Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:22 PM EDT

PDB ID	:	5LYB
Title	:	Crystal structure of the S.cerevisiae 80S ribosome in complex with the A-site bound aminoacyl-tRNA analog ACCPmn
Authors	:	Melnikov, S.; Mailliot, J.
Deposited on	:	2016-09-26
Resolution	:	3.25 Å(reported)

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

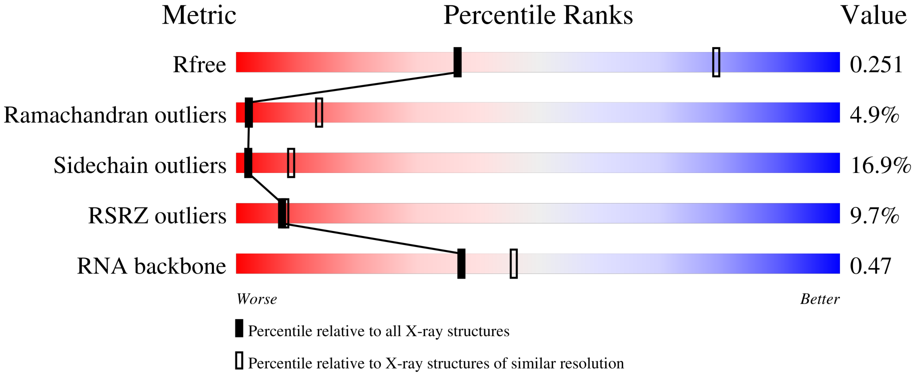
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

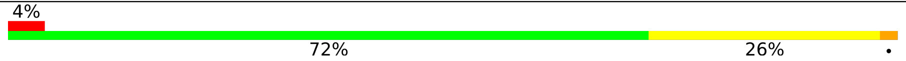
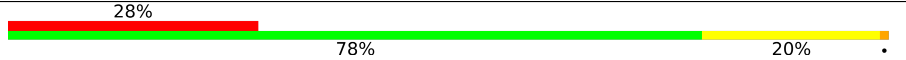
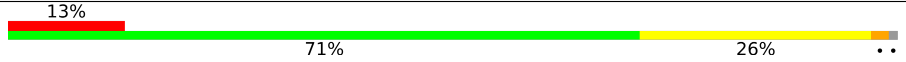
The reported resolution of this entry is 3.25 Å.

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	1191 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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 of 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	2	1800	
1	6	1800	
2	S0	206	
2	s0	206	
3	S1	216	

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Mol	Chain	Length	Quality of chain
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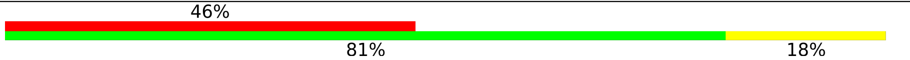
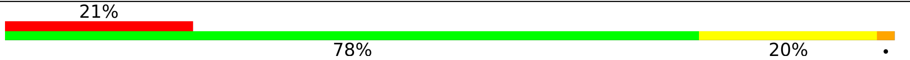
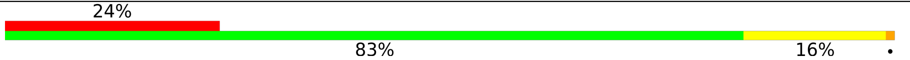
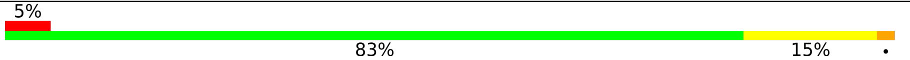
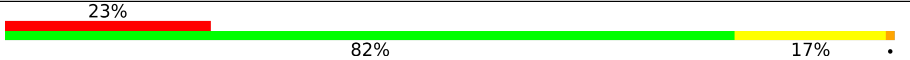
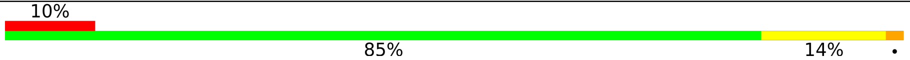
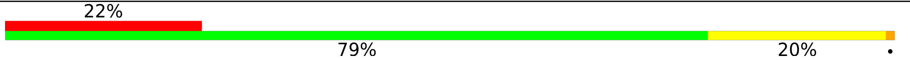
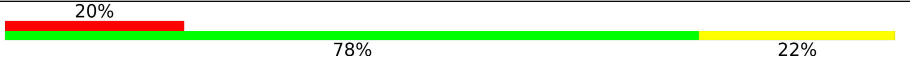
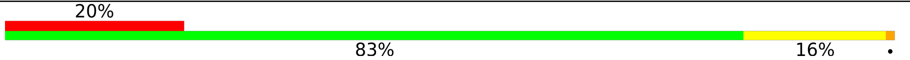
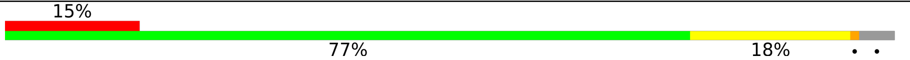
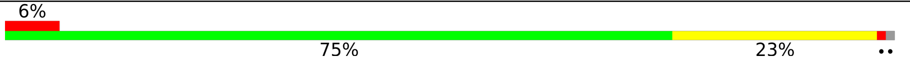
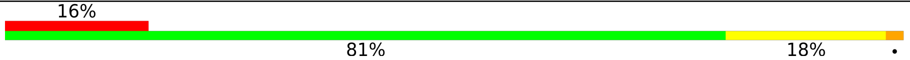
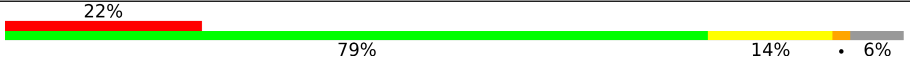
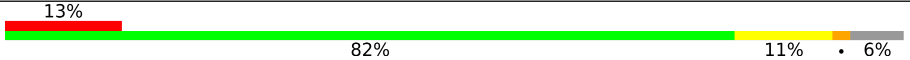
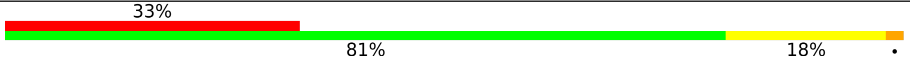
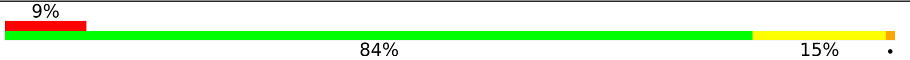
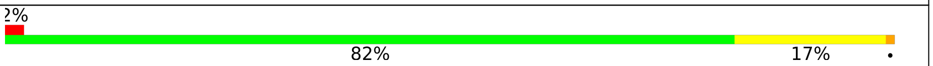
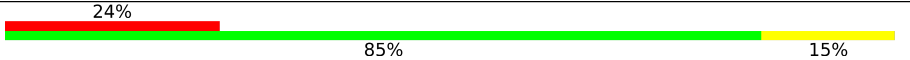
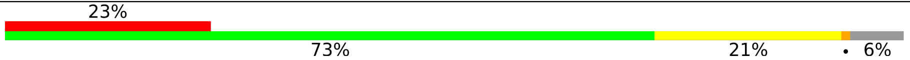
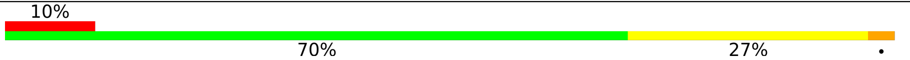
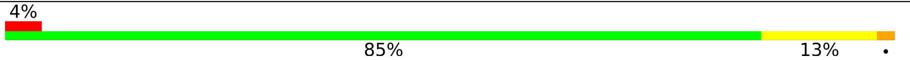
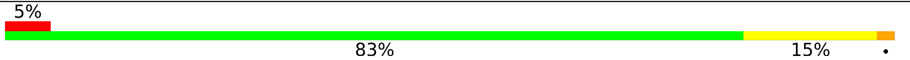
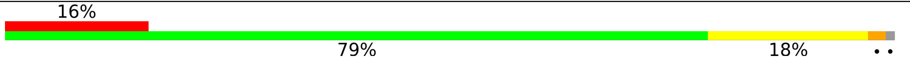
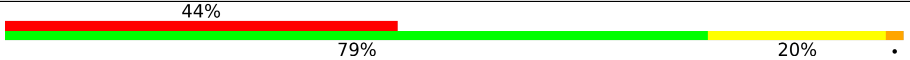
4	S2	217	
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	199	
10	s8	199	
11	S9	185	
11	s9	185	
12	C0	96	
13	C1	155	
13	c1	155	
14	C2	124	
15	C3	150	
15	c3	150	
16	C4	128	
16	c4	128	

