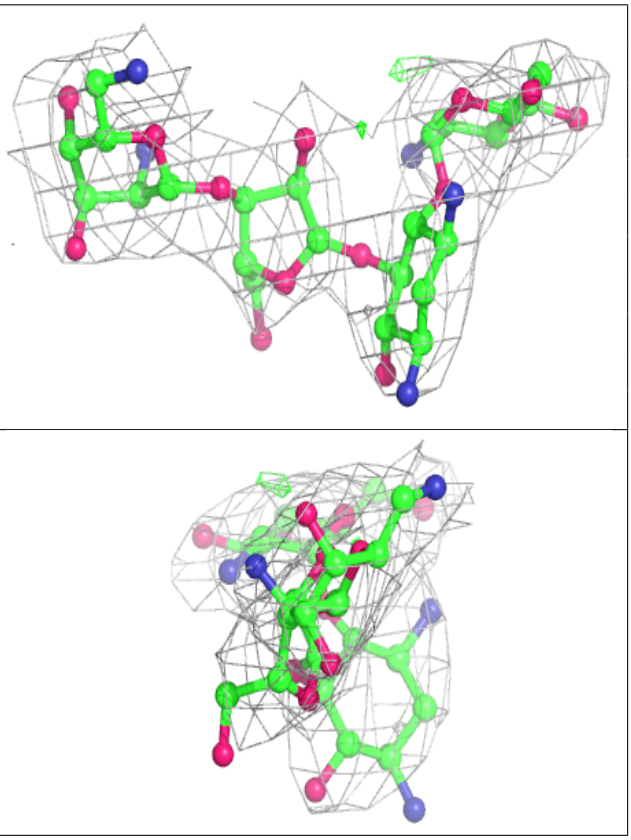
**Electron density around PAR 1 3426:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



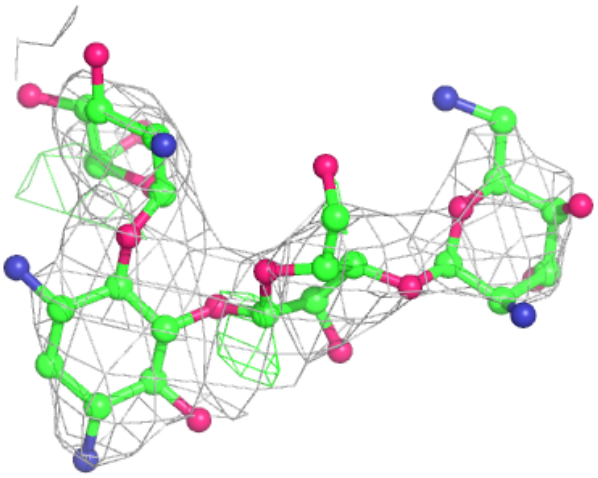
**Electron density around PAR 1 3401:**

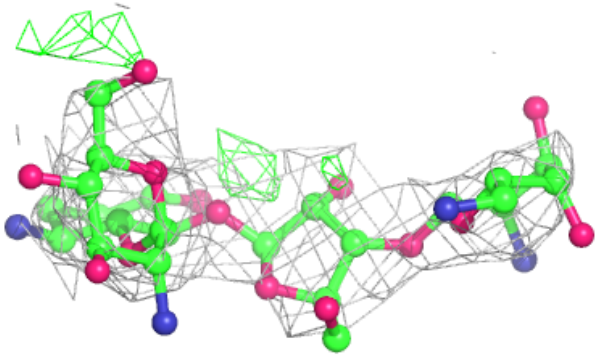
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

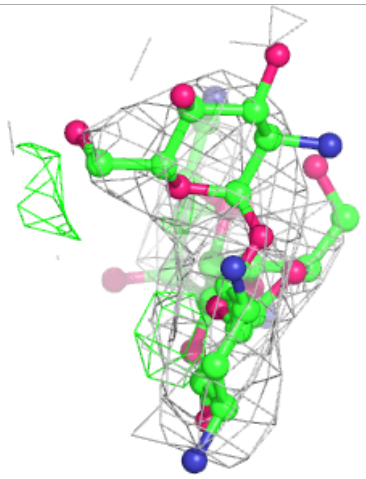


**Electron density around PAR 2 1901:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

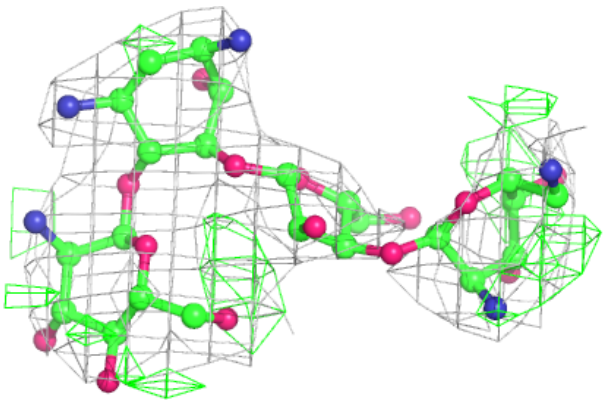


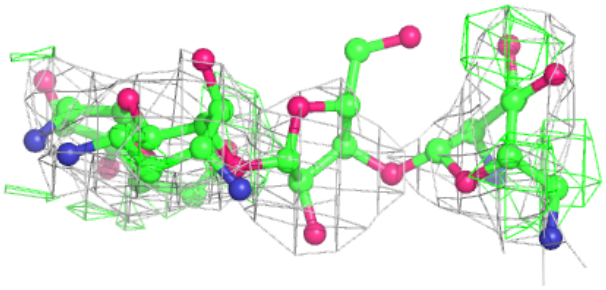


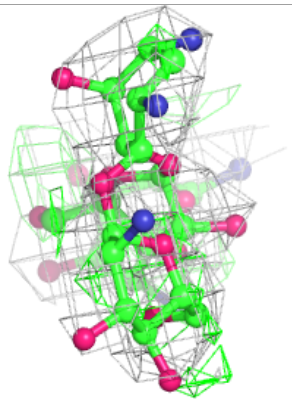


**Electron density around PAR 1 3405:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

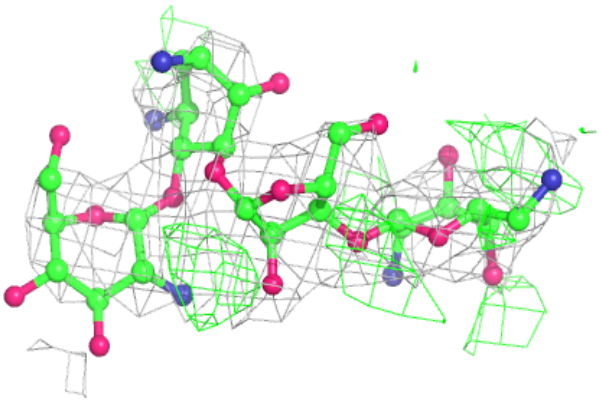


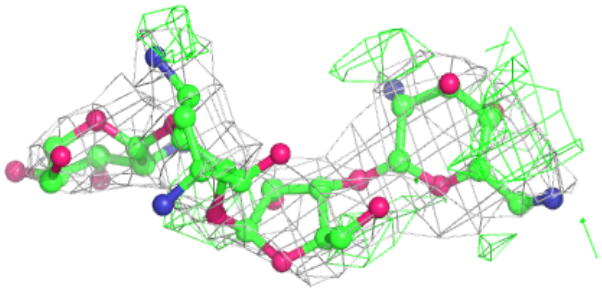


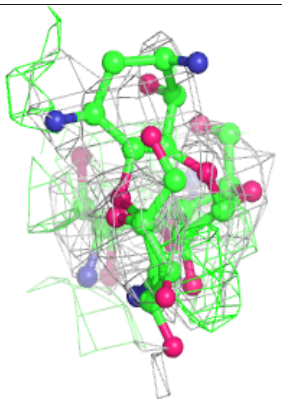


**Electron density around PAR 4 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

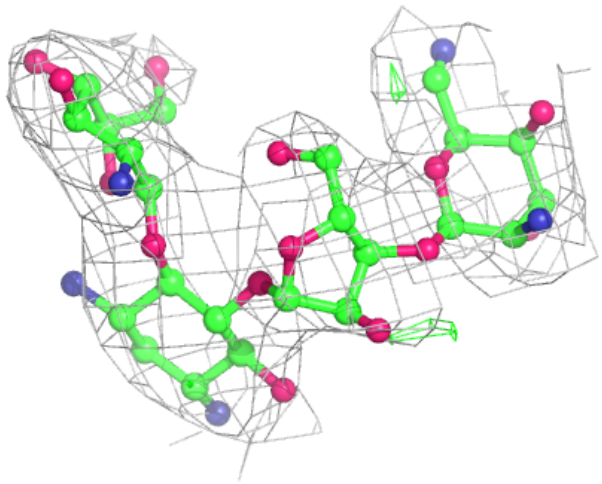


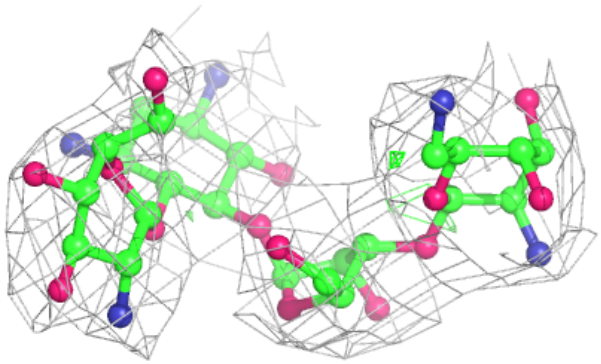


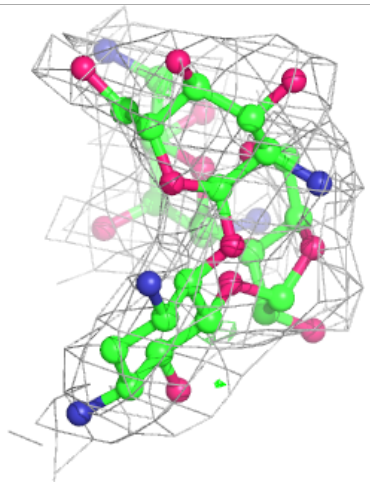


**Electron density around PAR 1 3436:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

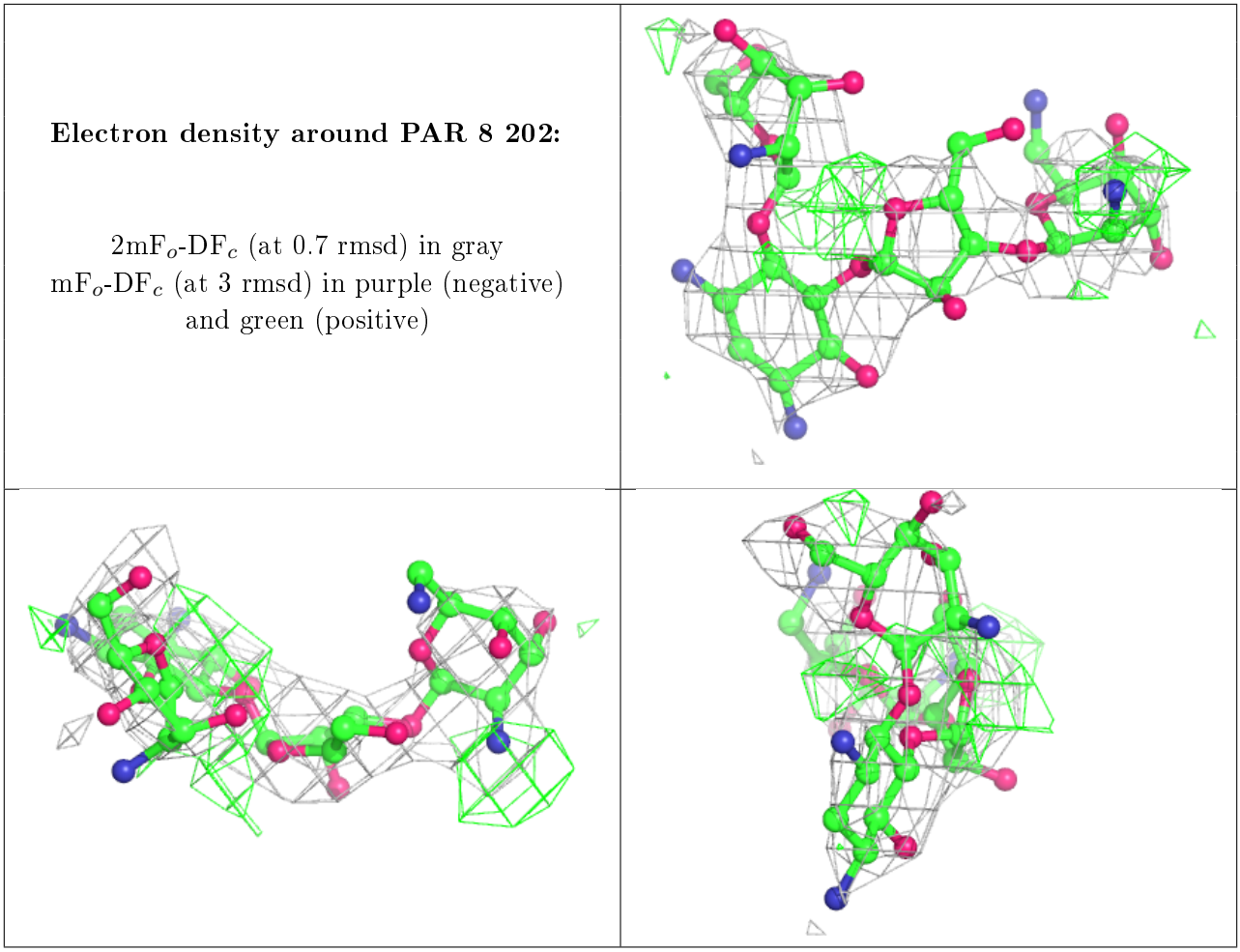






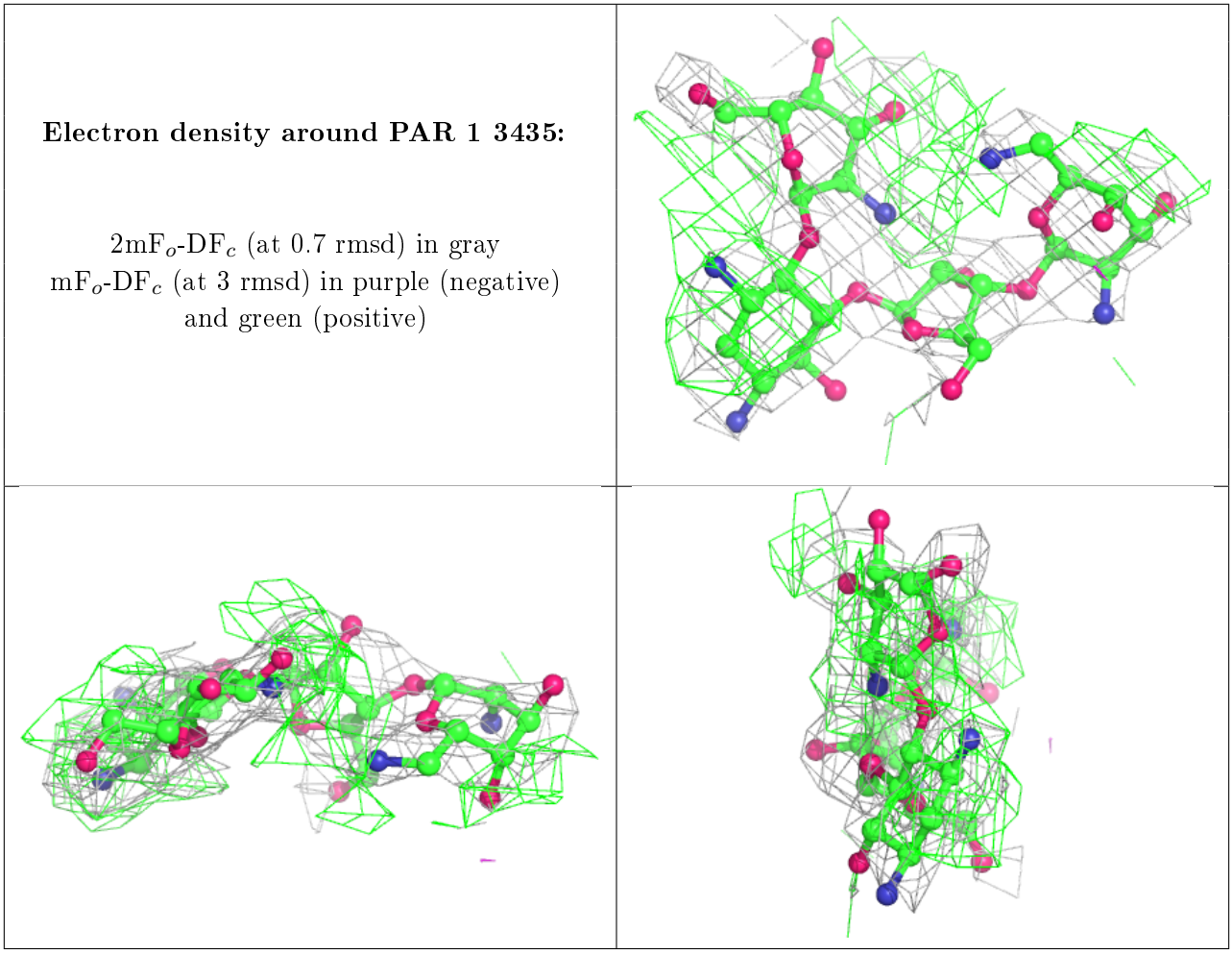
**Electron density around PAR 8 202:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



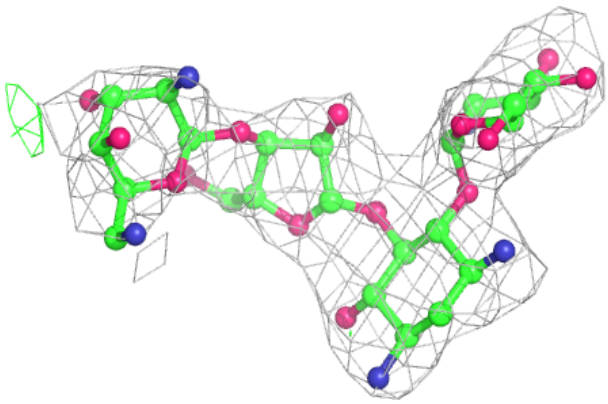
**Electron density around PAR 1 3435:**

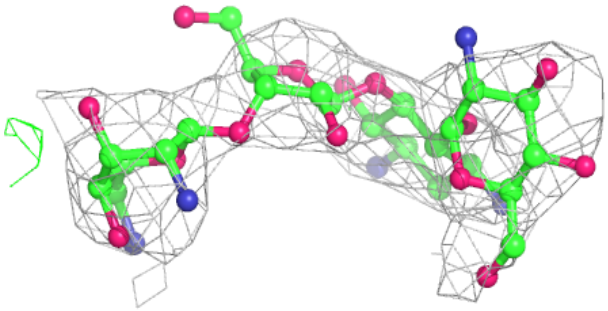
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

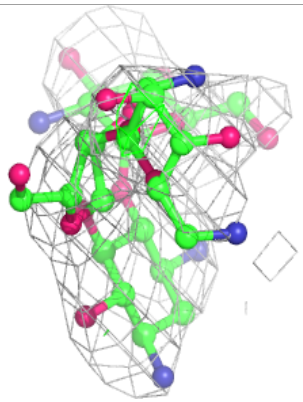


**Electron density around PAR 1 3431:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

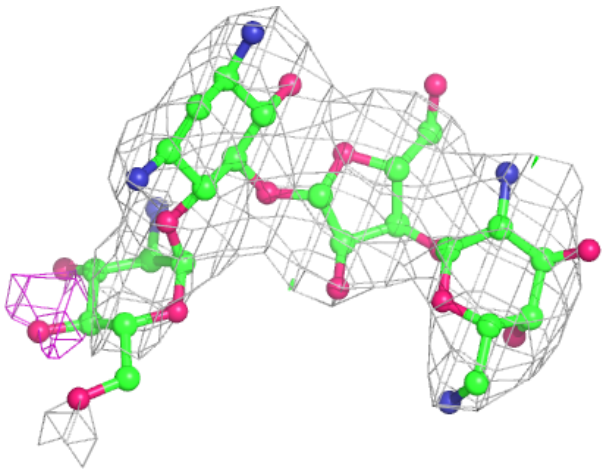


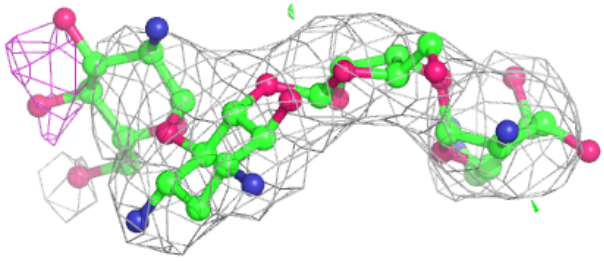


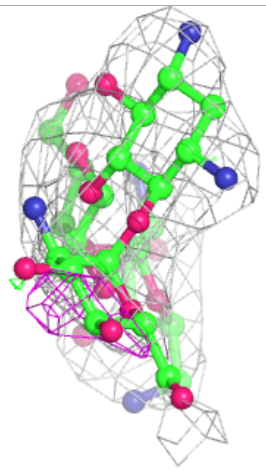


**Electron density around PAR 5 3411:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

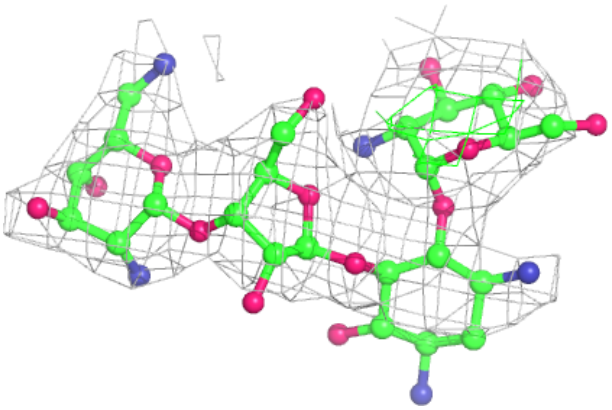


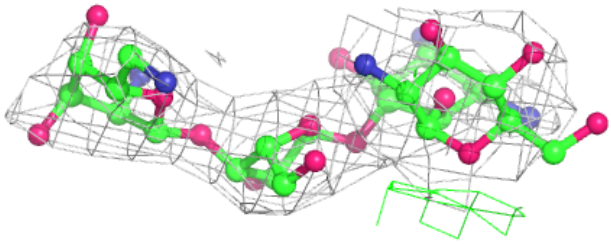


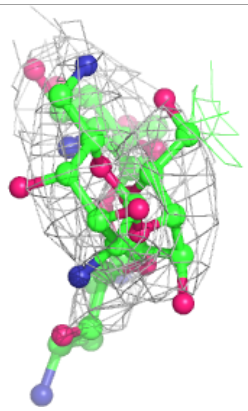


**Electron density around PAR 8 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

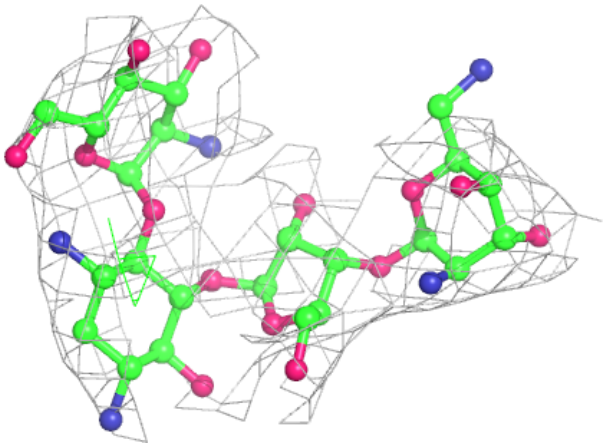


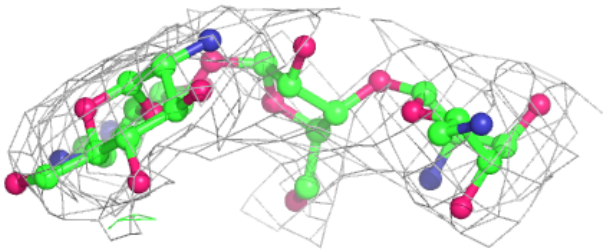


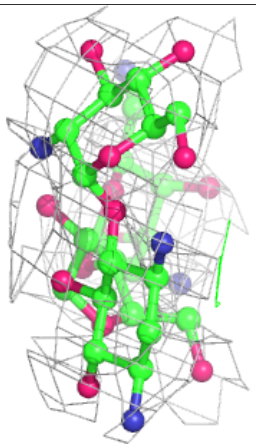


**Electron density around PAR 6 1905:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

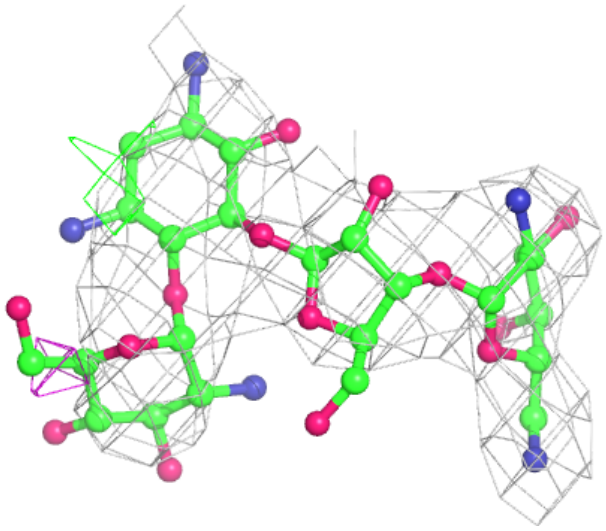


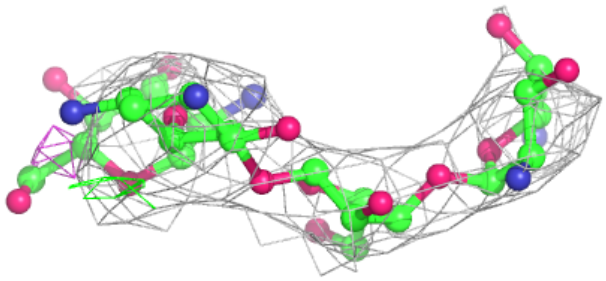


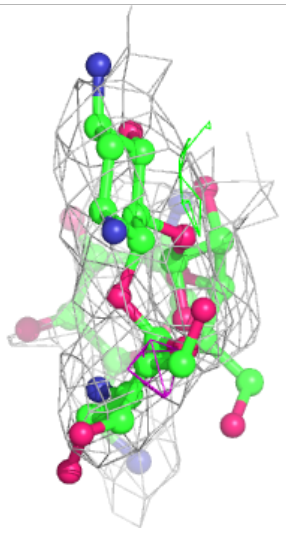


**Electron density around PAR 1 3406:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

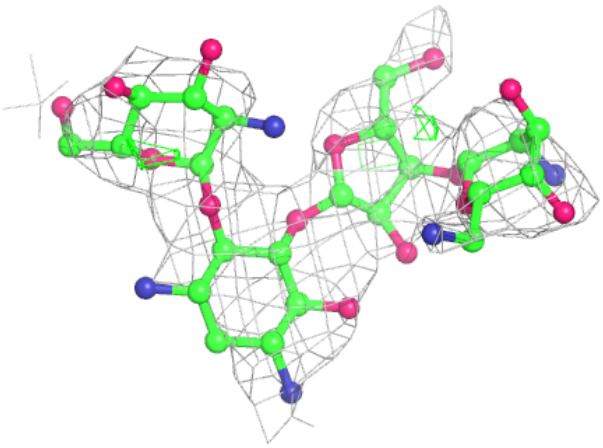


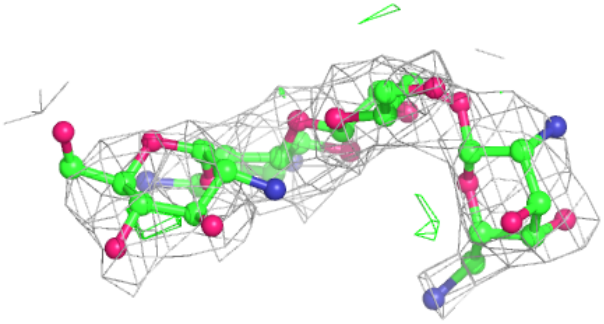


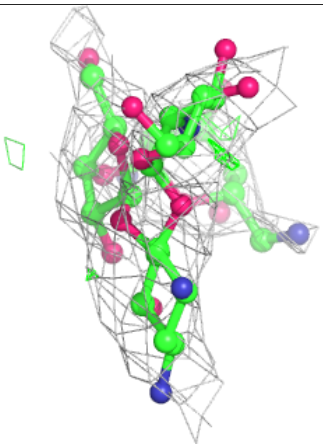


**Electron density around PAR 1 3437:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

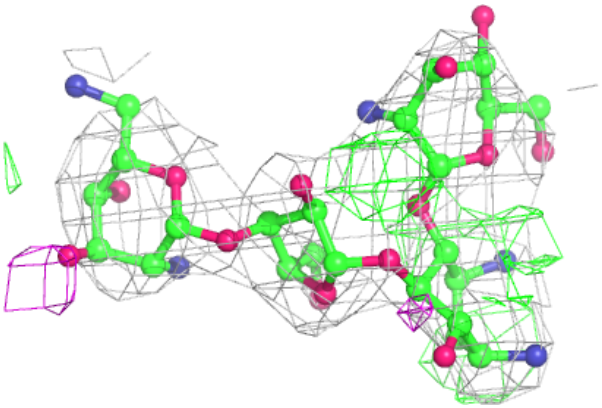


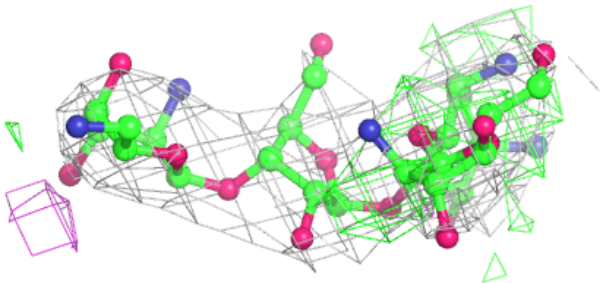


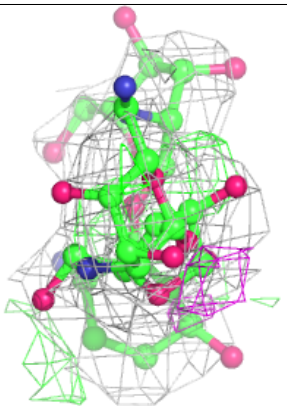


**Electron density around PAR 1 3410:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

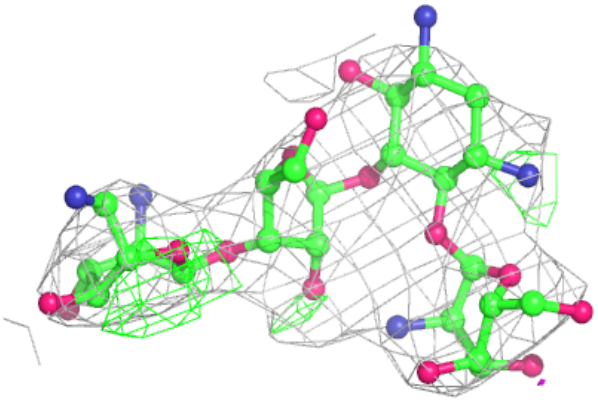


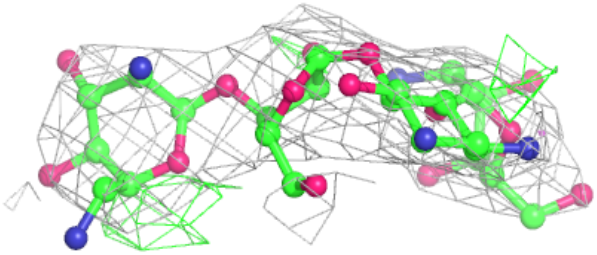


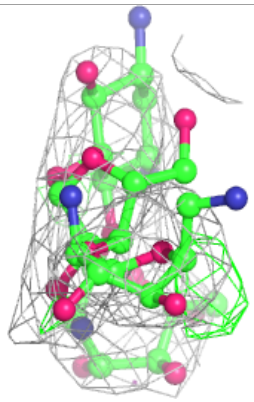


**Electron density around PAR 5 3409:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

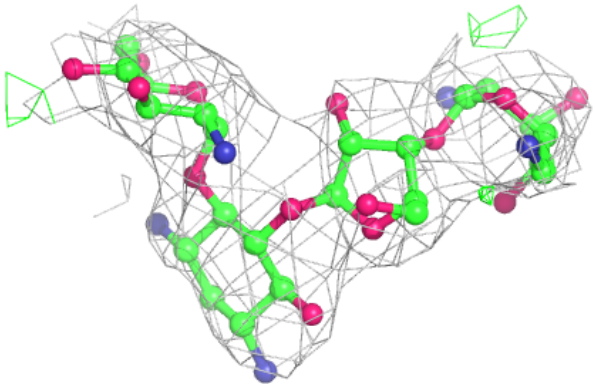


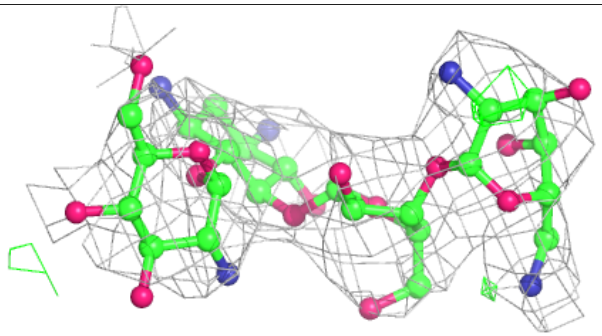


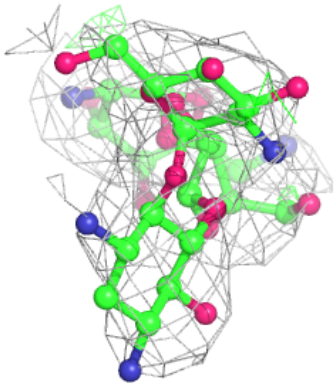