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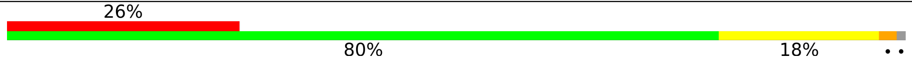
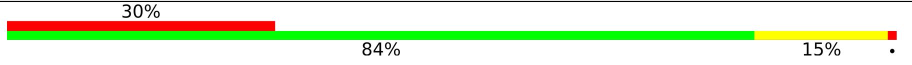
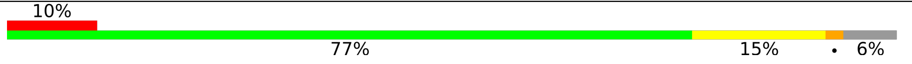
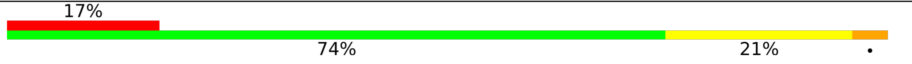
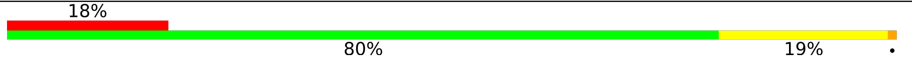
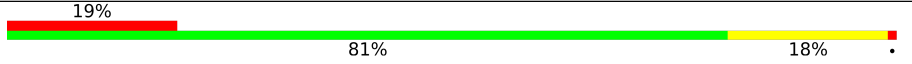
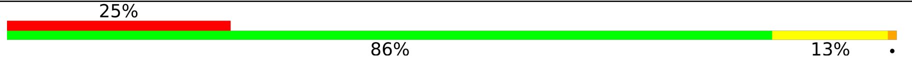
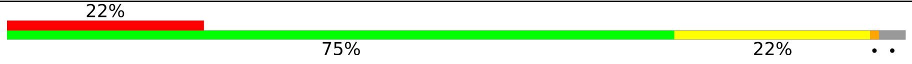
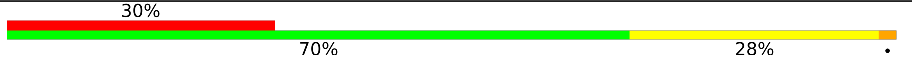
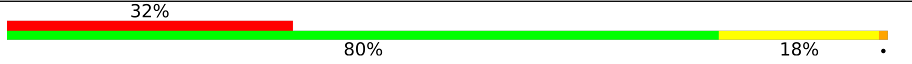
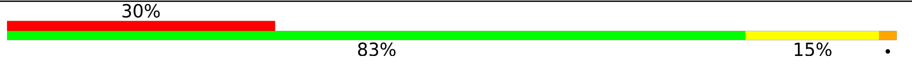
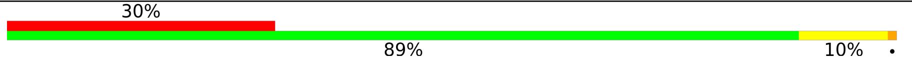
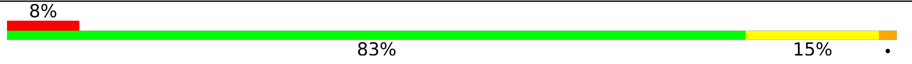
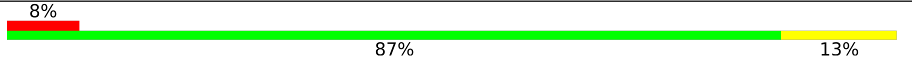
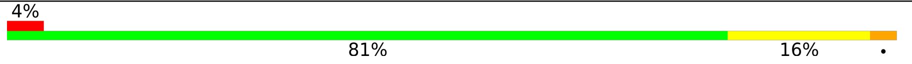
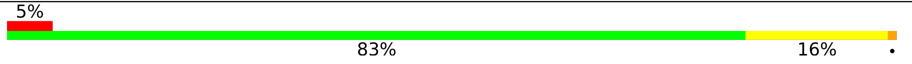
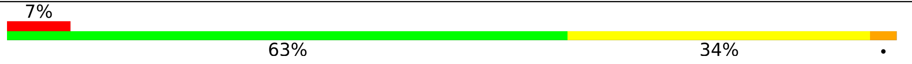
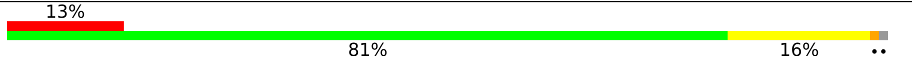
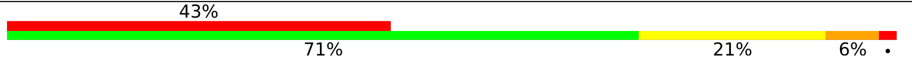
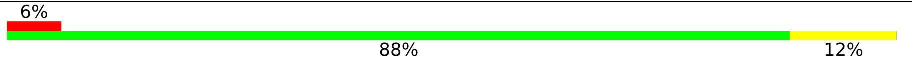
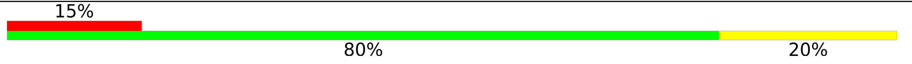
Mol	Chain	Length	Quality of chain
17	C5	131	
18	C6	142	
18	c6	142	
19	C7	125	
19	c7	125	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	110	
22	d0	110	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	70	
27	d5	70	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	