**Electron density around PAR 5 3402:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

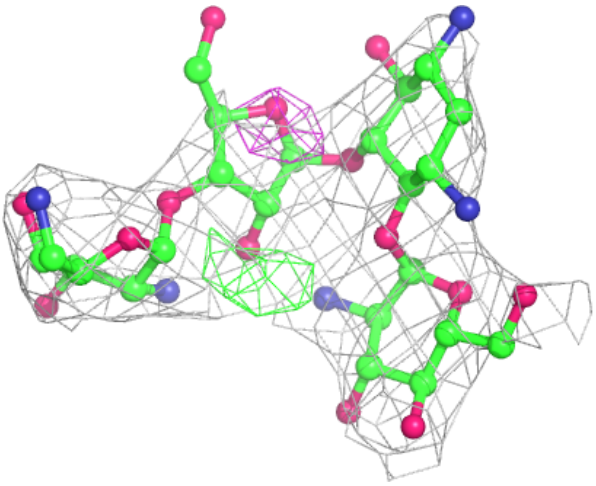


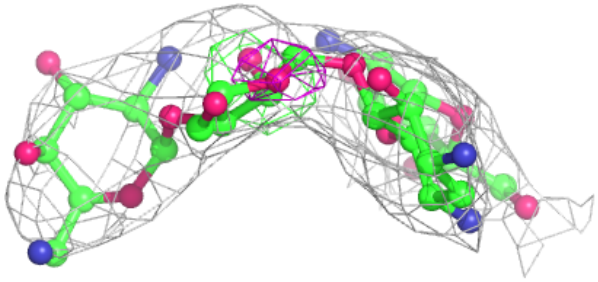


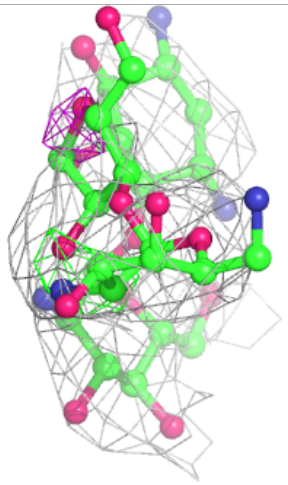


**Electron density around PAR 5 3413:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

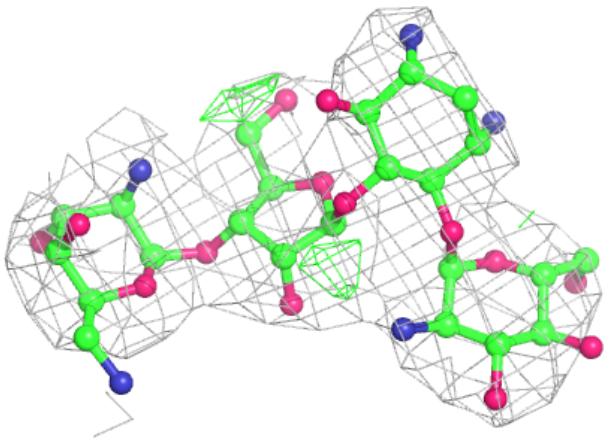


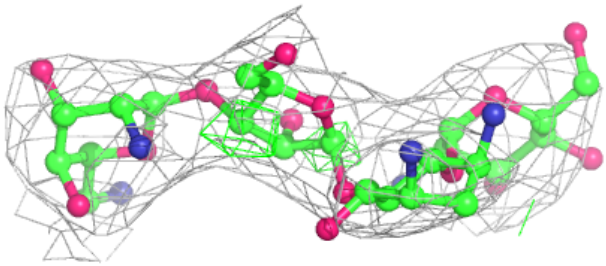


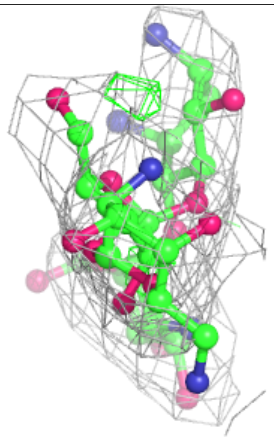


**Electron density around PAR 3 203:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

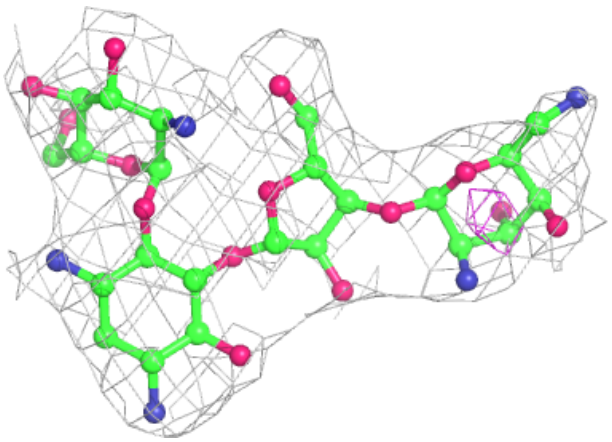


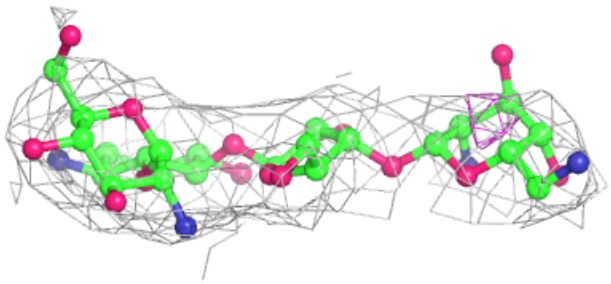


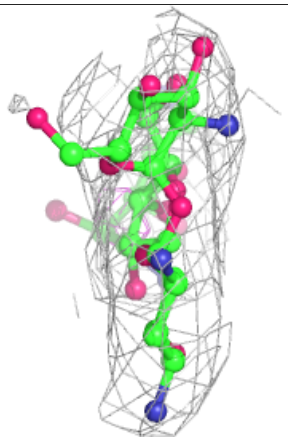


**Electron density around PAR 5 3421:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

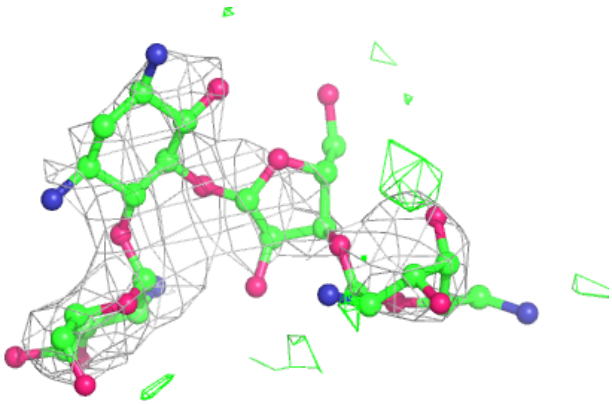


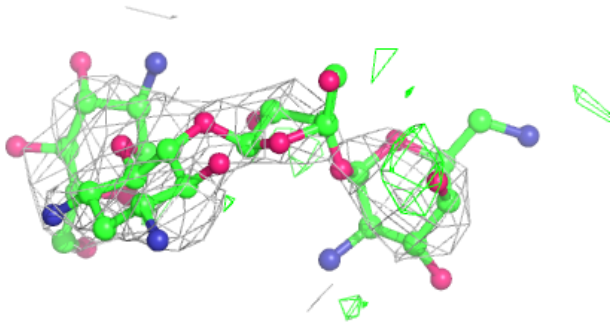


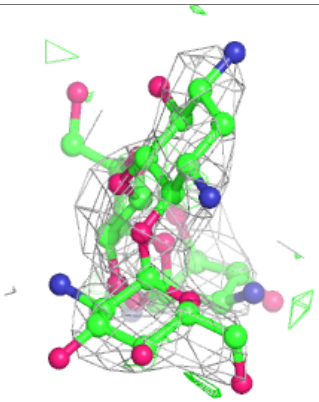


**Electron density around PAR 1 3404:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

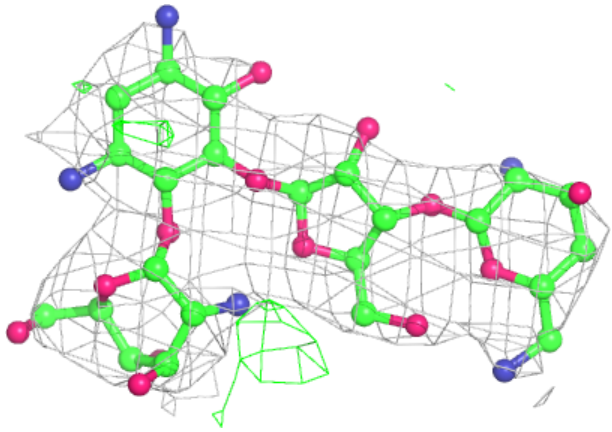


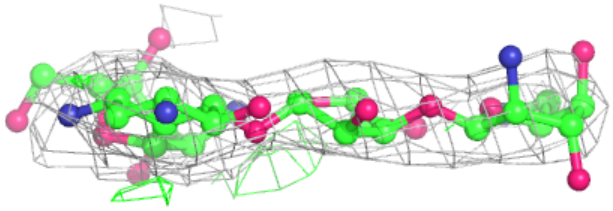


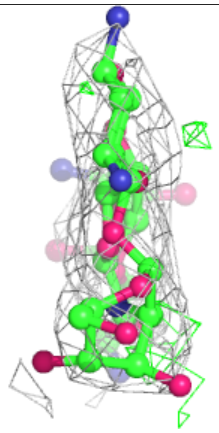


**Electron density around PAR 5 3425:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

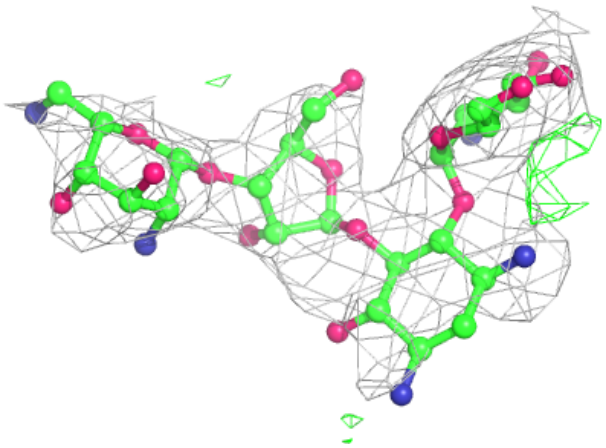


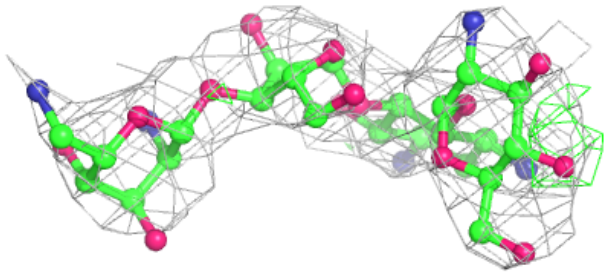


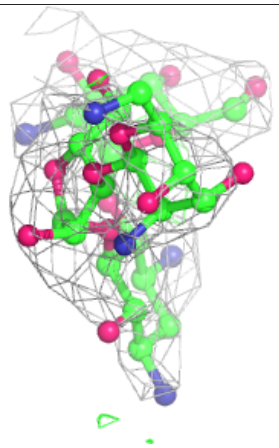


**Electron density around PAR 7 202:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

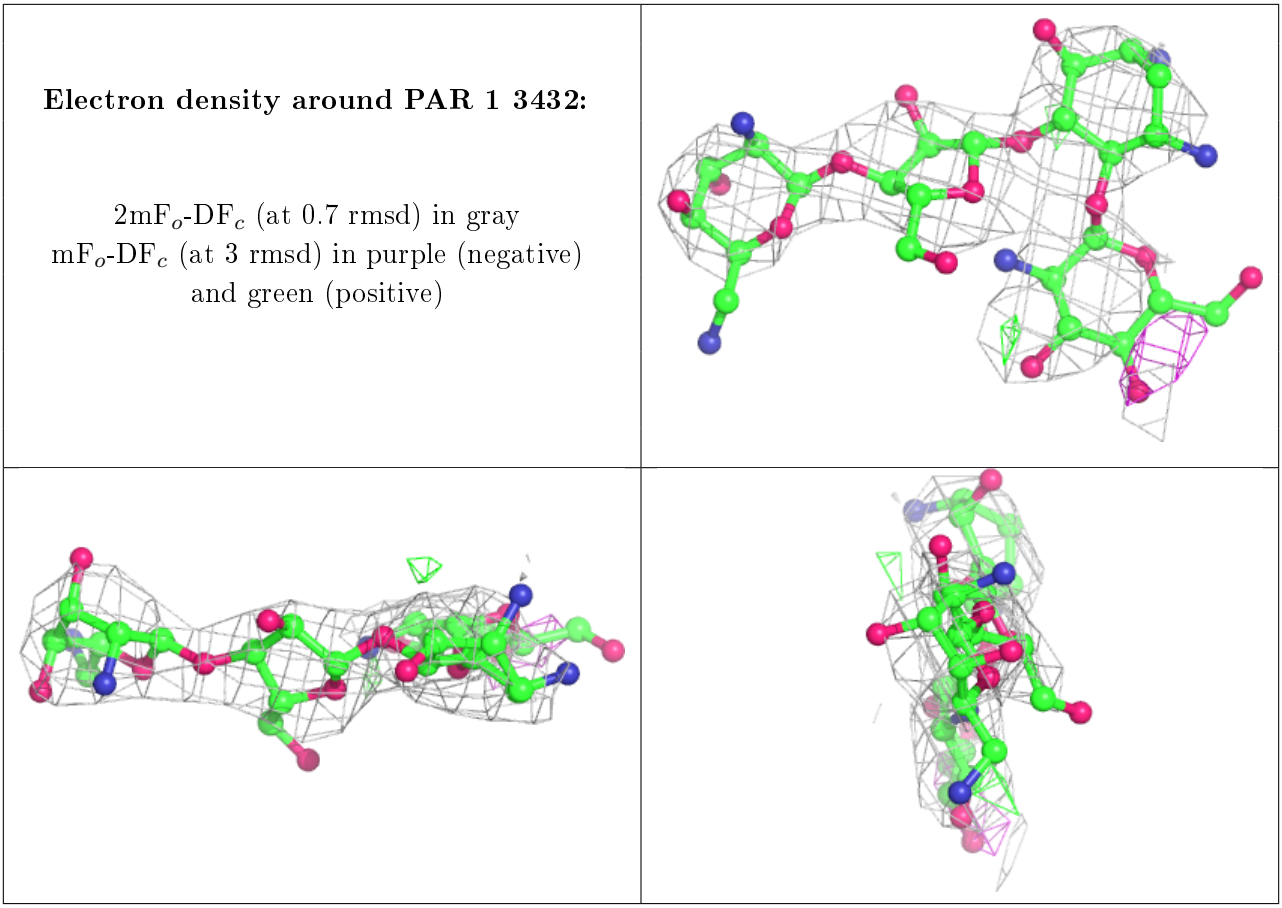






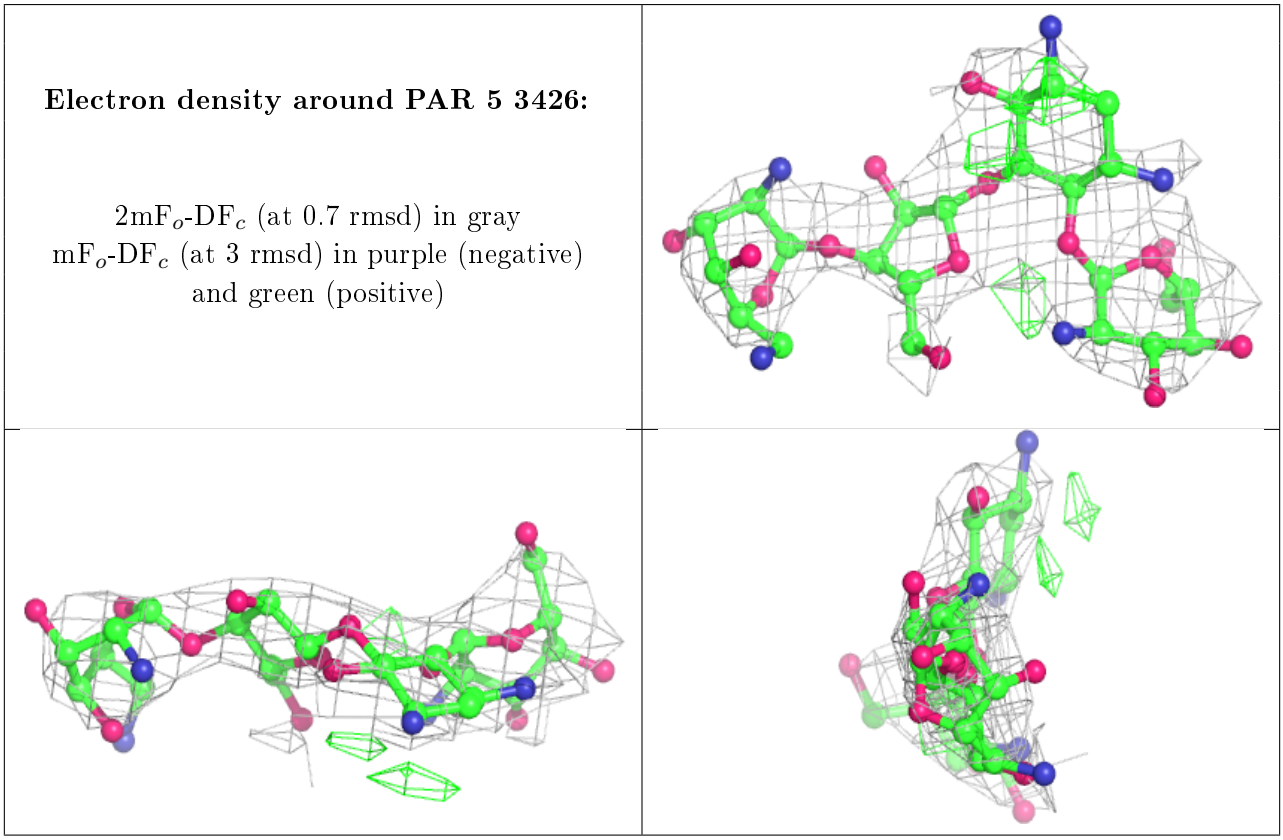
**Electron density around PAR 1 3432:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



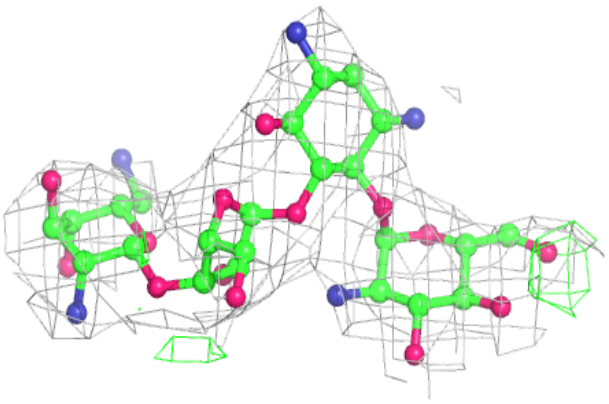
**Electron density around PAR 5 3426:**

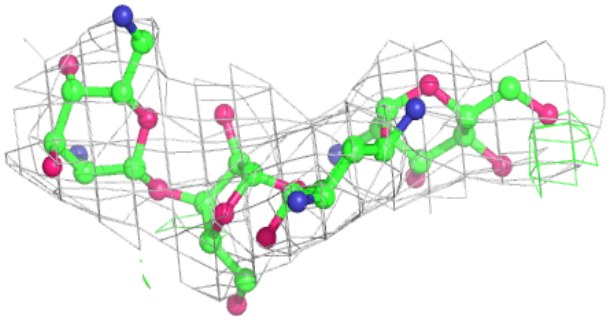
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

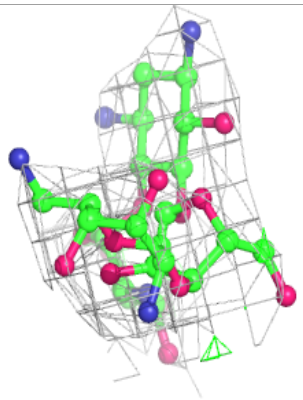


**Electron density around PAR 1 3434:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

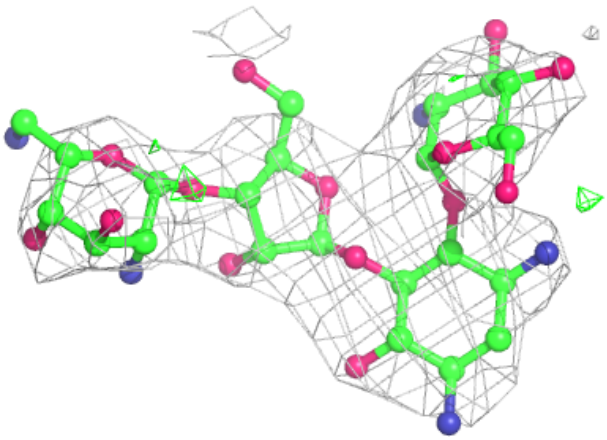


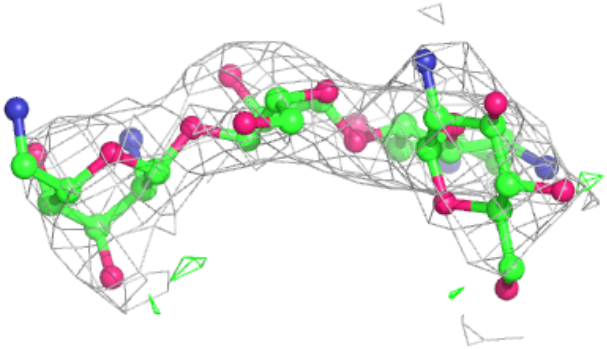


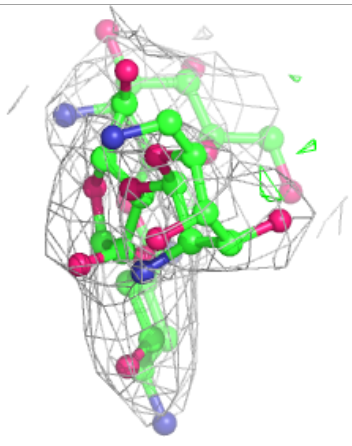


**Electron density around PAR 1 3417:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

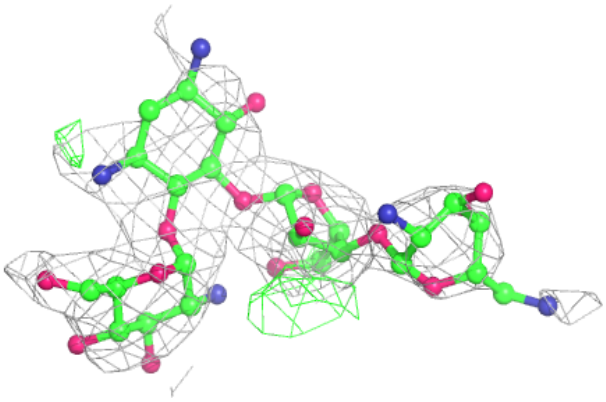


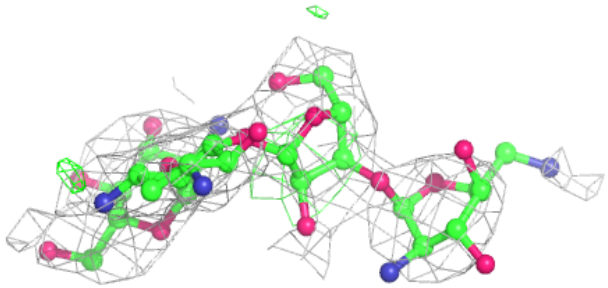


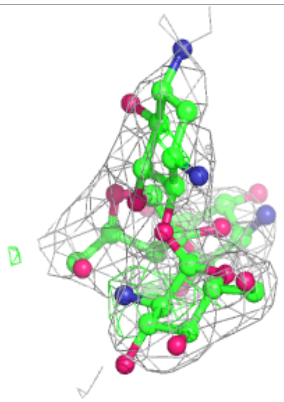


**Electron density around PAR 3 202:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

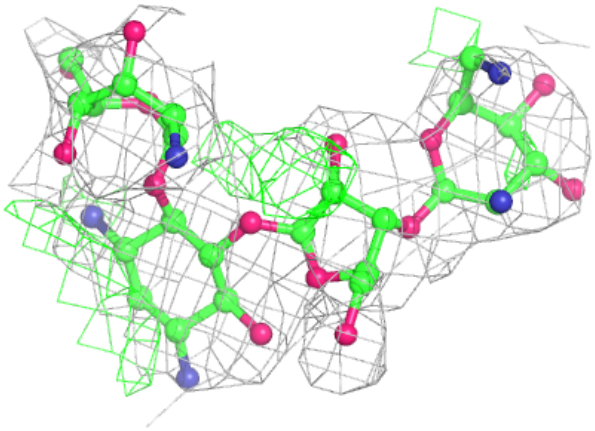


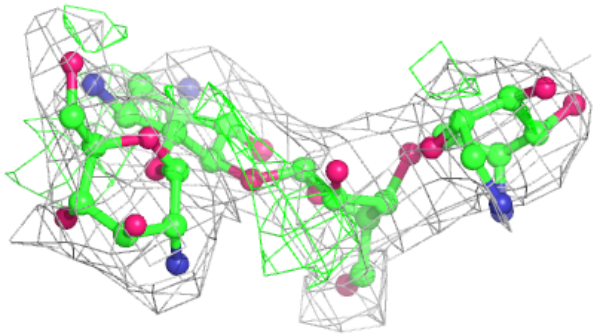


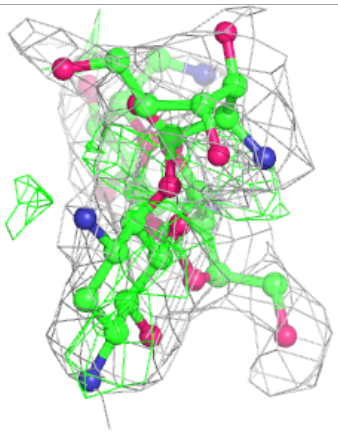


**Electron density around PAR 1 3414:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

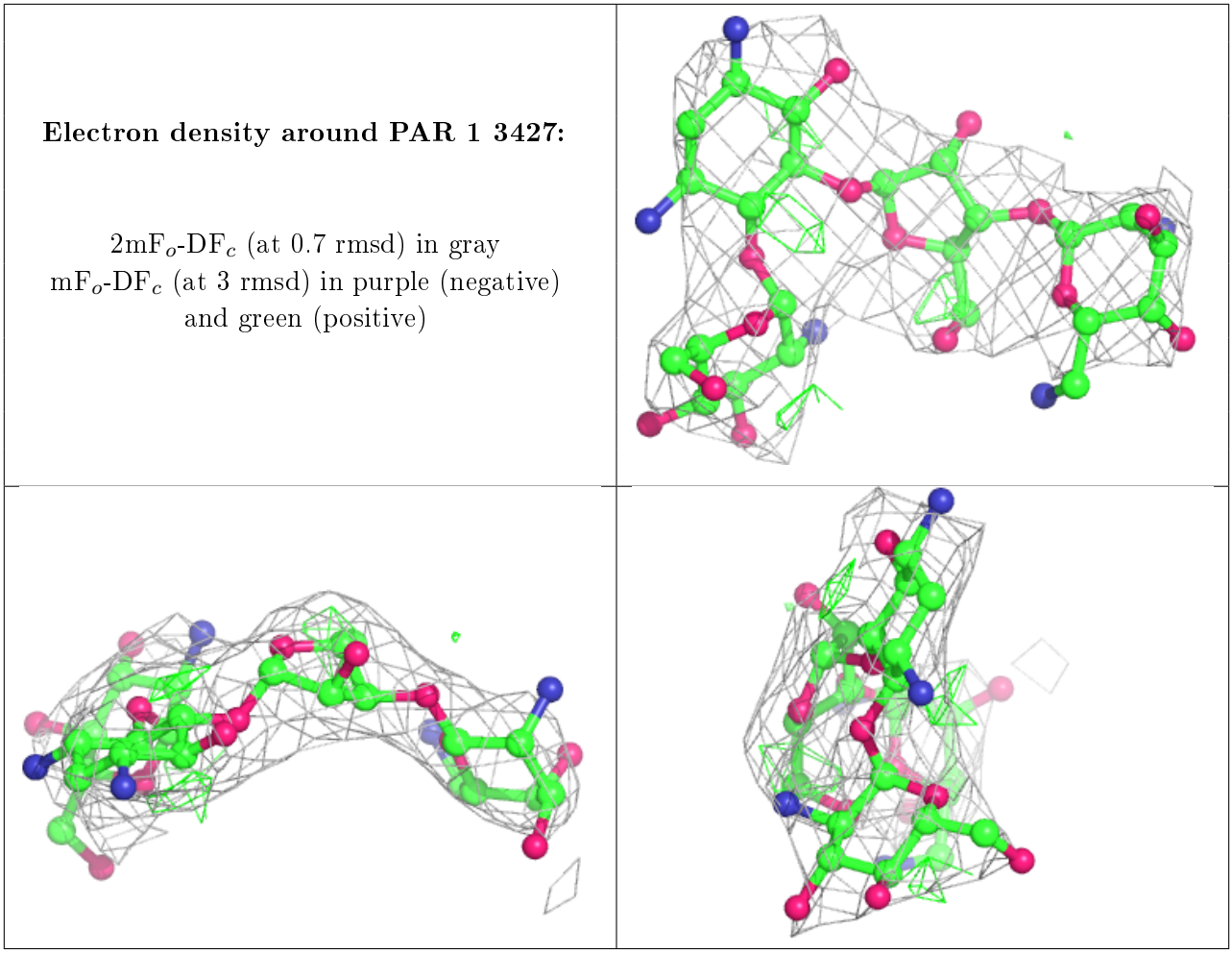






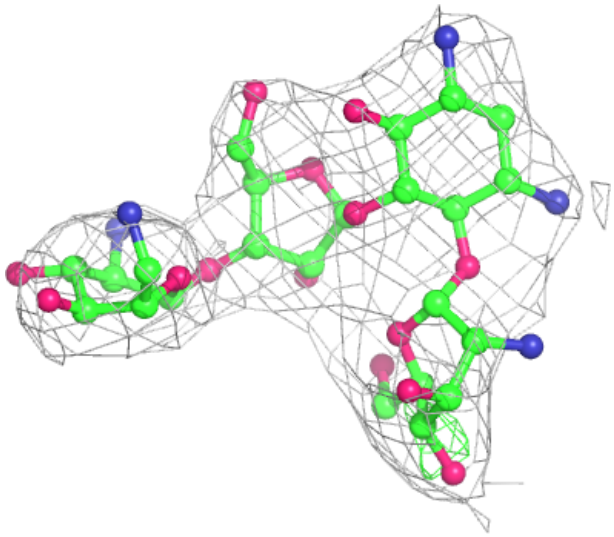
**Electron density around PAR 1 3427:**

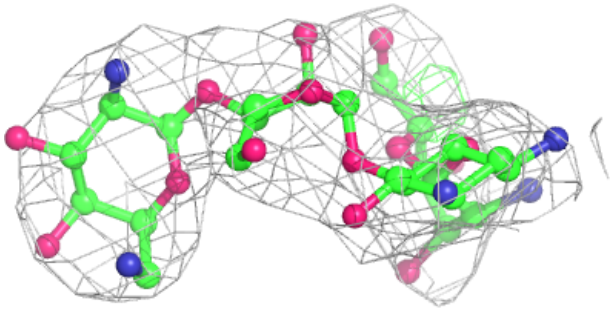
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

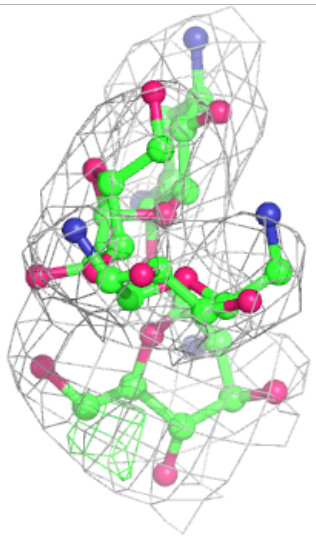


**Electron density around PAR 5 3415:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

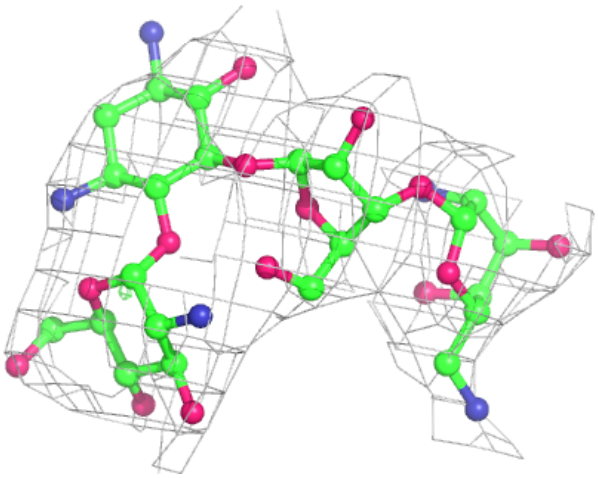


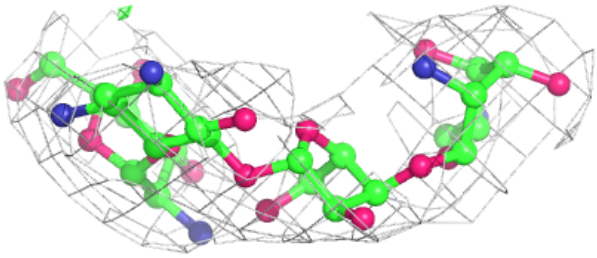


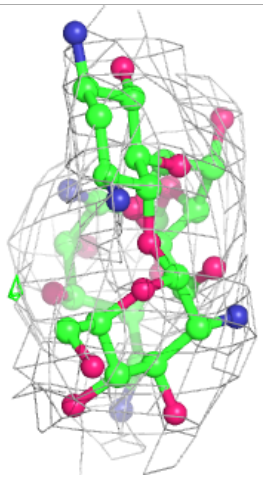


**Electron density around PAR 2 1904:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

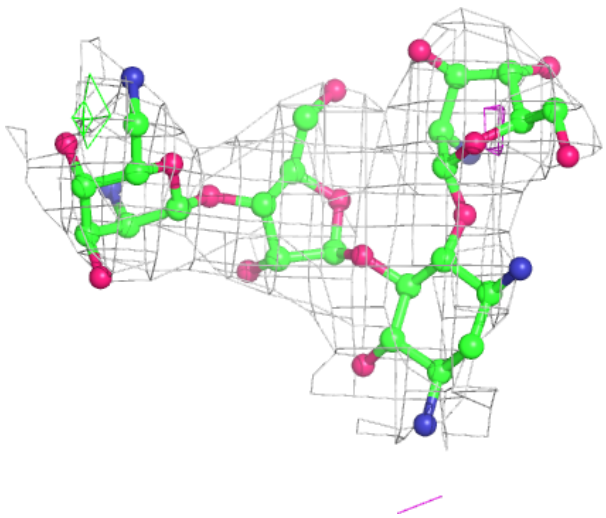


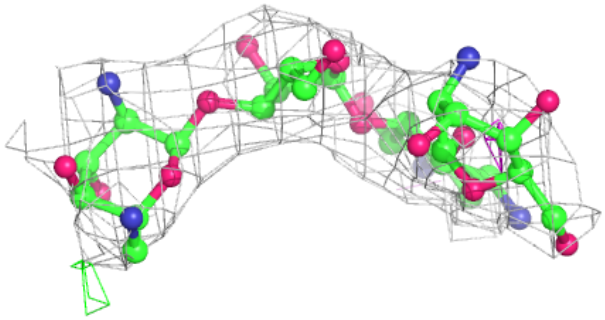


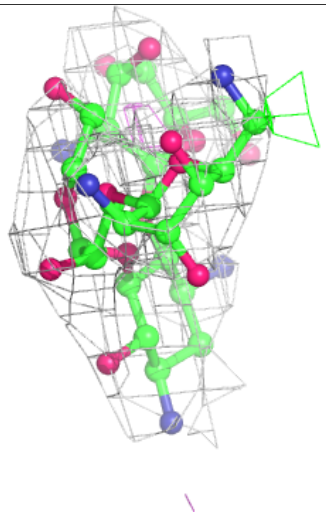


**Electron density around PAR 6 1901:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

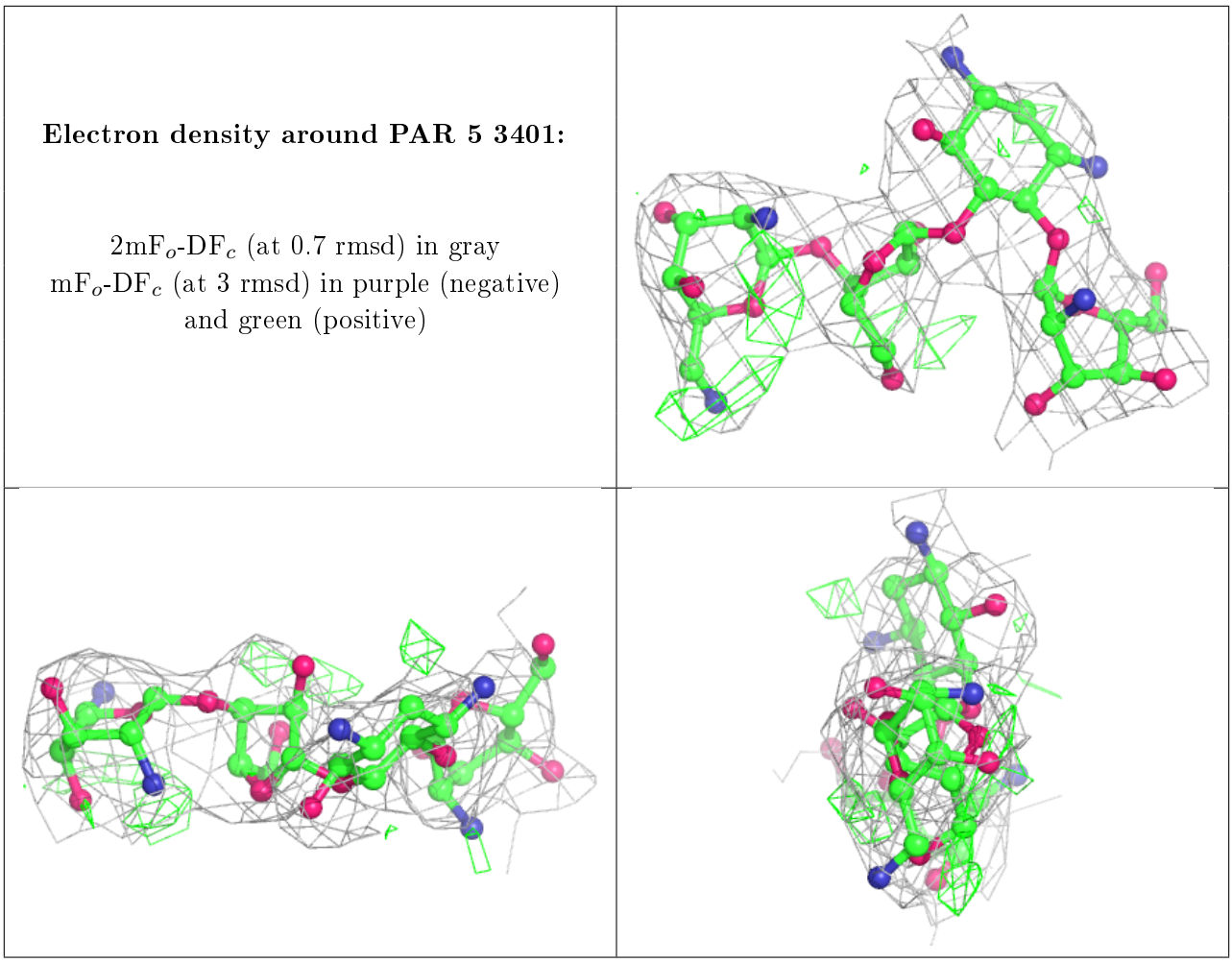






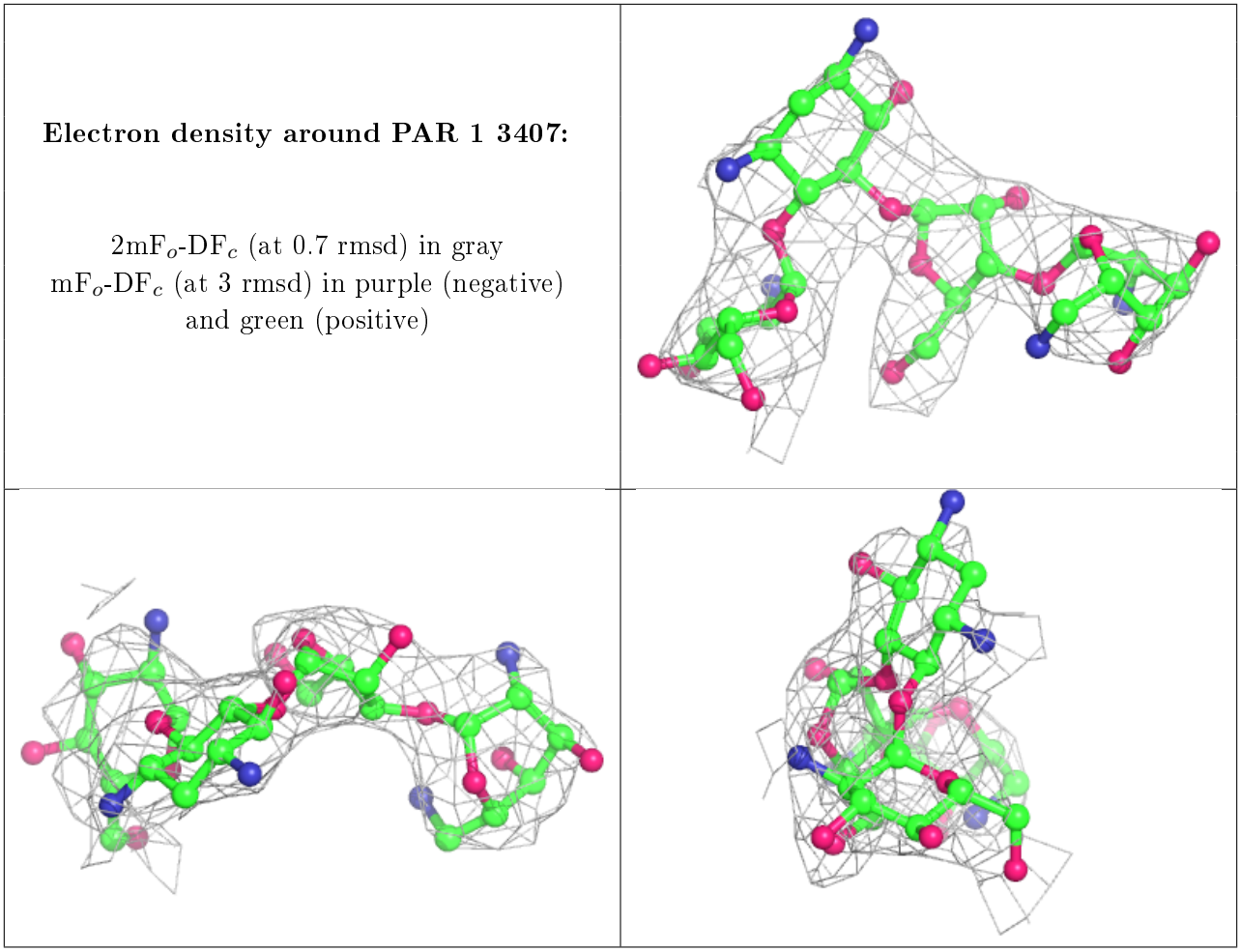
**Electron density around PAR 5 3401:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



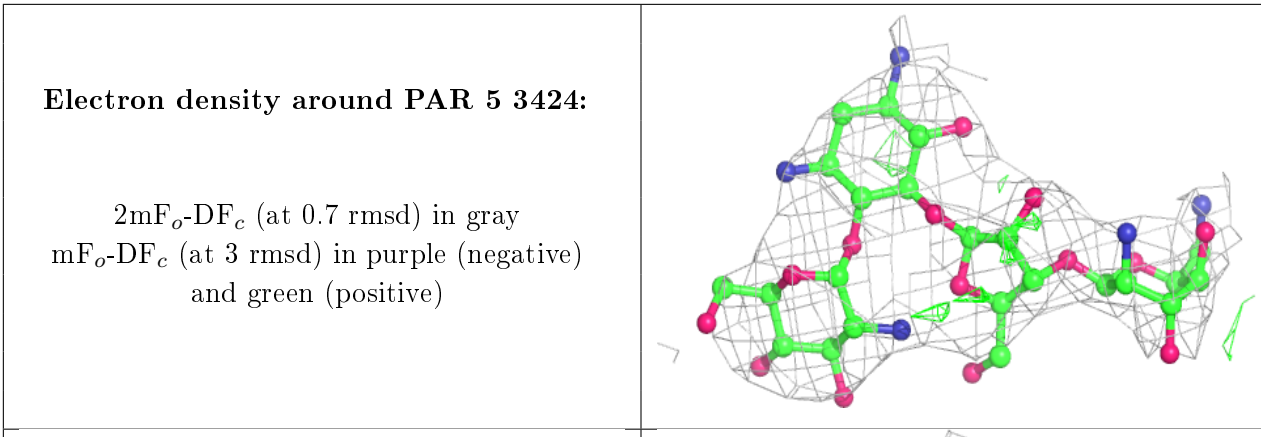
**Electron density around PAR 1 3407:**

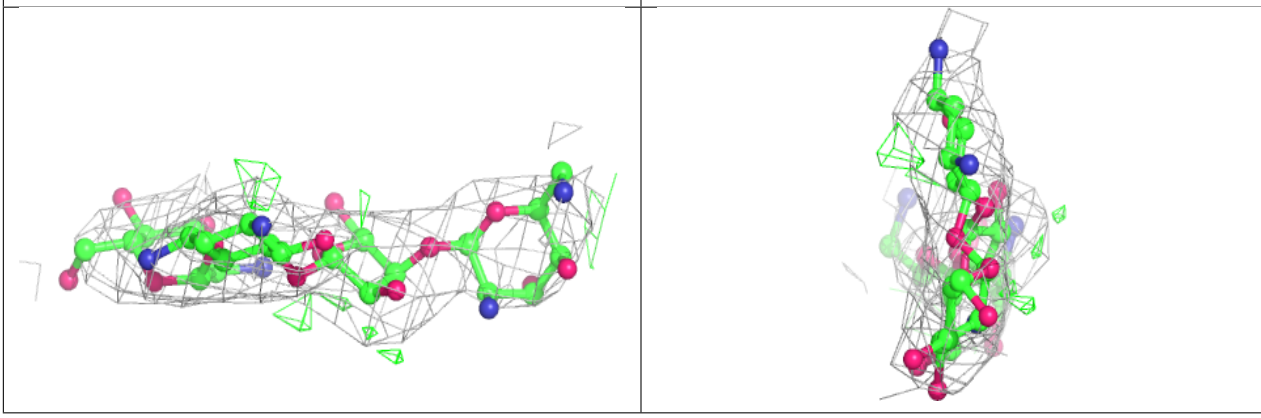
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