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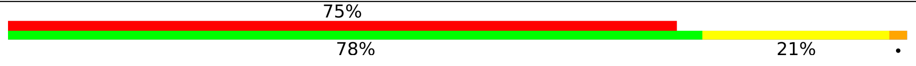
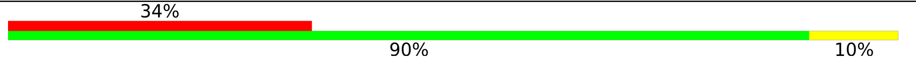
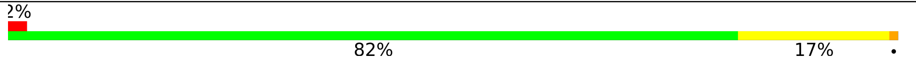
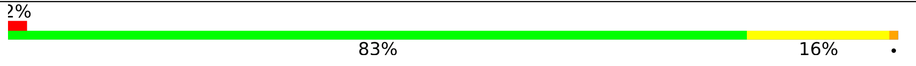
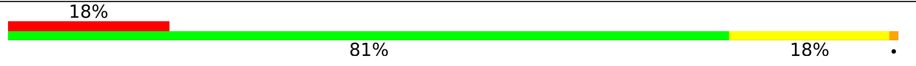
Mol	Chain	Length	Quality of chain
30	D8	63	 44% 78% 22%
30	d8	63	 75% 78% 21% •
31	D9	53	 4% 75% 23% •
31	d9	53	 8% 77% 23%
32	E0	62	 19% 84% 10% • •
32	e0	62	 2% 73% 23% 5%
33	E1	76	 20% 59% 29% 5% 7%
33	e1	76	 41% 61% 32% • •
34	SR	318	 34% 90% 10%
35	SM	159	 21% 84% 14% •
36	1	3394	 2% 67% 23% • 7%
36	5	3394	 % 66% 23% • 7%
37	3	121	 83% 16% •
37	7	121	 % 81% 17% •
38	4	158	 % 68% 30% •
38	8	158	 % 73% 25% •
39	L2	252	 5% 86% 13% •
39	l2	252	 2% 83% 15% •
40	L3	386	 2% 82% 17% •
40	l3	386	 2% 83% 16% •
41	L4	361	 82% 17%
41	l4	361	 3% 81% 17% •
42	L5	296	 18% 81% 18% •
42	l5	296	 2% 83% 15% ••
43	L6	175	 % 78% 10% • 11%

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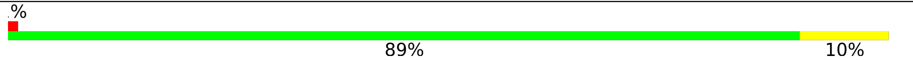
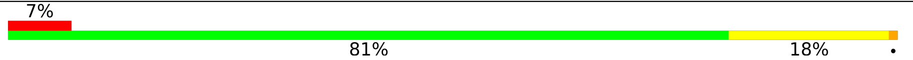
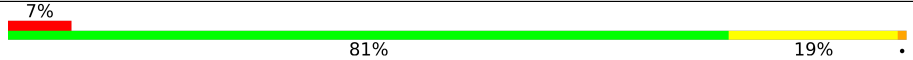
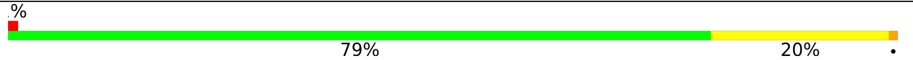
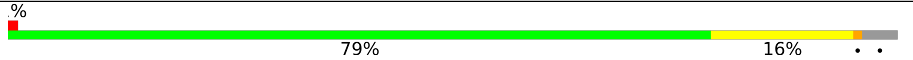
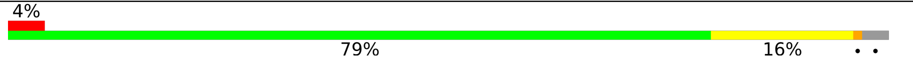
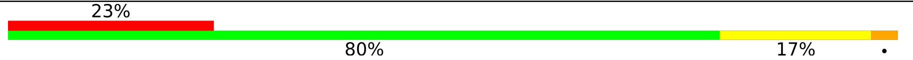
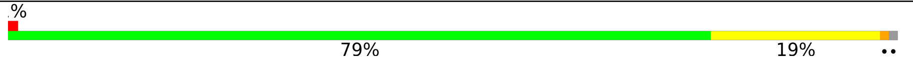
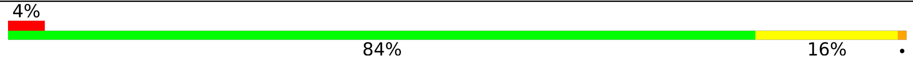
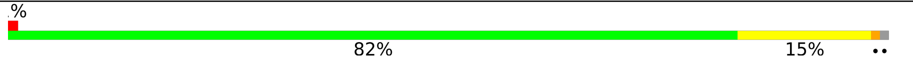
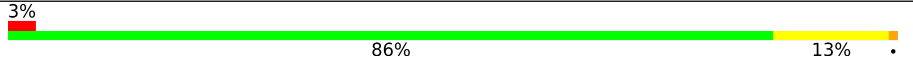
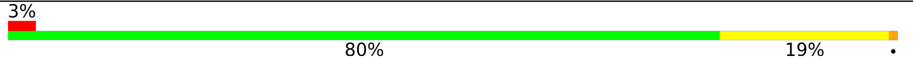
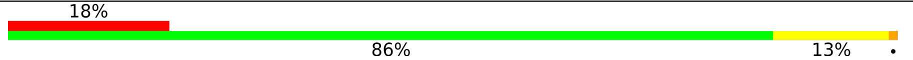
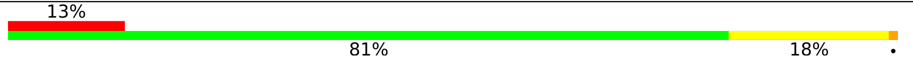
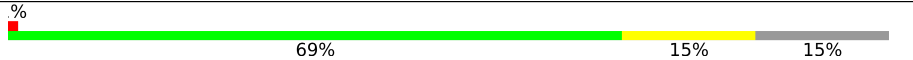
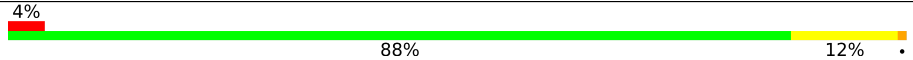
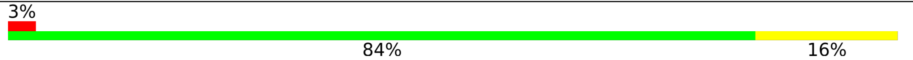
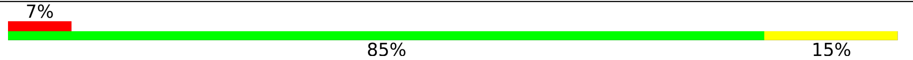
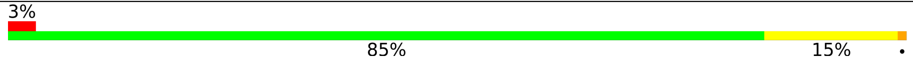
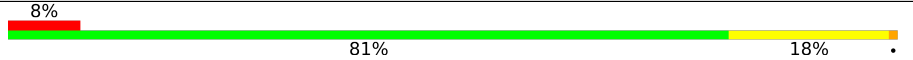
Mol	Chain	Length	Quality of chain
43	l6	175	
44	L7	223	
44	l7	223	
45	L8	233	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	

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Mol	Chain	Length	Quality of chain
56	n0	172	% 83% 17%
57	N1	159	4% 80% 19% •
57	n1	159	4% 81% 18% •
58	N2	100	12% 86% 14%
58	n2	100	7% 82% 16% •
59	N3	136	2% 85% 15%
59	n3	136	2% 91% 8% •
60	N4	98	35% 87% 13%
61	N5	121	10% 81% 18% •
61	n5	121	12% 79% 18% • •
62	N6	126	3% 75% 24% •
62	n6	126	75% 24% •
63	N7	135	10% 81% 16% •
63	n7	135	5% 76% 21% •
64	N8	148	7% 81% 18% •
64	n8	148	5% 84% 16%
65	N9	58	26% 81% 16% •
65	n9	58	9% 72% 22% 5%
66	O0	100	2% 83% 14% •
66	o0	100	5% 84% 16%
67	O1	109	13% 84% 14% •
67	o1	109	7% 80% 20%
68	O2	127	2% 89% 11%
68	o2	127	84% 15% •
69	O3	106	89% 10% •

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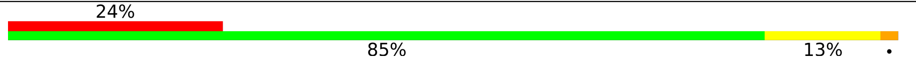
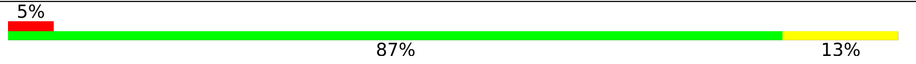
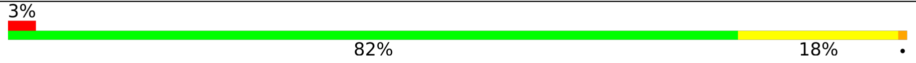
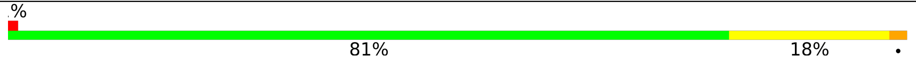
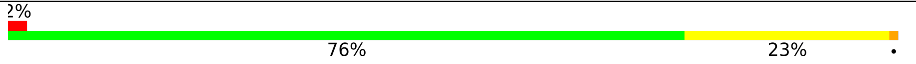
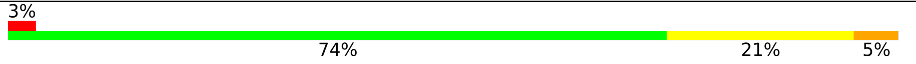
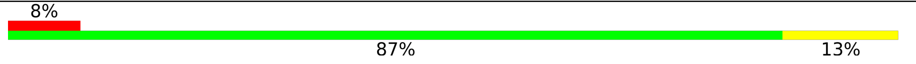
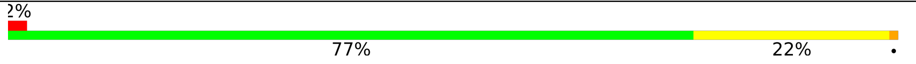
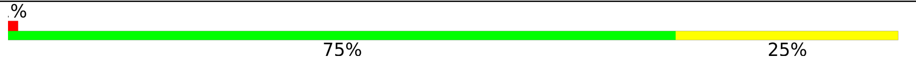
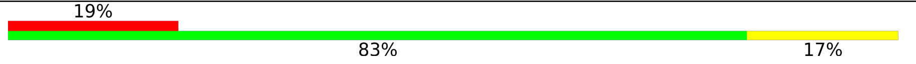
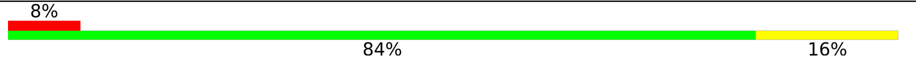
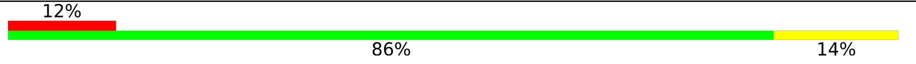
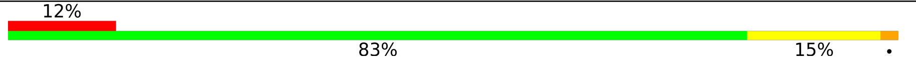
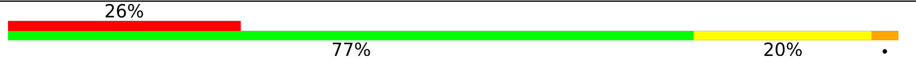
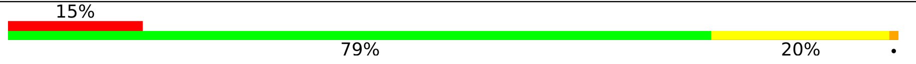
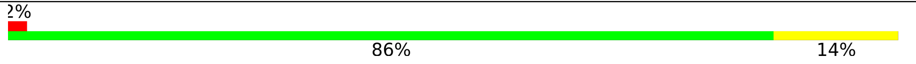
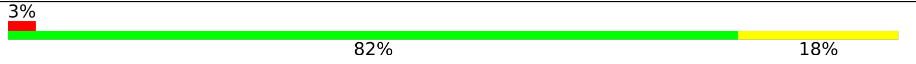
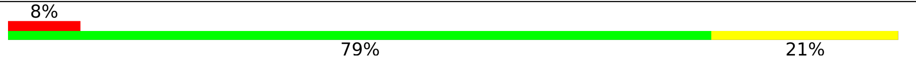
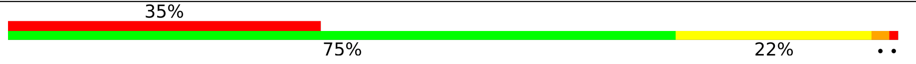
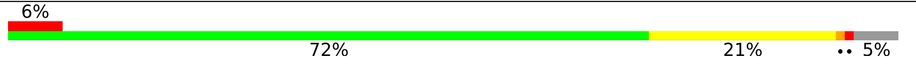
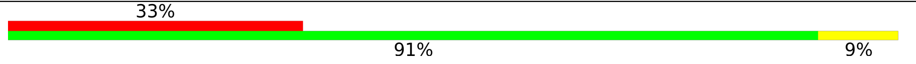
Mol	Chain	Length	Quality of chain
69	o3	106	
70	O4	112	
70	o4	112	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	c0	96	
81	c2	124	
82	c5	142	
83	sR	318	