**Electron density around PAR 5 3424:**

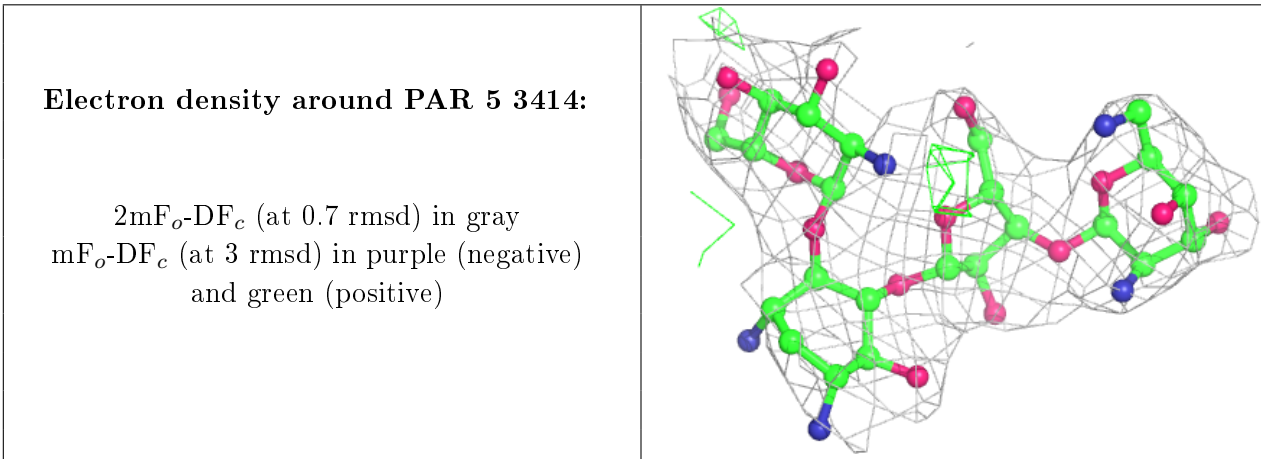
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

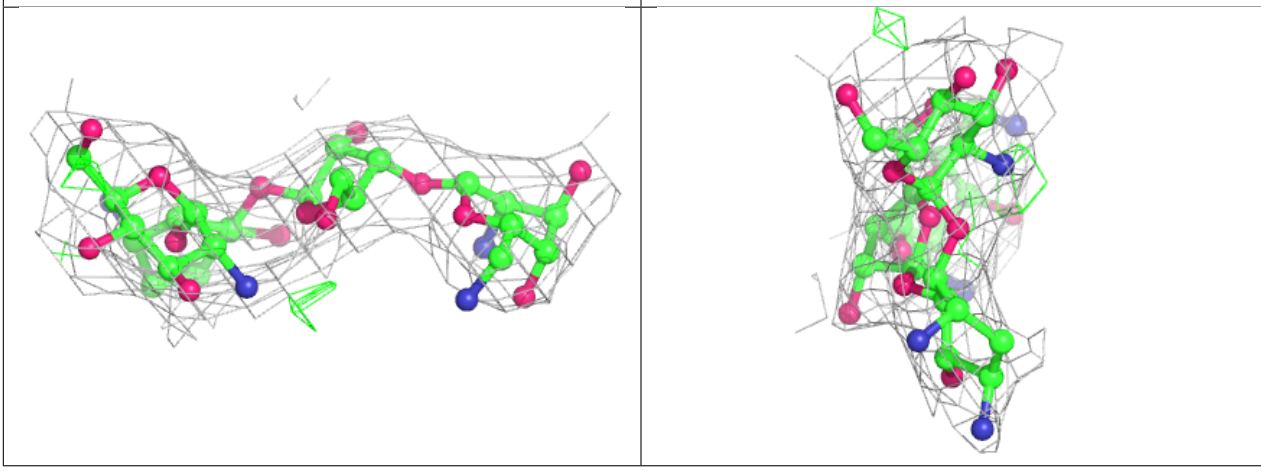




**Electron density around PAR 5 3414:**

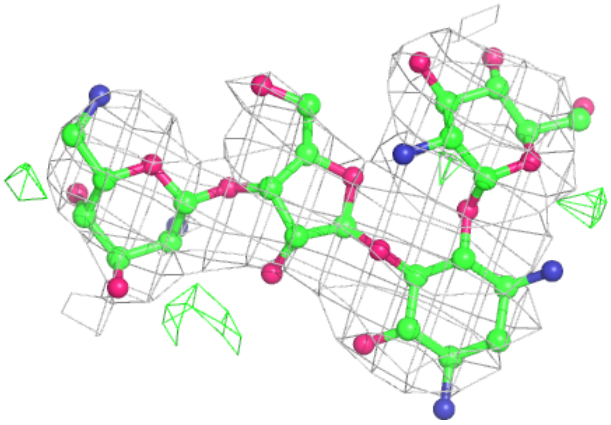
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

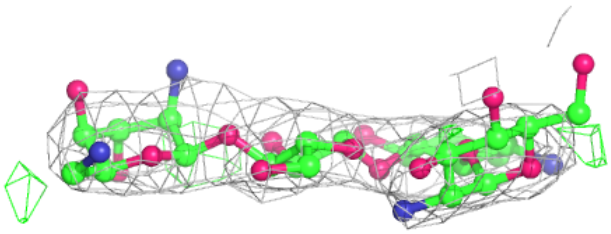


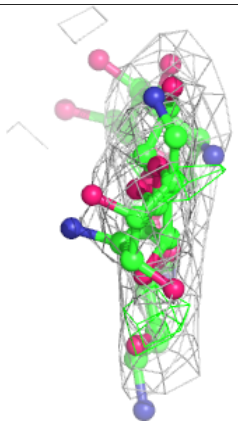


**Electron density around PAR 1 3422:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

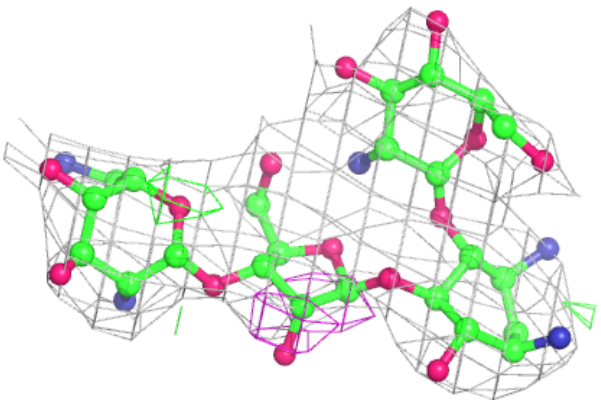


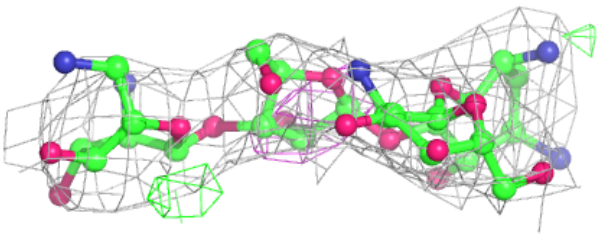


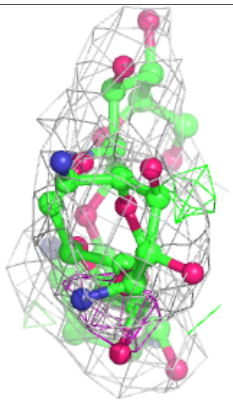


**Electron density around PAR 5 3419:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

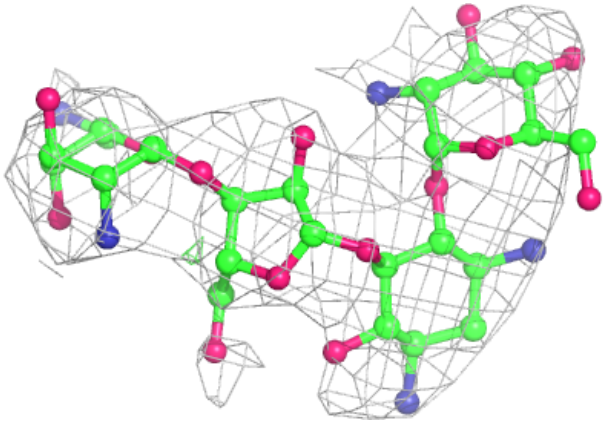


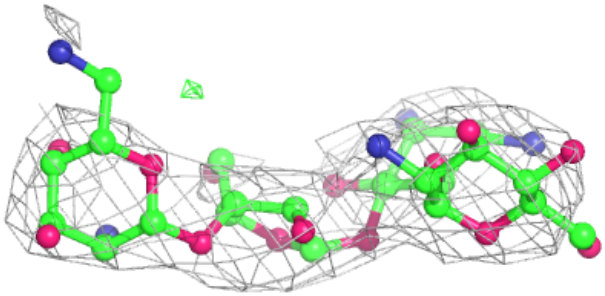


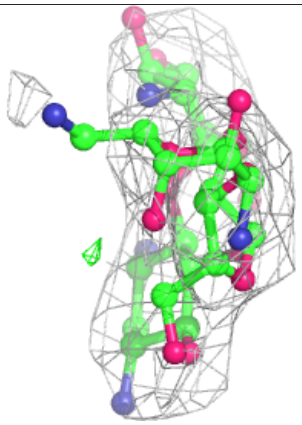


**Electron density around PAR 6 1904:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

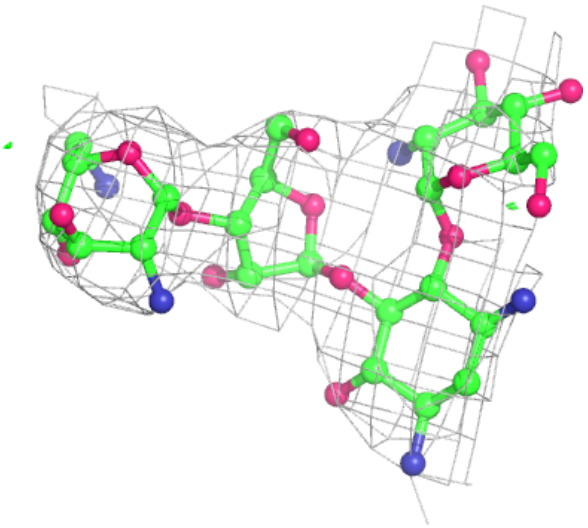


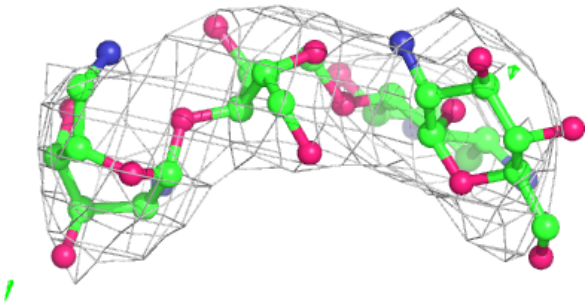


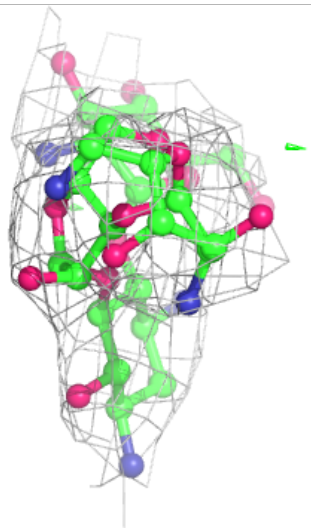


**Electron density around PAR 5 3418:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

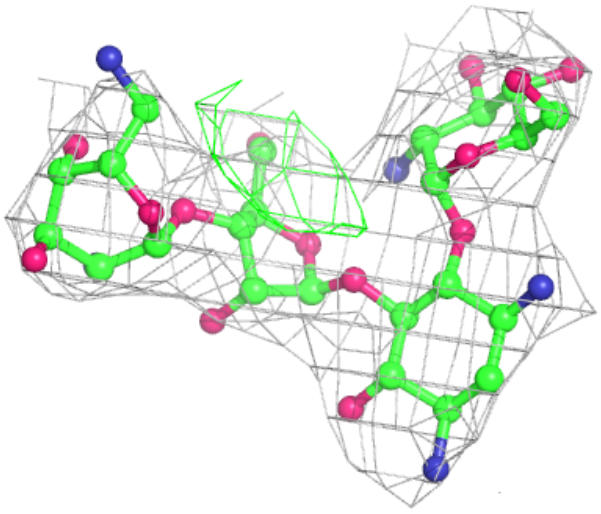


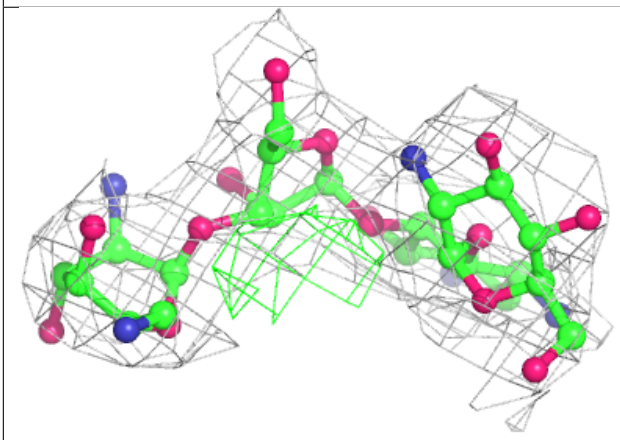


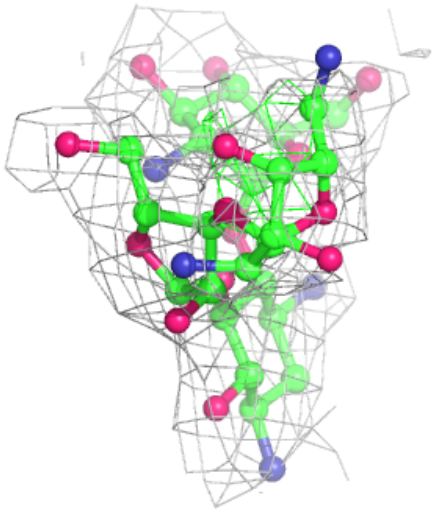


**Electron density around PAR 1 3418:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

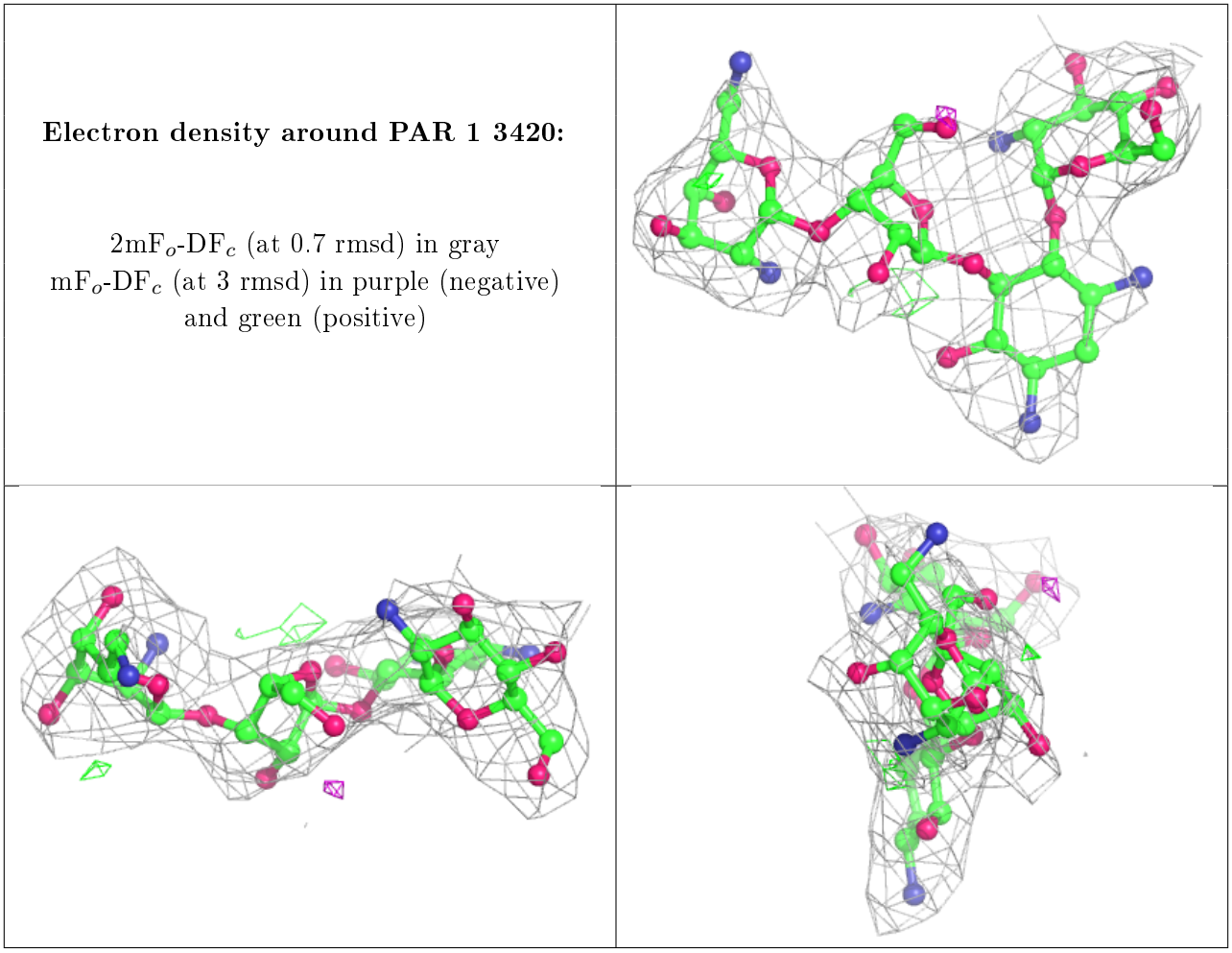






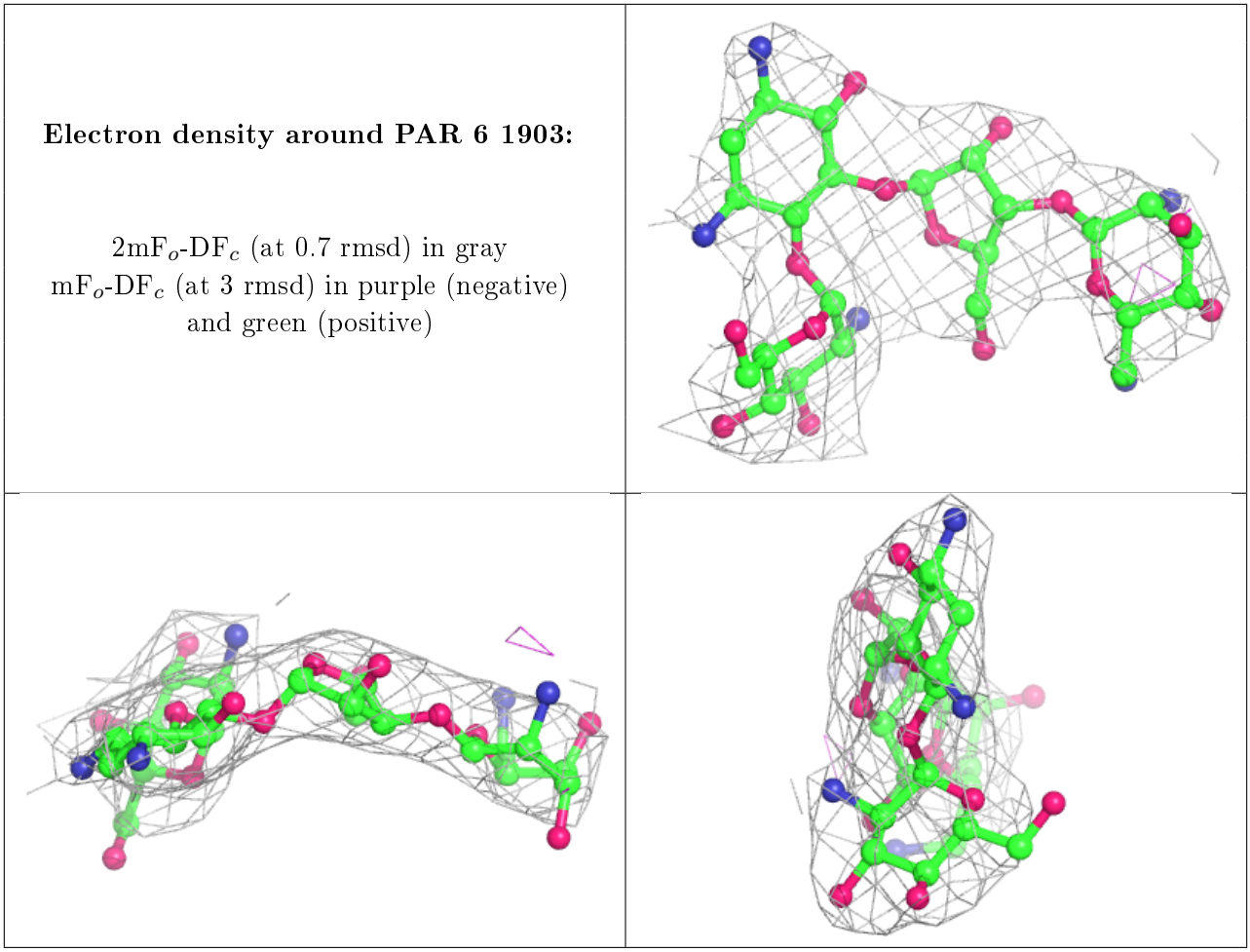
**Electron density around PAR 1 3420:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