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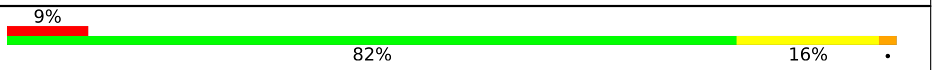
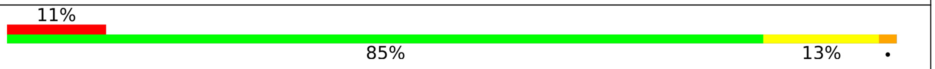
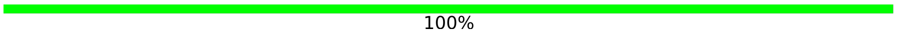
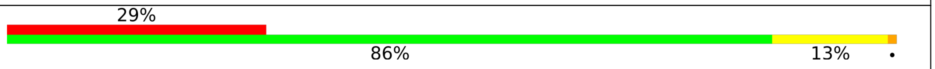
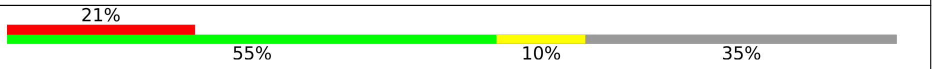
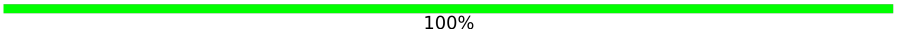
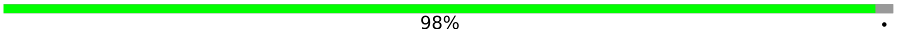
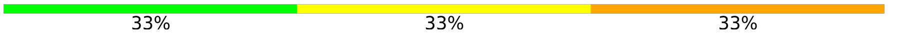
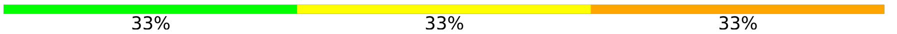
Mol	Chain	Length	Quality of chain
84	sM	104	
85	l8	231	
86	m2	150	
87	n4	135	
88	p0	219	
89	p1	47	
89	p2	47	
90	A	3	
90	a	3	

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
91	MG	1	3421	-	-	-	X
91	MG	1	3472	-	-	-	X
91	MG	1	3480	-	-	-	X
91	MG	1	3484	-	-	-	X
91	MG	1	3503	-	-	-	X
91	MG	1	3510	-	-	-	X
91	MG	1	3512	-	-	-	X
91	MG	1	3557	-	-	-	X
91	MG	1	3569	-	-	-	X
91	MG	1	3575	-	-	-	X
91	MG	1	3602	-	-	-	X
91	MG	1	3637	-	-	-	X
91	MG	1	3640	-	-	-	X
91	MG	1	3641	-	-	-	X
91	MG	1	3644	-	-	-	X
91	MG	1	3648	-	-	-	X
91	MG	1	3665	-	-	-	X
91	MG	1	3668	-	-	-	X
91	MG	1	3671	-	-	-	X
91	MG	1	3680	-	-	-	X
91	MG	1	3685	-	-	-	X
91	MG	1	3693	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	1	3697	-	-	-	X
91	MG	1	3710	-	-	-	X
91	MG	1	3712	-	-	-	X
91	MG	1	3714	-	-	-	X
91	MG	1	3715	-	-	-	X
91	MG	1	3719	-	-	-	X
91	MG	1	3721	-	-	-	X
91	MG	1	3723	-	-	-	X
91	MG	1	3734	-	-	-	X
91	MG	1	3741	-	-	-	X
91	MG	1	3748	-	-	-	X
91	MG	1	3749	-	-	-	X
91	MG	1	3760	-	-	-	X
91	MG	1	3766	-	-	-	X
91	MG	1	3768	-	-	-	X
91	MG	1	3772	-	-	-	X
91	MG	1	3776	-	-	-	X
91	MG	1	3779	-	-	-	X
91	MG	1	3785	-	-	-	X
91	MG	1	3788	-	-	-	X
91	MG	1	3791	-	-	-	X
91	MG	1	3808	-	-	-	X
91	MG	1	3822	-	-	-	X
91	MG	1	3838	-	-	-	X
91	MG	1	3844	-	-	-	X
91	MG	1	3850	-	-	-	X
91	MG	1	3857	-	-	-	X
91	MG	1	3860	-	-	-	X
91	MG	1	3868	-	-	-	X
91	MG	1	3869	-	-	-	X
91	MG	1	3872	-	-	-	X
91	MG	1	3875	-	-	-	X
91	MG	1	3876	-	-	-	X
91	MG	1	3882	-	-	-	X
91	MG	1	3889	-	-	-	X
91	MG	1	3895	-	-	-	X
91	MG	1	3903	-	-	-	X
91	MG	1	3922	-	-	-	X
91	MG	1	3930	-	-	-	X
91	MG	1	3939	-	-	-	X
91	MG	1	3943	-	-	-	X
91	MG	1	3947	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	1	3949	-	-	-	X
91	MG	1	3953	-	-	-	X
91	MG	1	3954	-	-	-	X
91	MG	1	3955	-	-	-	X
91	MG	1	3960	-	-	-	X
91	MG	1	3962	-	-	-	X
91	MG	1	3966	-	-	-	X
91	MG	1	3975	-	-	-	X
91	MG	1	3978	-	-	-	X
91	MG	1	3981	-	-	-	X
91	MG	1	3993	-	-	-	X
91	MG	1	3998	-	-	-	X
91	MG	1	4008	-	-	-	X
91	MG	1	4012	-	-	-	X
91	MG	1	4019	-	-	-	X
91	MG	1	4021	-	-	-	X
91	MG	1	4026	-	-	-	X
91	MG	1	4029	-	-	-	X
91	MG	1	4044	-	-	-	X
91	MG	1	4051	-	-	-	X
91	MG	1	4055	-	-	-	X
91	MG	1	4063	-	-	-	X
91	MG	1	4069	-	-	-	X
91	MG	1	4076	-	-	-	X
91	MG	1	4077	-	-	-	X
91	MG	1	4082	-	-	-	X
91	MG	1	4083	-	-	-	X
91	MG	1	4084	-	-	-	X
91	MG	1	4088	-	-	-	X
91	MG	1	4094	-	-	-	X
91	MG	1	4098	-	-	-	X
91	MG	2	1912	-	-	-	X
91	MG	2	1918	-	-	-	X
91	MG	2	1920	-	-	-	X
91	MG	2	1927	-	-	-	X
91	MG	2	1945	-	-	-	X
91	MG	2	1946	-	-	-	X
91	MG	2	1947	-	-	-	X
91	MG	2	1955	-	-	-	X
91	MG	2	1958	-	-	-	X
91	MG	2	1964	-	-	-	X
91	MG	2	1966	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	2	1972	-	-	-	X
91	MG	2	1981	-	-	-	X
91	MG	2	1992	-	-	-	X
91	MG	2	1993	-	-	-	X
91	MG	2	1999	-	-	-	X
91	MG	2	2002	-	-	-	X
91	MG	2	2005	-	-	-	X
91	MG	2	2007	-	-	-	X
91	MG	2	2009	-	-	-	X
91	MG	2	2013	-	-	-	X
91	MG	2	2014	-	-	-	X
91	MG	2	2016	-	-	-	X
91	MG	2	2023	-	-	-	X
91	MG	2	2024	-	-	-	X
91	MG	2	2025	-	-	-	X
91	MG	2	2026	-	-	-	X
91	MG	2	2029	-	-	-	X
91	MG	2	2035	-	-	-	X
91	MG	2	2038	-	-	-	X
91	MG	2	2047	-	-	-	X
91	MG	2	2053	-	-	-	X
91	MG	2	2055	-	-	-	X
91	MG	2	2057	-	-	-	X
91	MG	2	2059	-	-	-	X
91	MG	3	217	-	-	-	X
91	MG	4	227	-	-	-	X
91	MG	4	229	-	-	-	X
91	MG	5	3418	-	-	-	X
91	MG	5	3440	-	-	-	X
91	MG	5	3452	-	-	-	X
91	MG	5	3476	-	-	-	X
91	MG	5	3532	-	-	-	X
91	MG	5	3567	-	-	-	X
91	MG	5	3621	-	-	-	X
91	MG	5	3635	-	-	-	X
91	MG	5	3650	-	-	-	X
91	MG	5	3653	-	-	-	X
91	MG	5	3664	-	-	-	X
91	MG	5	3668	-	-	-	X
91	MG	5	3669	-	-	-	X
91	MG	5	3676	-	-	-	X
91	MG	5	3678	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	3681	-	-	-	X
91	MG	5	3688	-	-	-	X
91	MG	5	3690	-	-	-	X
91	MG	5	3703	-	-	-	X
91	MG	5	3715	-	-	-	X
91	MG	5	3718	-	-	-	X
91	MG	5	3719	-	-	-	X
91	MG	5	3730	-	-	-	X
91	MG	5	3744	-	-	-	X
91	MG	5	3747	-	-	-	X
91	MG	5	3752	-	-	-	X
91	MG	5	3760	-	-	-	X
91	MG	5	3767	-	-	-	X
91	MG	5	3768	-	-	-	X
91	MG	5	3779	-	-	-	X
91	MG	5	3784	-	-	-	X
91	MG	5	3788	-	-	-	X
91	MG	5	3798	-	-	-	X
91	MG	5	3803	-	-	-	X
91	MG	5	3804	-	-	-	X
91	MG	5	3806	-	-	-	X
91	MG	5	3809	-	-	-	X
91	MG	5	3819	-	-	-	X
91	MG	5	3823	-	-	-	X
91	MG	5	3832	-	-	-	X
91	MG	5	3834	-	-	-	X
91	MG	5	3840	-	-	-	X
91	MG	5	3842	-	-	-	X
91	MG	5	3846	-	-	-	X
91	MG	5	3861	-	-	-	X
91	MG	5	3863	-	-	-	X
91	MG	5	3870	-	-	-	X
91	MG	5	3875	-	-	-	X
91	MG	5	3881	-	-	-	X
91	MG	5	3891	-	-	-	X
91	MG	5	3898	-	-	-	X
91	MG	5	3904	-	-	-	X
91	MG	5	3909	-	-	-	X
91	MG	5	3917	-	-	-	X
91	MG	5	3920	-	-	-	X
91	MG	5	3927	-	-	-	X
91	MG	5	3931	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	3932	-	-	-	X
91	MG	5	3936	-	-	-	X
91	MG	5	3944	-	-	-	X
91	MG	5	3948	-	-	-	X
91	MG	5	3964	-	-	-	X
91	MG	5	3965	-	-	-	X
91	MG	5	3966	-	-	-	X
91	MG	5	3969	-	-	-	X
91	MG	5	3970	-	-	-	X
91	MG	5	3971	-	-	-	X
91	MG	5	3977	-	-	-	X
91	MG	5	3982	-	-	-	X
91	MG	5	3983	-	-	-	X
91	MG	5	3989	-	-	-	X
91	MG	5	3992	-	-	-	X
91	MG	5	4003	-	-	-	X
91	MG	5	4004	-	-	-	X
91	MG	5	4007	-	-	-	X
91	MG	5	4014	-	-	-	X
91	MG	5	4029	-	-	-	X
91	MG	5	4030	-	-	-	X
91	MG	5	4033	-	-	-	X
91	MG	5	4047	-	-	-	X
91	MG	5	4051	-	-	-	X
91	MG	5	4054	-	-	-	X
91	MG	5	4061	-	-	-	X
91	MG	5	4062	-	-	-	X
91	MG	5	4063	-	-	-	X
91	MG	5	4064	-	-	-	X
91	MG	5	4068	-	-	-	X
91	MG	5	4086	-	-	-	X
91	MG	5	4088	-	-	-	X
91	MG	5	4093	-	-	-	X
91	MG	5	4097	-	-	-	X
91	MG	5	4100	-	-	-	X
91	MG	5	4102	-	-	-	X
91	MG	5	4103	-	-	-	X
91	MG	5	4105	-	-	-	X
91	MG	5	4106	-	-	-	X
91	MG	5	4120	-	-	-	X
91	MG	5	4135	-	-	-	X
91	MG	5	4138	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	4140	-	-	-	X
91	MG	5	4142	-	-	-	X
91	MG	5	4150	-	-	-	X
91	MG	5	4151	-	-	-	X
91	MG	5	4154	-	-	-	X
91	MG	5	4155	-	-	-	X
91	MG	6	1909	-	-	-	X
91	MG	6	1915	-	-	-	X
91	MG	6	1917	-	-	-	X
91	MG	6	1926	-	-	-	X
91	MG	6	1934	-	-	-	X
91	MG	6	1970	-	-	-	X
91	MG	6	1972	-	-	-	X
91	MG	6	1974	-	-	-	X
91	MG	6	1984	-	-	-	X
91	MG	6	1995	-	-	-	X
91	MG	6	1997	-	-	-	X
91	MG	6	2001	-	-	-	X
91	MG	6	2003	-	-	-	X
91	MG	6	2020	-	-	-	X
91	MG	6	2026	-	-	-	X
91	MG	6	2027	-	-	-	X
91	MG	6	2036	-	-	-	X
91	MG	6	2043	-	-	-	X
91	MG	6	2044	-	-	-	X
91	MG	6	2057	-	-	-	X
91	MG	6	2058	-	-	-	X
91	MG	6	2065	-	-	-	X
91	MG	6	2068	-	-	-	X
91	MG	6	2069	-	-	-	X
91	MG	6	2079	-	-	-	X
91	MG	6	2083	-	-	-	X
91	MG	6	2086	-	-	-	X
91	MG	6	2087	-	-	-	X
91	MG	6	2088	-	-	-	X
91	MG	6	2096	-	-	-	X
91	MG	6	2099	-	-	-	X
91	MG	6	2107	-	-	-	X
91	MG	6	2110	-	-	-	X
91	MG	6	2111	-	-	-	X
91	MG	6	2114	-	-	-	X
91	MG	6	2119	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	6	2131	-	-	-	X
91	MG	6	2132	-	-	-	X
91	MG	6	2137	-	-	-	X
91	MG	6	2139	-	-	-	X
91	MG	6	2140	-	-	-	X
91	MG	6	2341	-	-	-	X
91	MG	7	209	-	-	-	X
91	MG	7	222	-	-	-	X
91	MG	7	225	-	-	-	X
91	MG	8	216	-	-	-	X
91	MG	C5	201	-	-	-	X
91	MG	D0	201	-	-	-	X
91	MG	D3	201	-	-	-	X
91	MG	L3	401	-	-	-	X
91	MG	L4	406	-	-	-	X
91	MG	M5	306	-	-	-	X
91	MG	M5	308	-	-	-	X
91	MG	M7	205	-	-	-	X
91	MG	N3	204	-	-	-	X
91	MG	O2	201	-	-	-	X
91	MG	O2	202	-	-	-	X
91	MG	O3	202	-	-	-	X
91	MG	S4	301	-	-	-	X
91	MG	c6	201	-	-	-	X
91	MG	c6	202	-	-	-	X
91	MG	c6	203	-	-	-	X
91	MG	d2	201	-	-	-	X
91	MG	l2	304	-	-	-	X
91	MG	l3	404	-	-	-	X
91	MG	l4	401	-	-	-	X
91	MG	l4	402	-	-	-	X
91	MG	l5	306	-	-	-	X
91	MG	l7	304	-	-	-	X
91	MG	l8	301	-	-	-	X
91	MG	l9	202	-	-	-	X
91	MG	l9	203	-	-	-	X
91	MG	m6	204	-	-	-	X
91	MG	m7	206	-	-	-	X
91	MG	n3	203	-	-	-	X
91	MG	o3	203	-	-	-	X
91	MG	o3	204	-	-	-	X
91	MG	o3	205	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	q1	101	-	-	-	X
91	MG	s8	303	-	-	-	X
92	OHX	1	4423	-	-	-	X
92	OHX	1	4429	-	-	-	X
92	OHX	1	4434	-	-	-	X
92	OHX	1	4450	-	-	-	X
92	OHX	1	4463	-	-	-	X
92	OHX	1	4477	-	-	-	X
92	OHX	1	4485	-	-	-	X
92	OHX	2	2197	-	-	-	X
92	OHX	2	2231	-	-	-	X
92	OHX	2	2246	-	-	-	X
92	OHX	5	4495	-	-	-	X
92	OHX	5	4513	-	-	-	X
92	OHX	5	4520	-	-	-	X
92	OHX	5	4528	-	-	-	X
92	OHX	5	4534	-	-	-	X
92	OHX	5	4536	-	-	-	X
92	OHX	5	4541	-	-	-	X
92	OHX	5	4549	-	-	-	X
92	OHX	5	4562	-	-	-	X
92	OHX	6	2305	-	-	-	X
92	OHX	6	2314	-	-	-	X
92	OHX	6	2322	-	-	-	X
92	OHX	6	2328	-	-	-	X
92	OHX	6	2336	-	-	-	X
92	OHX	7	239	-	-	-	X