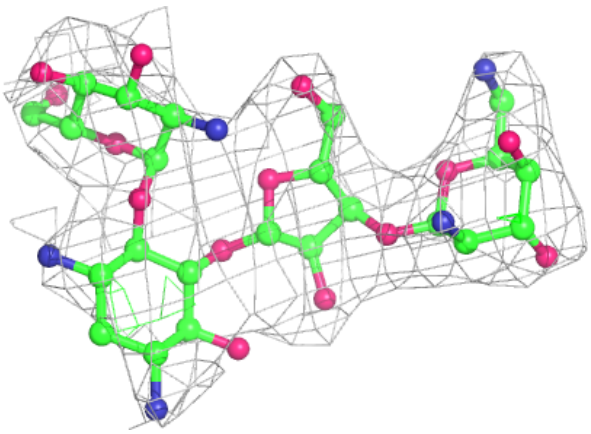
**Electron density around PAR 6 1903:**

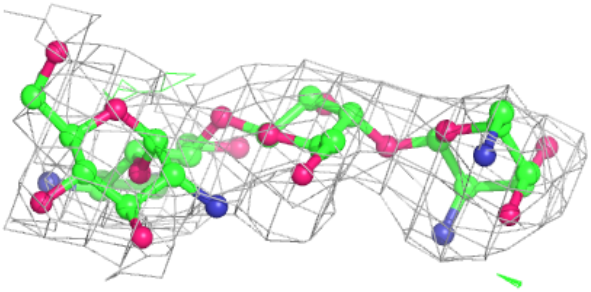
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

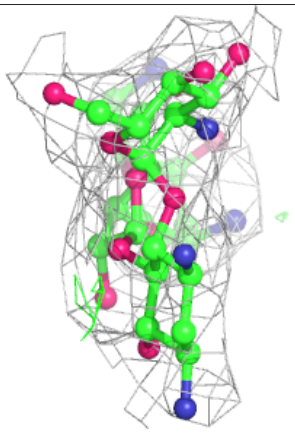


**Electron density around PAR 1 3402:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

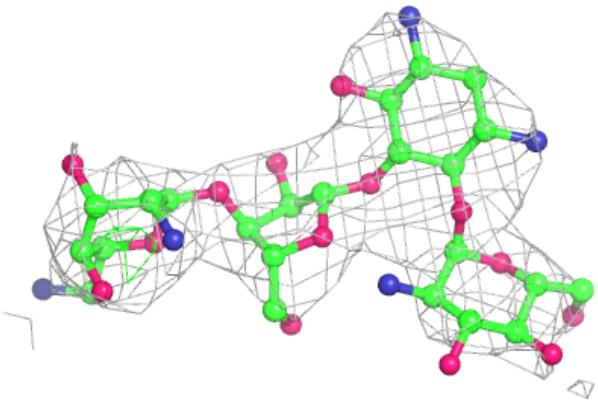


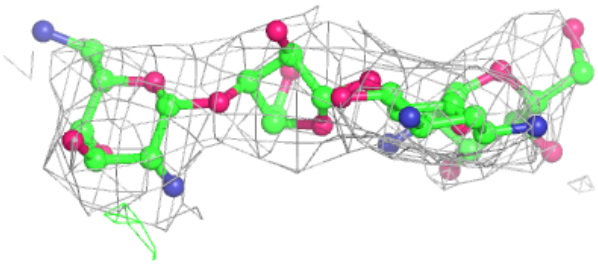


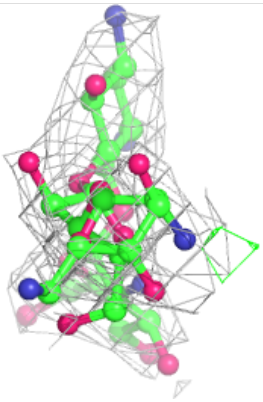


**Electron density around PAR 1 3415:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

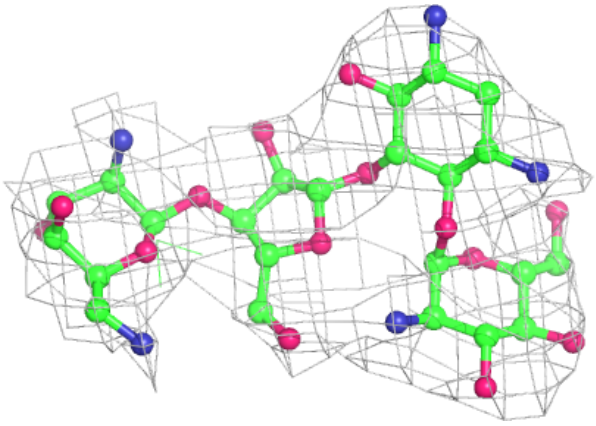


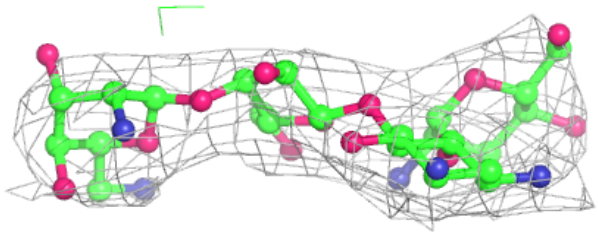


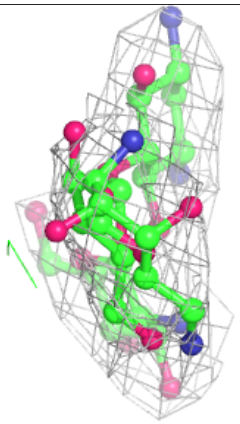


**Electron density around PAR 7 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

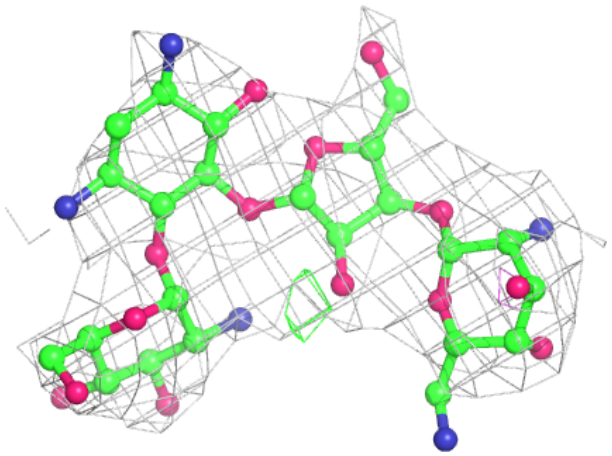


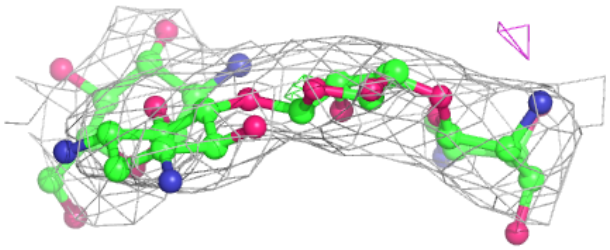


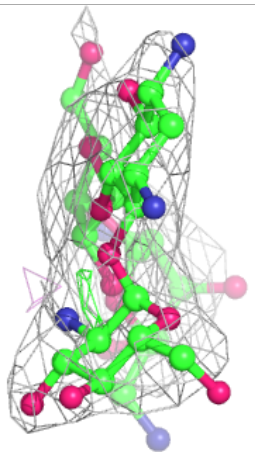


**Electron density around PAR 2 1902:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

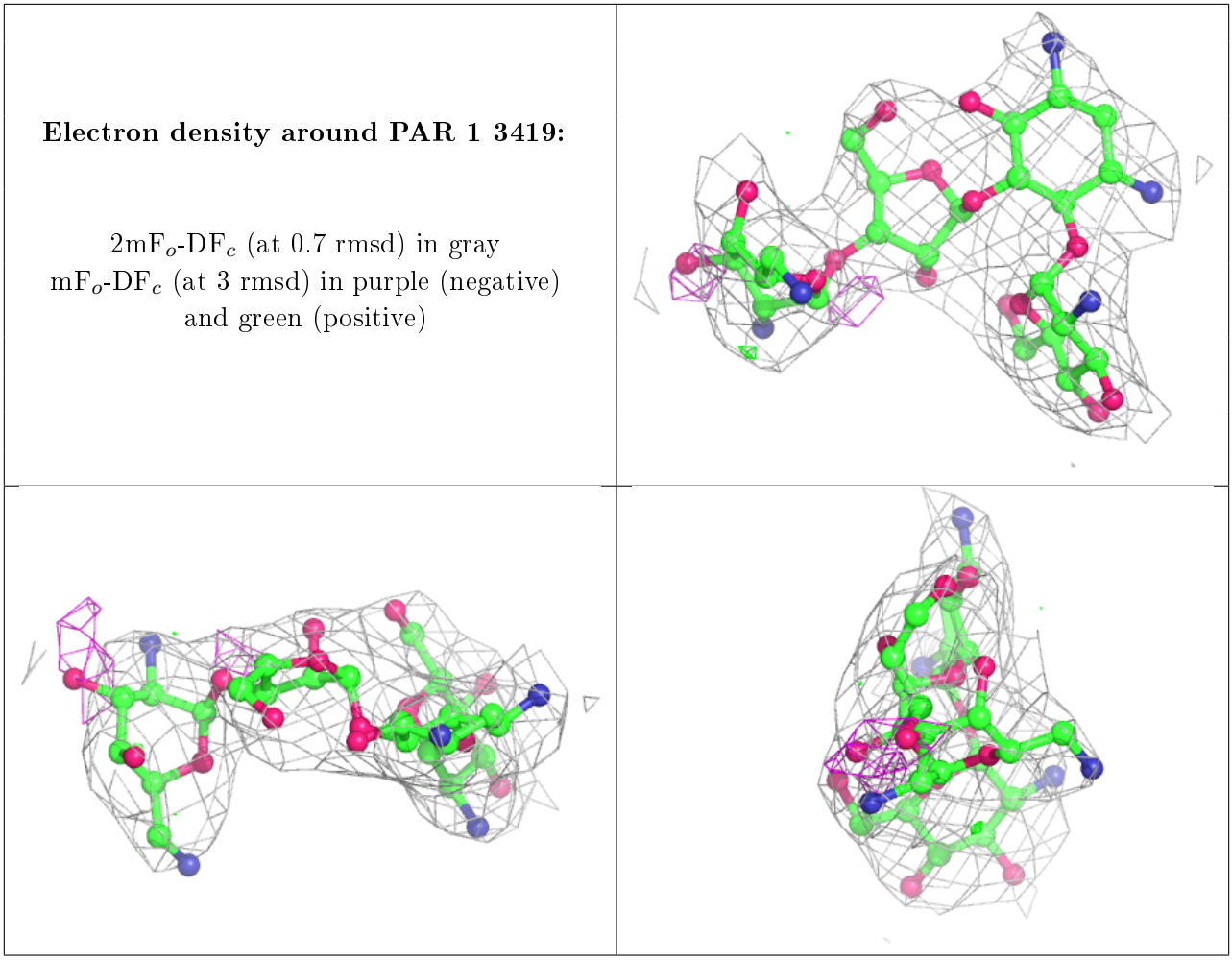






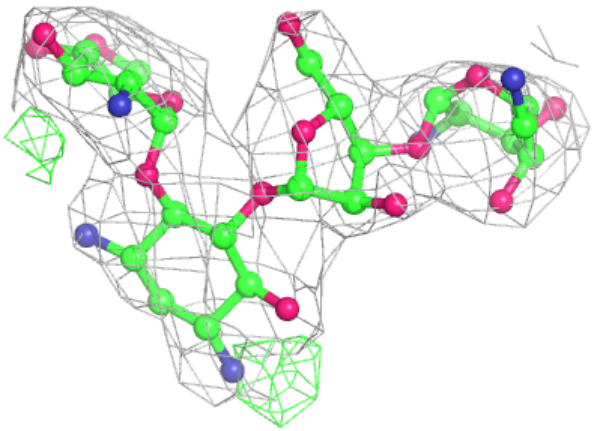
**Electron density around PAR 1 3419:**

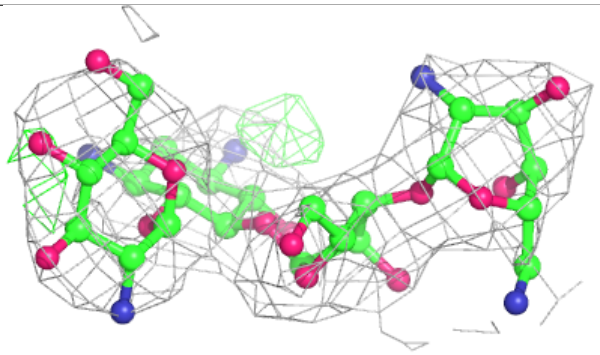
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



**Electron density around PAR 1 3430:**

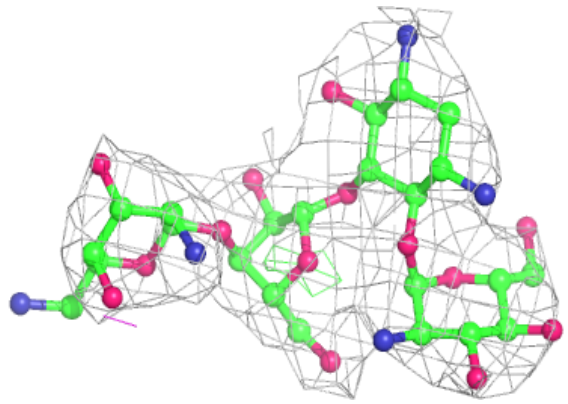
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