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 414290 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 18S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total 37970	C 16975	N 6720	O 12493	P 1782	0	1	0
1	6	1795	Total 38260	C 17105	N 6763	O 12596	P 1796	0	1	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total 1577	C 1014	N 278	O 283	S 2	0	0	0
2	s0	206	Total 1583	C 1017	N 281	O 283	S 2	0	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total 1709	C 1084	N 310	O 311	S 4	0	0	0
3	s1	216	Total 1722	C 1091	N 312	O 315	S 4	0	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

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

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

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

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	s8	188	Total C N O S 1489 925 298 264 2	0	0	0

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	S9	185	Total C N O S 1494 943 289 261 1	0	0	0
11	s9	185	Total C N O S 1494 943 289 261 1	0	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	C0	96	Total C N O S 773 500 126 145 2	0	0	0

- Molecule 13 is a protein called 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	C1	155	Total C N O S 1214 775 230 206 3	0	0	0
13	c1	146	Total C N O S 1168 747 221 197 3	0	0	0

- Molecule 14 is a protein called 40S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	C2	124	Total C N O S 890 560 156 172 2	0	0	0

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called 40S Ribosomal Protein S14.

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

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
21	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total 855	C 539	N 156	O 159	S 1	0	0	0
22	d0	110	Total 882	C 554	N 161	O 166	S 1	0	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total 1121	C 708	N 220	O 191	S 2	0	0	0
25	d3	144	Total 1121	C 708	N 220	O 191	S 2	0	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total 442	C 274	N 92	O 72	S 4	0	0	0
31	d9	53	Total 442	C 274	N 92	O 72	S 4	0	0	0

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total 475	C 299	N 98	O 77	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	e0	62	491	309	101	80	1	0	0	0

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	E1	71	566	362	106	94	4	0	0	0
33	e1	76	608	388	117	99	4	0	0	0

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	SR	318	2437	1541	418	470	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	654	221	229	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	134	LEU	ASP	conflict	UNP P39015

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	1	3149	67355	30086	12142	21978	3149	0	0	0
36	5	3150	67376	30095	12145	21987	3149	0	0	0

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
37	3	121	2579	1152	461	845	121	0	0	0
37	7	121	2579	1152	461	845	121	0	0	0

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
38	4	158	3353	1500	586	1109	158	0	0	0
38	8	158	3353	1500	586	1109	158	0	0	0

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	L2	252	1914	1191	388	334	1	0	0	0
39	l2	252	1912	1190	388	333	1	0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3075	1950	584	533	8	0	0	0
40	l3	386	3075	1950	584	533	8	0	0	0

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	L4	361	2748	1729	522	494	3	0	0	0
41	l4	361	2748	1729	522	494	3	0	0	0

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	L5	296	2375	1501	414	458	2	0	0	0
42	l5	294	2359	1489	412	456	2	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	L7	222	1784	1151	324	308	1	0	0	0
44	l7	223	1791	1155	325	310	1	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	1804	1151	323	327	3	0	0	0

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	L9	191	1518	963	274	277	4	0	0	0
46	l9	191	1518	963	274	277	4	0	0	0

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	M0	211	1705	1083	322	294	6	0	0	0
47	m0	213	1722	1094	325	297	6	0	0	0

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

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

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	M7	183	Total 1420	C 882	N 281	O 257	0	0	0
53	m7	155	Total 1227	C 764	N 238	O 225	0	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	M9	188	Total 1521	C 935	N 326	O 260	0	0	0
55	m9	188	Total 1521	C 935	N 326	O 260	0	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total 796	C 516	N 131	O 149	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total 1173	C 749	N 231	O 190	S 3	0	0	0
64	n8	148	Total 1173	C 749	N 231	O 190	S 3	0	0	0