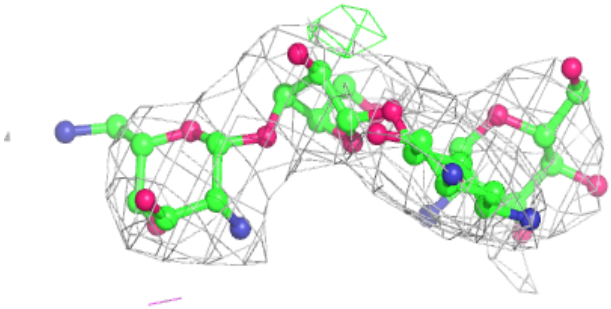


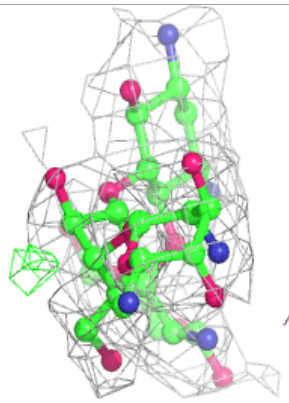


**Electron density around PAR 1 3412:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

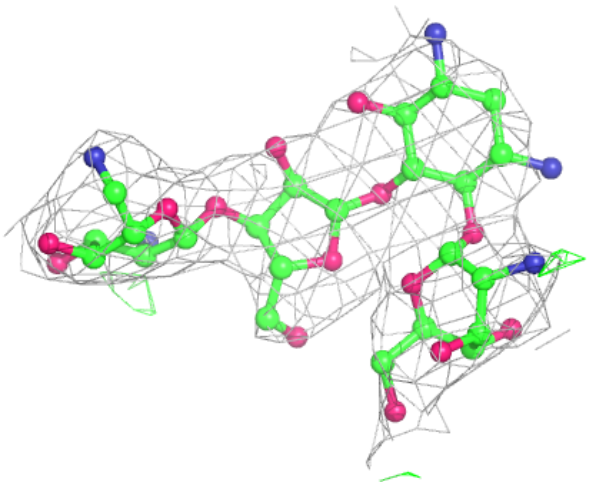


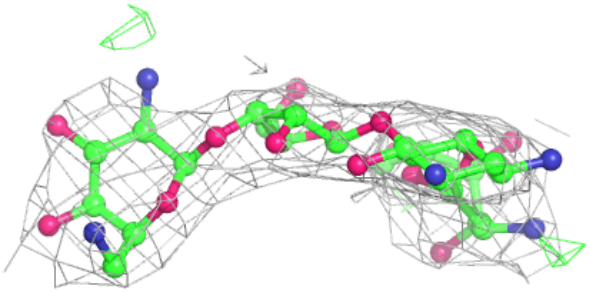


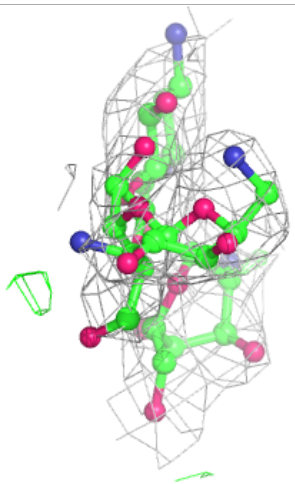


**Electron density around PAR 1 3425:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

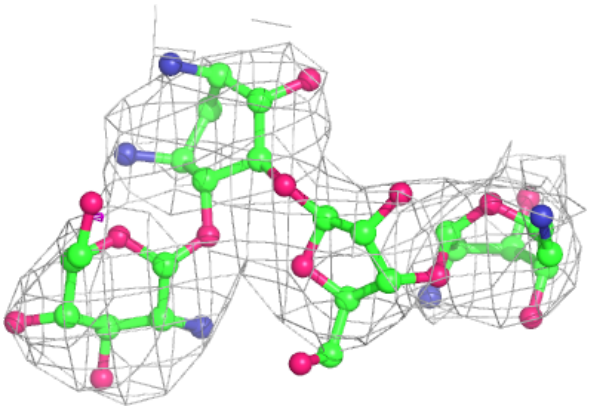


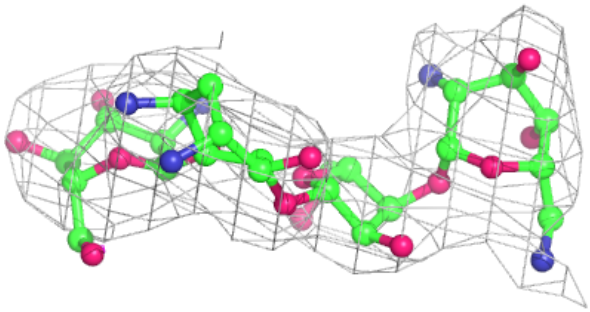


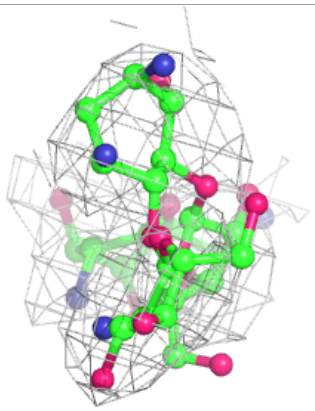


**Electron density around PAR 5 3420:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

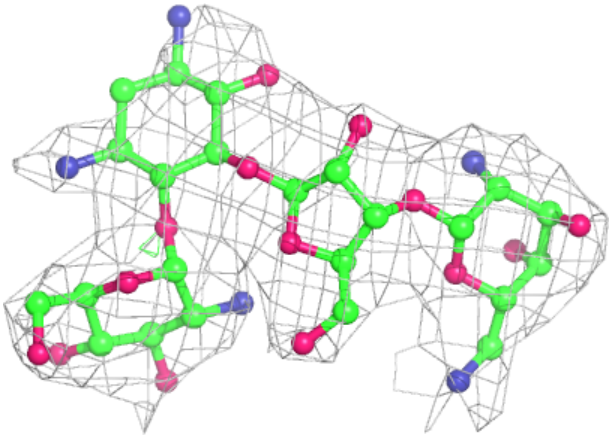


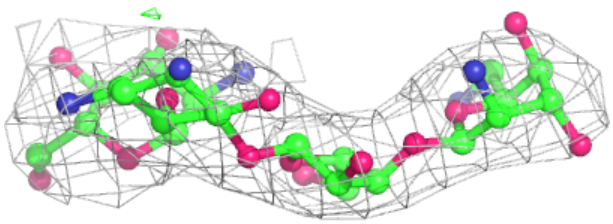


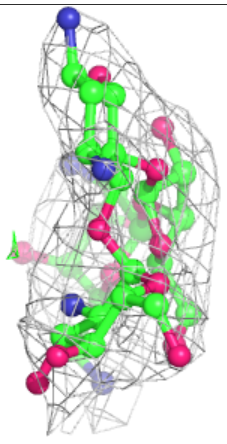


**Electron density around PAR 4 202:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

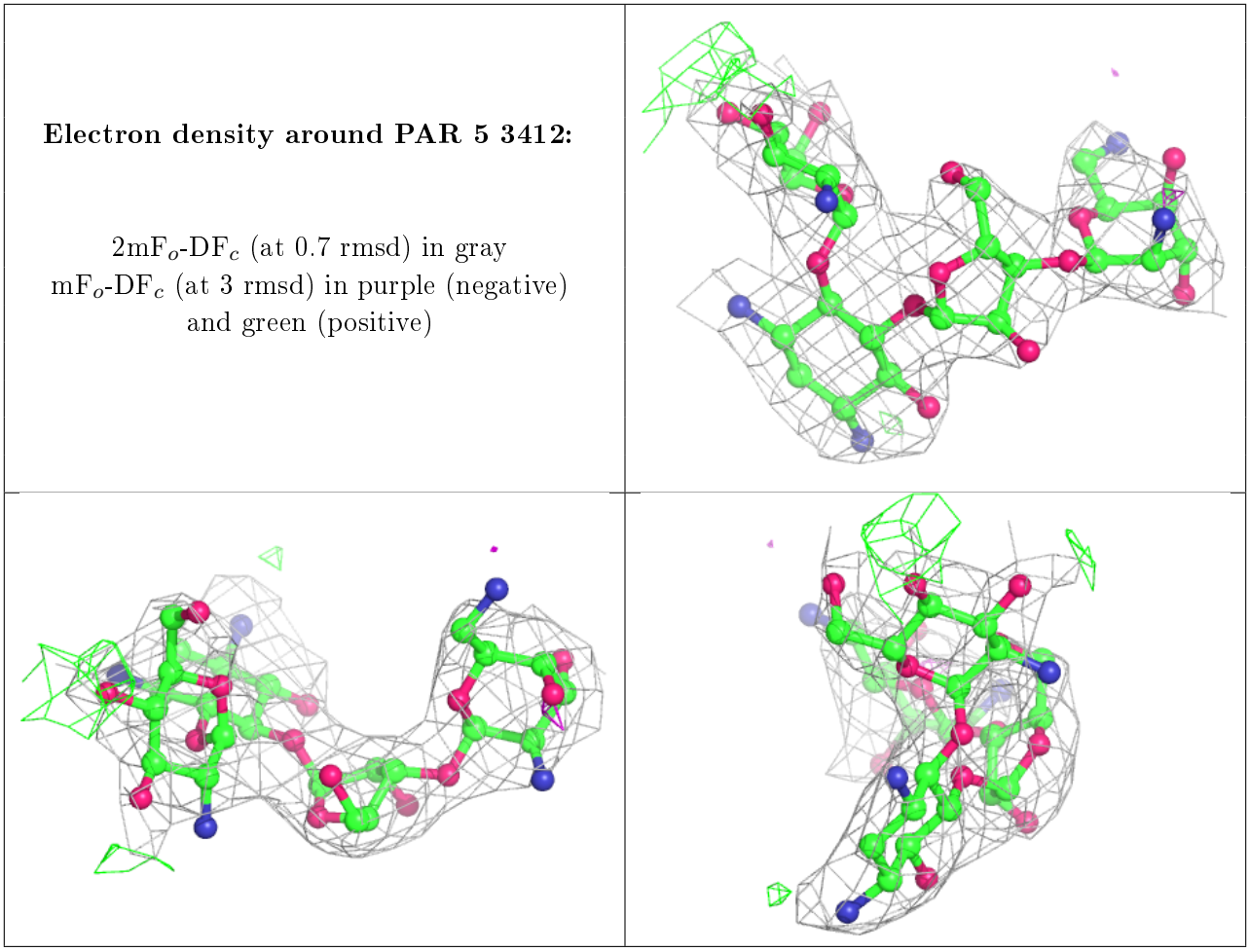






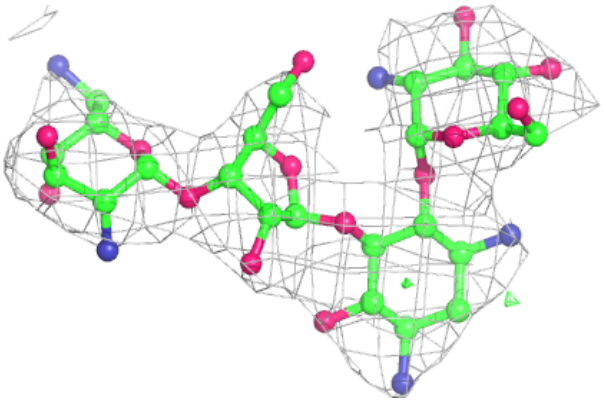
**Electron density around PAR 5 3412:**

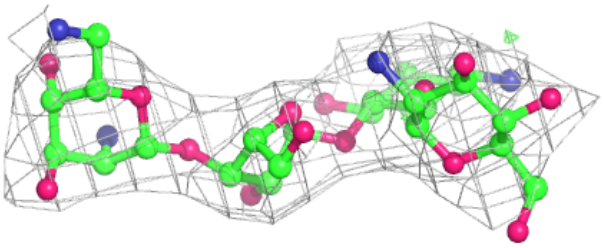
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

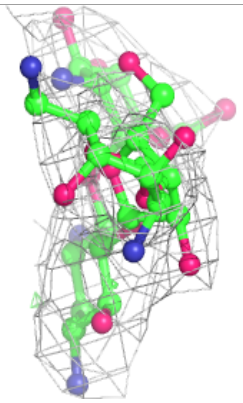


**Electron density around PAR 5 3416:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

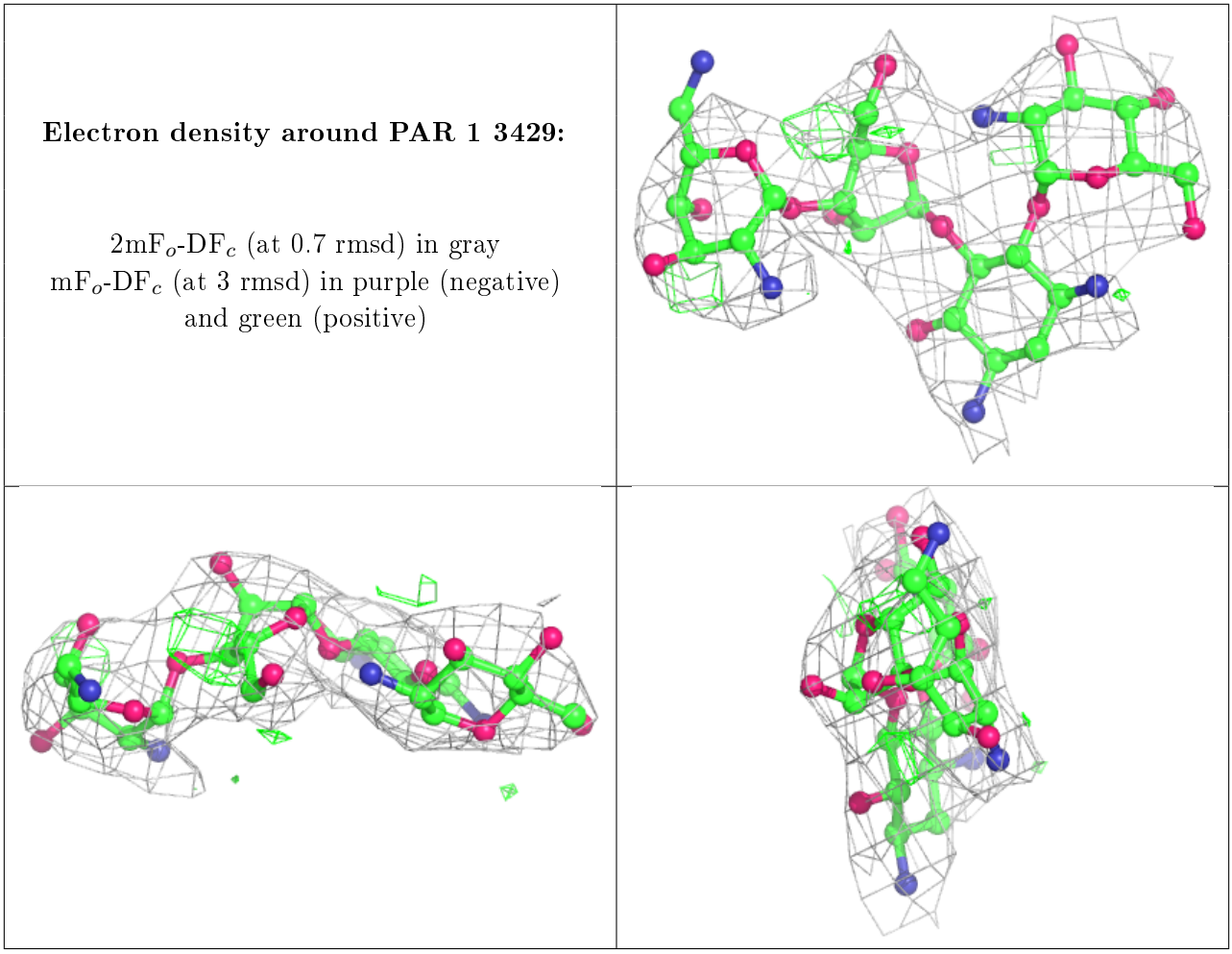






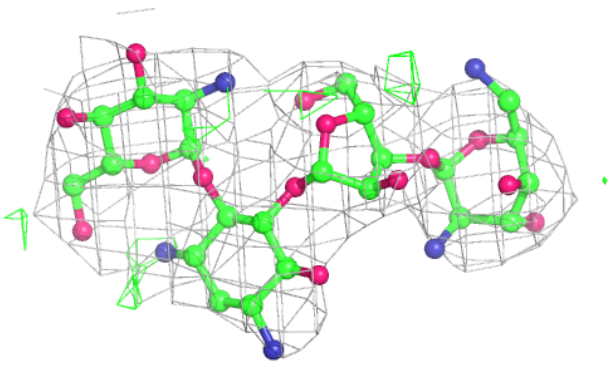
**Electron density around PAR 1 3429:**

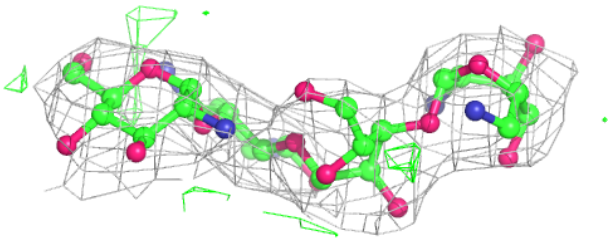
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

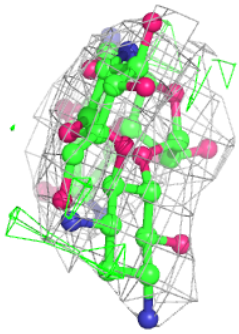


**Electron density around PAR 5 3407:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

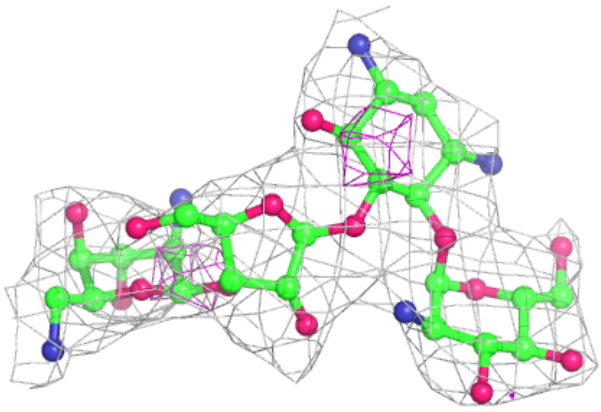


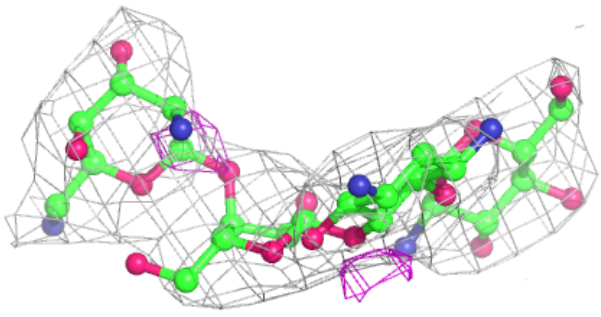




**Electron density around PAR 1 3416:**

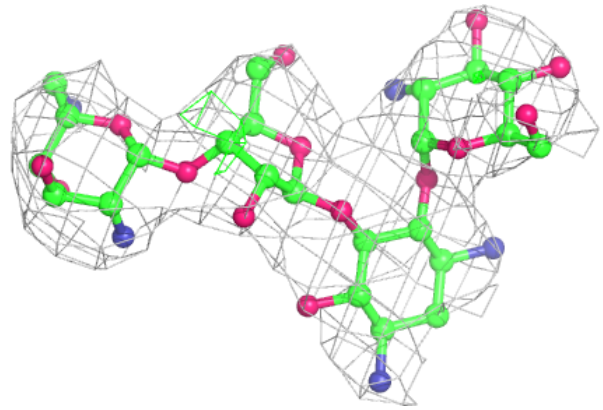
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

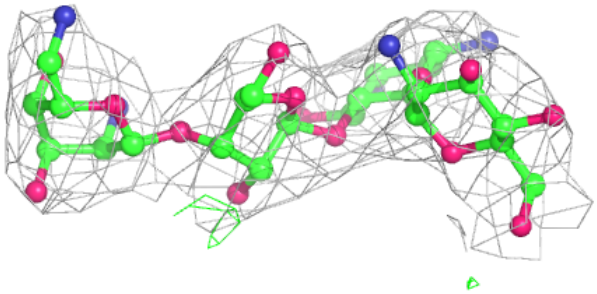


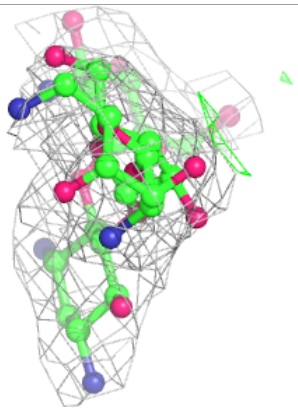


**Electron density around PAR 1 3428:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

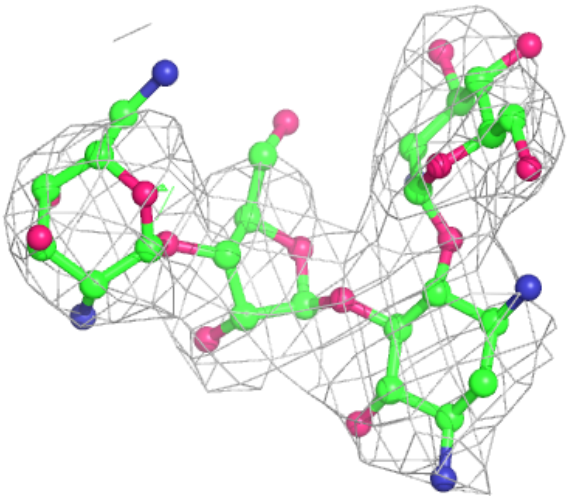


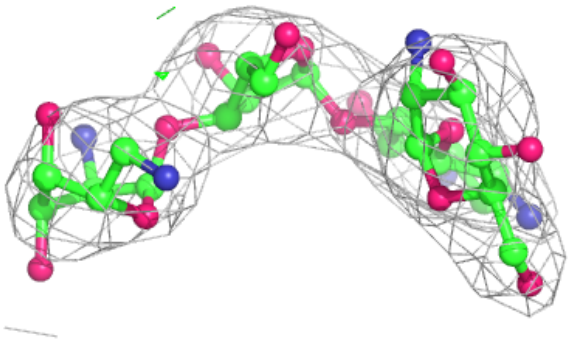


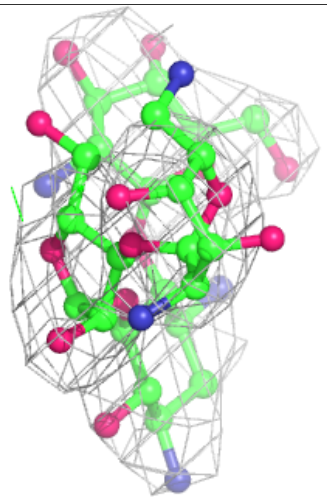


**Electron density around PAR 1 3408:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

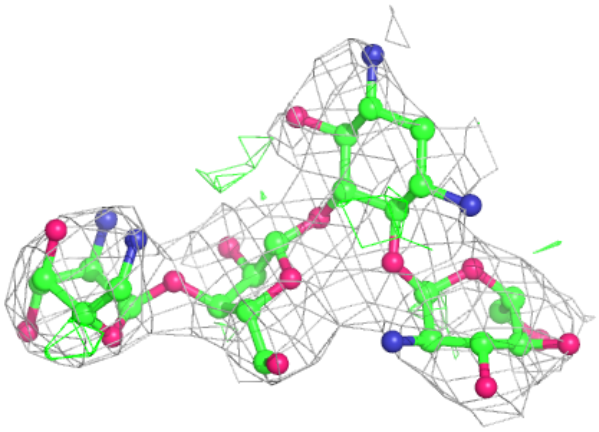


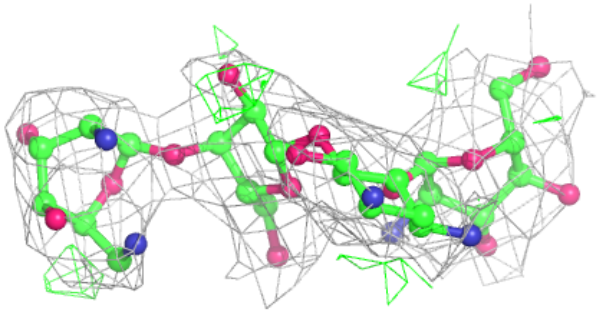


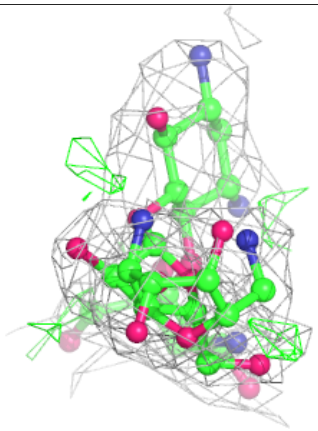


**Electron density around PAR 5 3406:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

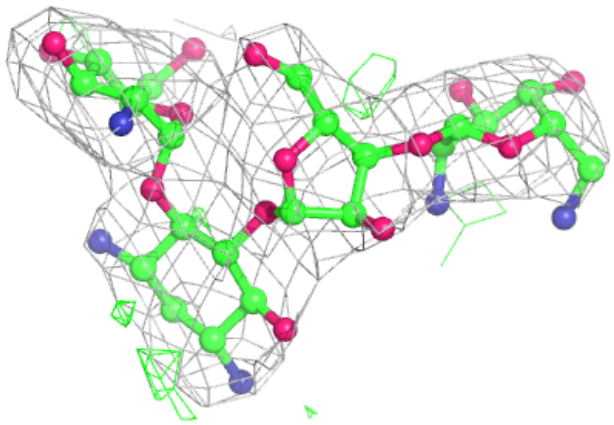


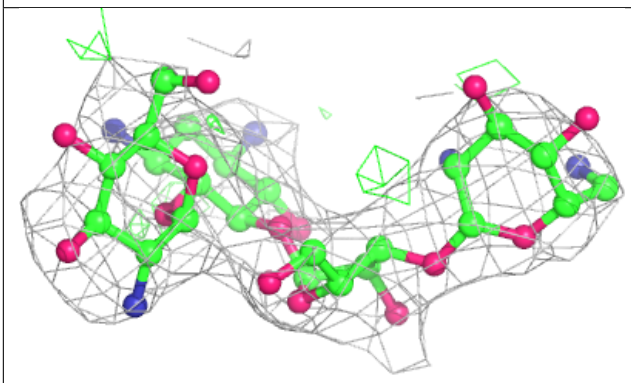


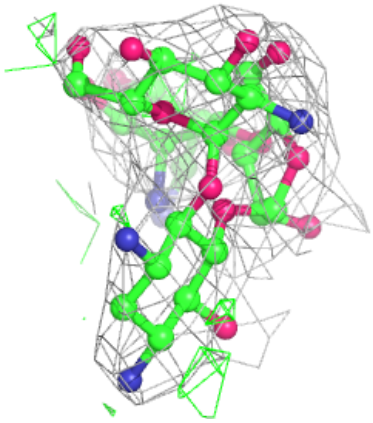


**Electron density around PAR 5 3408:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

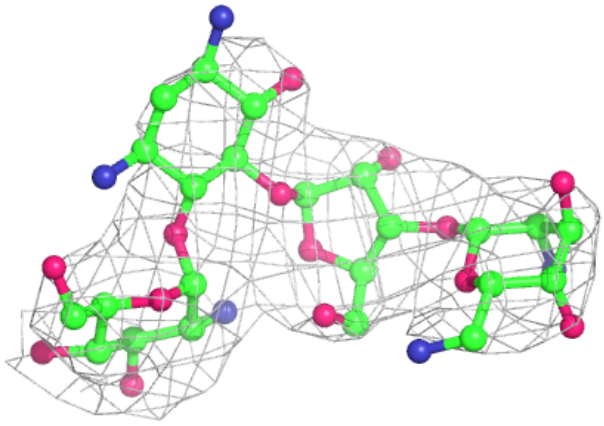


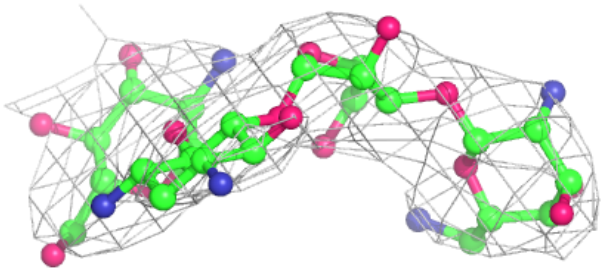


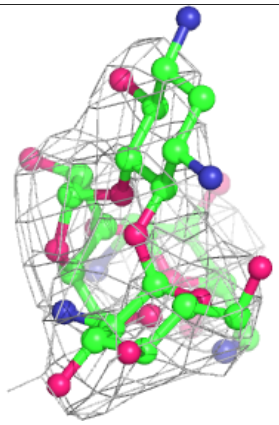


**Electron density around PAR 5 3410:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

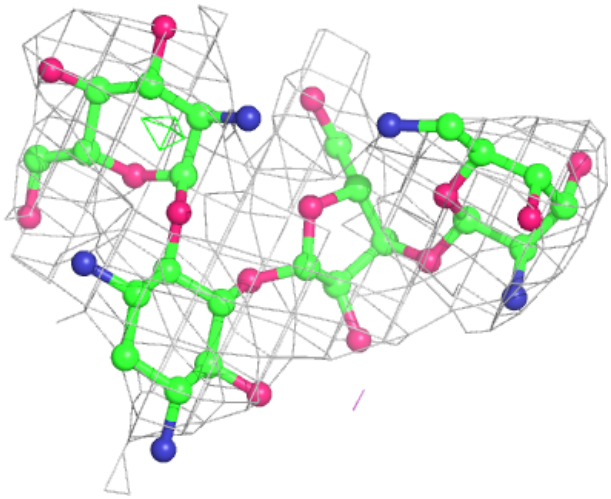


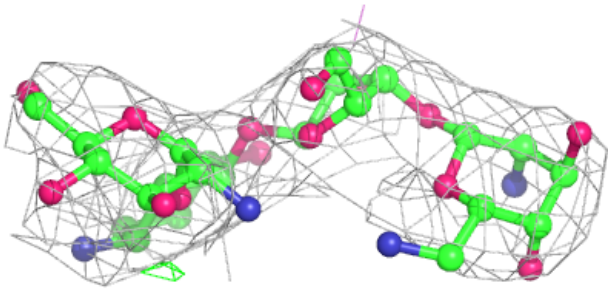


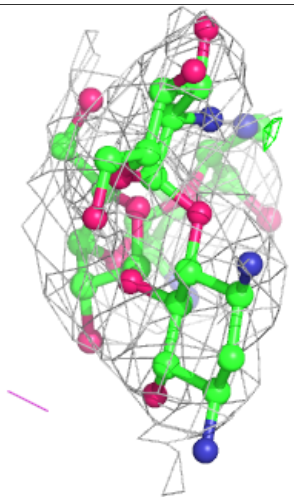


**Electron density around PAR 1 3424:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

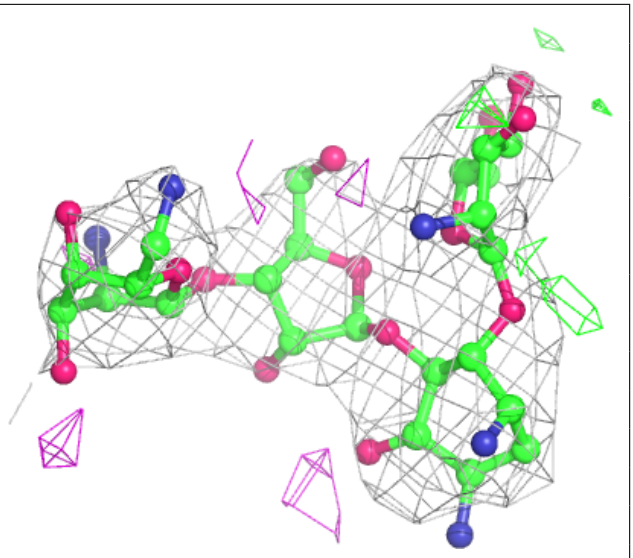


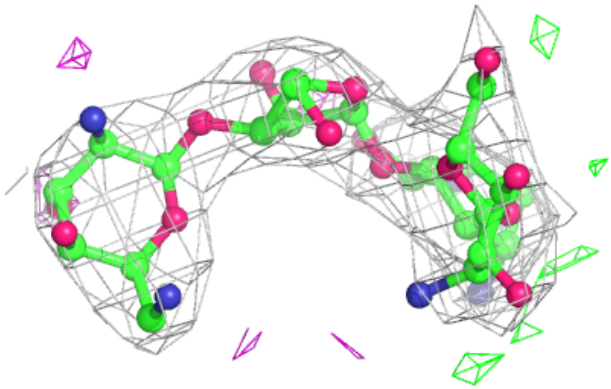


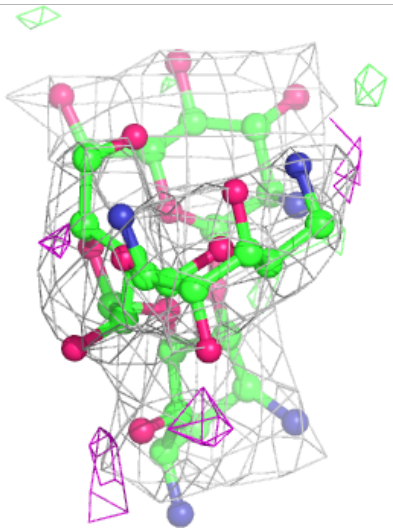


**Electron density around PAR 1 3409:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

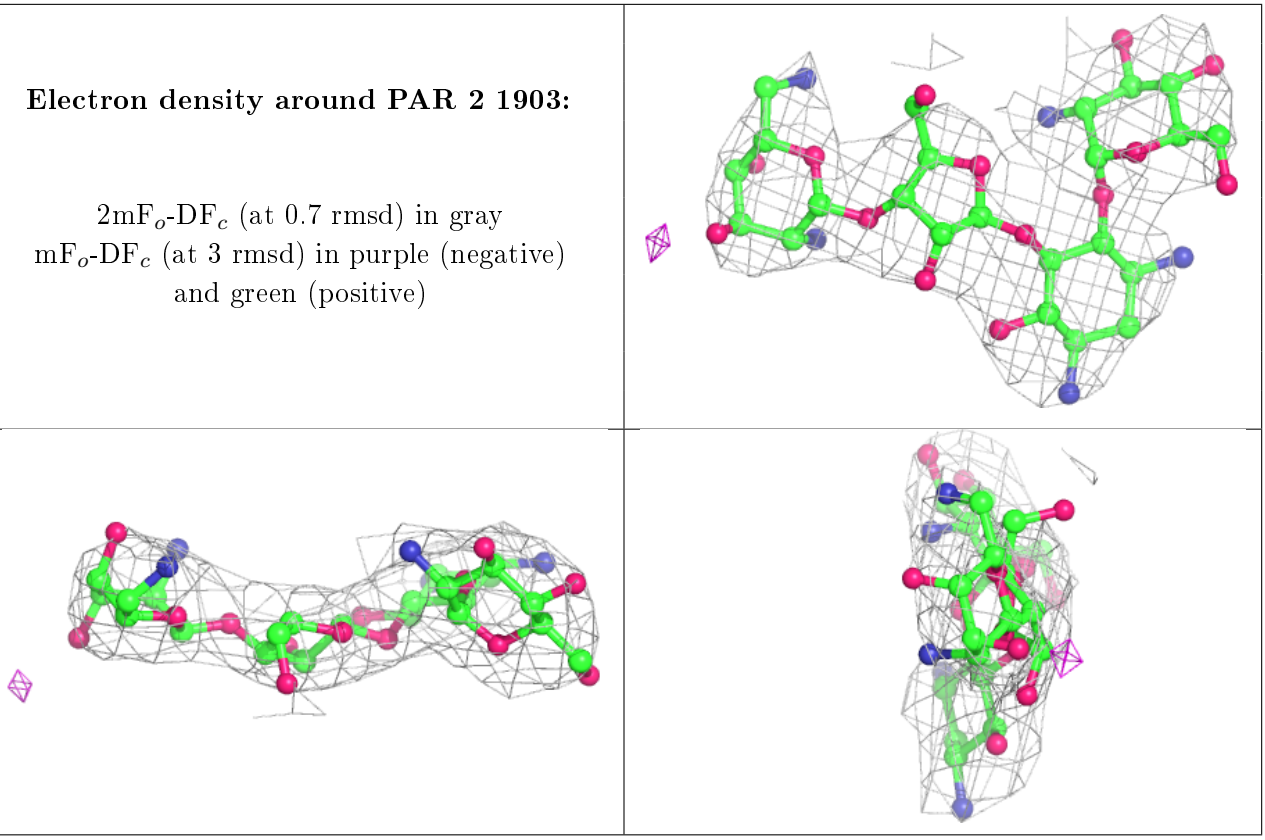






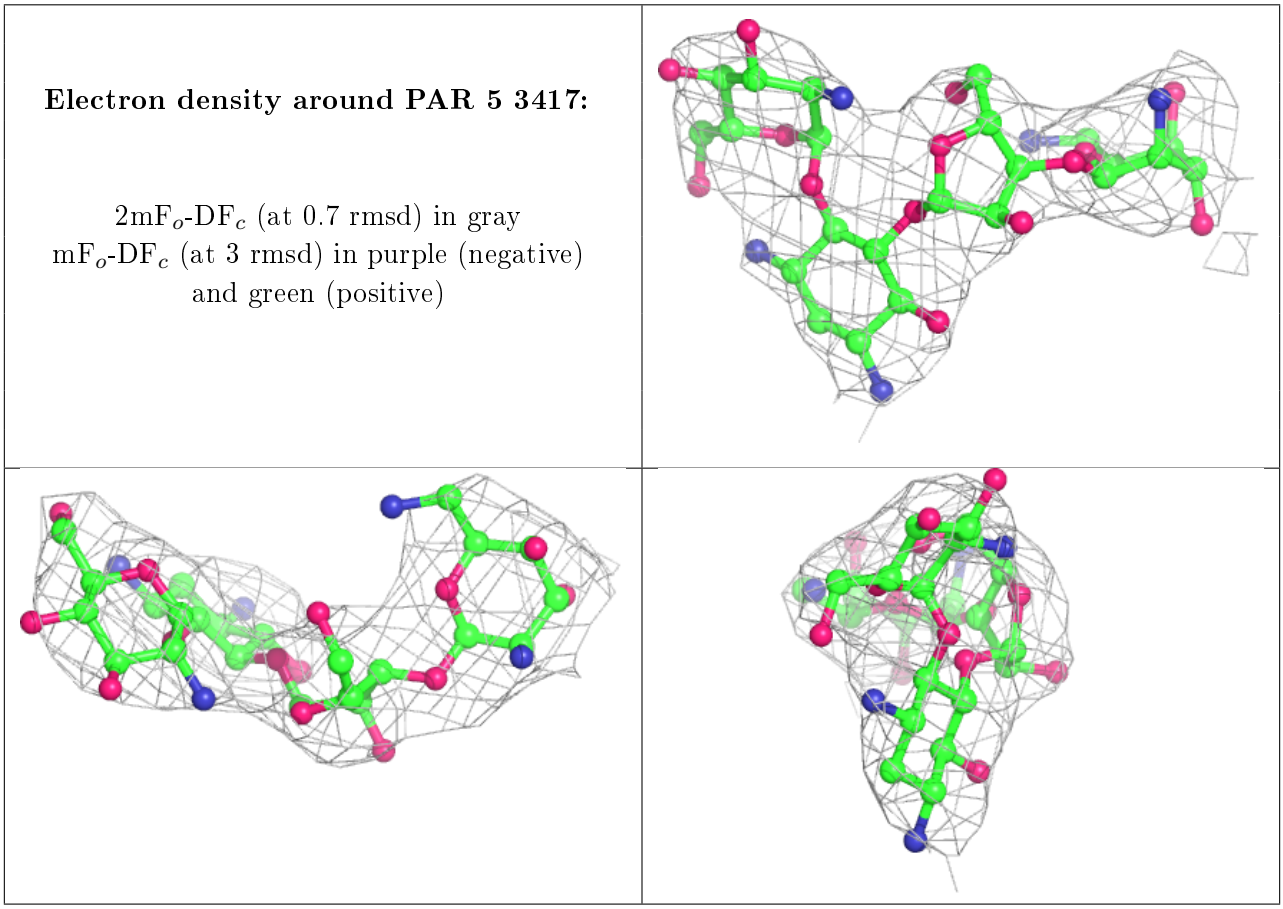
**Electron density around PAR 2 1903:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



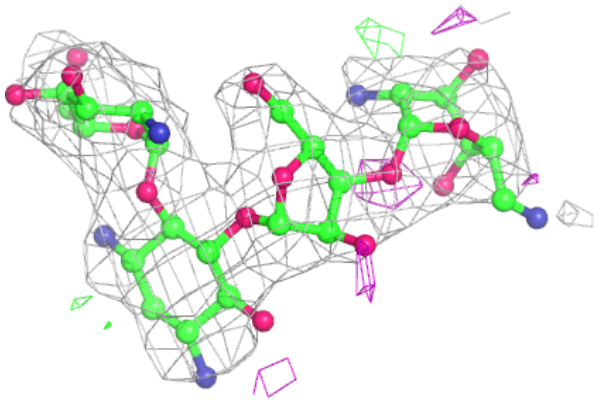
**Electron density around PAR 5 3417:**

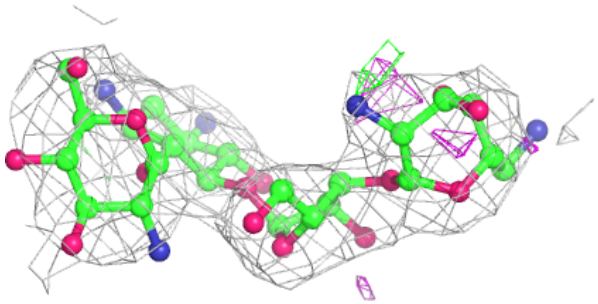
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

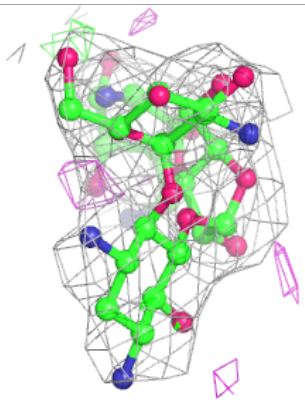


**Electron density around PAR 1 3411:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

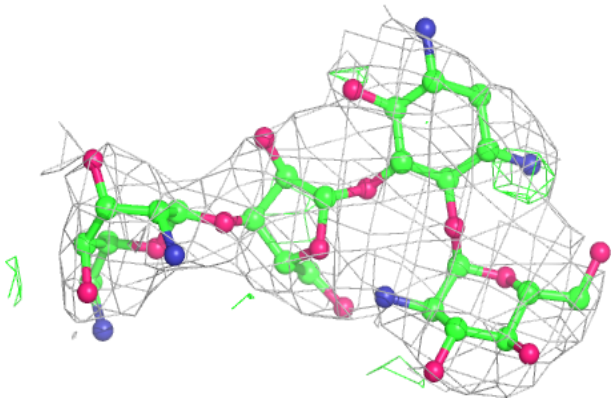


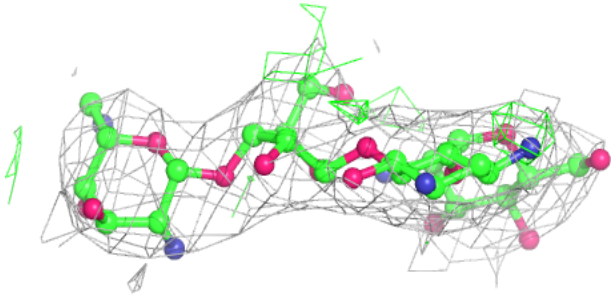


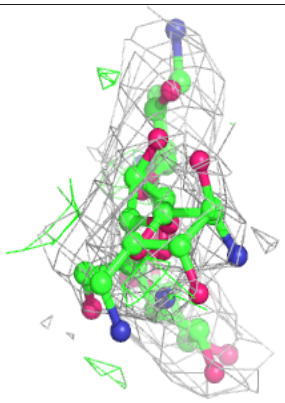


**Electron density around PAR 1 3421:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

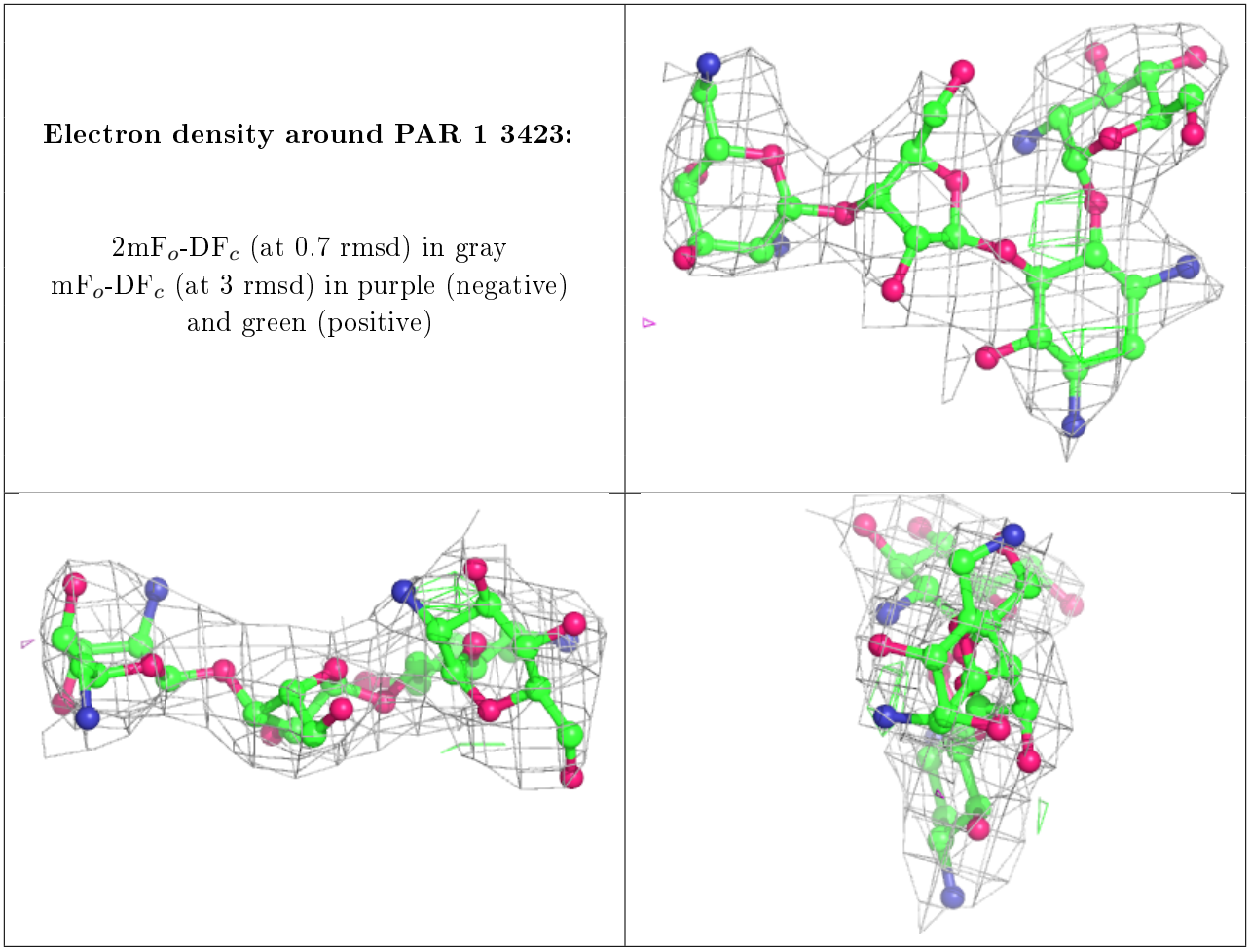






**Electron density around PAR 1 3423:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.