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total 462	C 289	N 100	O 73	0	0	0
65	n9	58	Total 462	C 289	N 100	O 73	0	0	0

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total 743	C 479	N 124	O 139	S 1	0	0	0
66	o0	100	Total 767	C 492	N 128	O 146	S 1	0	0	0

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total 876	C 556	N 167	O 152	S 1	0	0	0
67	o1	109	Total 883	C 559	N 167	O 156	S 1	0	0	0

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total 1020	C 647	N 205	O 167	S 1	0	0	0
68	o2	127	Total 1020	C 647	N 205	O 167	S 1	0	0	0

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

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

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

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	O4	112	880	545	179	152	4	0	0	0
70	o4	112	880	545	179	152	4	0	0	0

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
72	O6	99	771	481	156	132	2	0	0	0
72	o6	99	770	481	156	131	2	0	0	0

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
73	O7	87	681	414	148	114	5	0	0	0
73	o7	87	681	414	148	114	5	0	0	0

- Molecule 74 is a protein called 60S ribosomal protein L38.

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

- Molecule 75 is a protein called 60S ribosomal protein L39.

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

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 80 is a protein called 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	c0	96	762	491	125	144	2	0	0	0

- Molecule 81 is a protein called 40S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	c2	124	892	562	156	172	2	0	0	0

- Molecule 82 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
82	c5	135	1039	658	196	178	7	0	0	0

- Molecule 83 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
83	sR	318	2442	1544	418	472	8	0	0	0

- Molecule 84 is a protein called Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
84	sM	104	681	404	140	137	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
sM	59	ALA	GLY	conflict	UNP P39015

- Molecule 85 is a protein called 60S ribosomal protein L8-A,60S ribosomal protein L8-A,60S Ribosomal Protein L8.

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

- Molecule 86 is a protein called 60S Ribosomal Protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
86	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 87 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
87	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 88 is a protein called 60S acidic ribosomal protein P0,60S acidic ribosomal protein P0,60S Ribosomal Protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
88	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 89 is a protein called 60S Ribosomal Protein P1/2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
89	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			
89	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 90 is a RNA chain called aminoacyl-tRNA fragment ACCPmn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
90	A	3	Total	C	N	O	P	0	0	0
			77	40	13	21	3			
90	a	3	Total	C	N	O	P	0	0	0
			77	40	13	21	3			

- Molecule 91 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	2	169	Total	Mg	0	0
			169	169		
91	S1	1	Total	Mg	0	0
			1	1		
91	S2	2	Total	Mg	0	0
			2	2		
91	S4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	S6	1	Total Mg 1 1	0	0
91	S8	2	Total Mg 2 2	0	0
91	C1	2	Total Mg 2 2	0	0
91	C5	1	Total Mg 1 1	0	0
91	C8	1	Total Mg 1 1	0	0
91	D0	1	Total Mg 1 1	0	0
91	D3	1	Total Mg 1 1	0	0
91	D6	1	Total Mg 1 1	0	0
91	D9	2	Total Mg 2 2	0	0
91	E1	1	Total Mg 1 1	0	0
91	1	700	Total Mg 700 700	1	0
91	3	18	Total Mg 18 18	0	0
91	4	32	Total Mg 32 32	0	0
91	L2	4	Total Mg 4 4	0	0
91	L3	6	Total Mg 6 6	0	0
91	L4	7	Total Mg 7 7	0	0
91	L6	1	Total Mg 1 1	0	0
91	L7	1	Total Mg 1 1	0	0
91	L8	1	Total Mg 1 1	0	0
91	M0	4	Total Mg 4 4	0	0
91	M1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	M3	4	Total Mg 4 4	0	0
91	M4	1	Total Mg 1 1	0	0
91	M5	8	Total Mg 8 8	0	0
91	M6	4	Total Mg 4 4	0	0
91	M7	8	Total Mg 8 8	0	0
91	M8	3	Total Mg 3 3	0	0
91	M9	3	Total Mg 3 3	0	0
91	N0	2	Total Mg 2 2	0	0
91	N1	1	Total Mg 1 1	0	0
91	N3	4	Total Mg 4 4	0	0
91	N6	1	Total Mg 1 1	0	0
91	N8	7	Total Mg 7 7	0	0
91	N9	1	Total Mg 1 1	0	0
91	O1	1	Total Mg 1 1	0	0
91	O2	2	Total Mg 2 2	0	0
91	O3	3	Total Mg 3 3	0	0
91	O4	1	Total Mg 1 1	0	0
91	O7	5	Total Mg 5 5	0	0
91	O9	1	Total Mg 1 1	0	0
91	Q0	2	Total Mg 2 2	0	0
91	Q2	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	6	242	Total Mg 242 242	0	0
91	s1	1	Total Mg 1 1	0	0
91	s4	1	Total Mg 1 1	0	0
91	s8	4	Total Mg 4 4	0	0
91	c6	3	Total Mg 3 3	0	0
91	c8	3	Total Mg 3 3	0	0
91	c9	1	Total Mg 1 1	0	0
91	d2	1	Total Mg 1 1	0	0
91	d3	1	Total Mg 1 1	0	0
91	d5	1	Total Mg 1 1	0	0
91	d6	1	Total Mg 1 1	0	0
91	d9	2	Total Mg 2 2	0	0
91	sM	1	Total Mg 1 1	0	0
91	5	758	Total Mg 758 758	0	0
91	7	27	Total Mg 27 27	0	0
91	8	21	Total Mg 21 21	0	0
91	l2	5	Total Mg 5 5	0	0
91	l3	11	Total Mg 11 11	0	0
91	l4	3	Total Mg 3 3	0	0
91	l5	7	Total Mg 7 7	0	0
91	l7	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	l8	1	Total Mg 1 1	0	0
91	l9	3	Total Mg 3 3	0	0
91	m0	1	Total Mg 1 1	0	0
91	m1	2	Total Mg 2 2	0	0
91	m3	2	Total Mg 2 2	0	0
91	m4	1	Total Mg 1 1	0	0
91	m5	2	Total Mg 2 2	0	0
91	m6	6	Total Mg 6 6	0	0
91	m7	7	Total Mg 7 7	0	0
91	m8	2	Total Mg 2 2	0	0
91	m9	1	Total Mg 1 1	0	0
91	n0	5	Total Mg 5 5	0	0
91	n1	3	Total Mg 3 3	0	0
91	n3	3	Total Mg 3 3	0	0
91	n6	1	Total Mg 1 1	0	0
91	n8	4	Total Mg 4 4	0	0
91	n9	2	Total Mg 2 2	0	0
91	o2	3	Total Mg 3 3	0	0
91	o3	5	Total Mg 5 5	0	0
91	o4	3	Total Mg 3 3	0	0
91	o6	1	Total Mg 1 1	0	0

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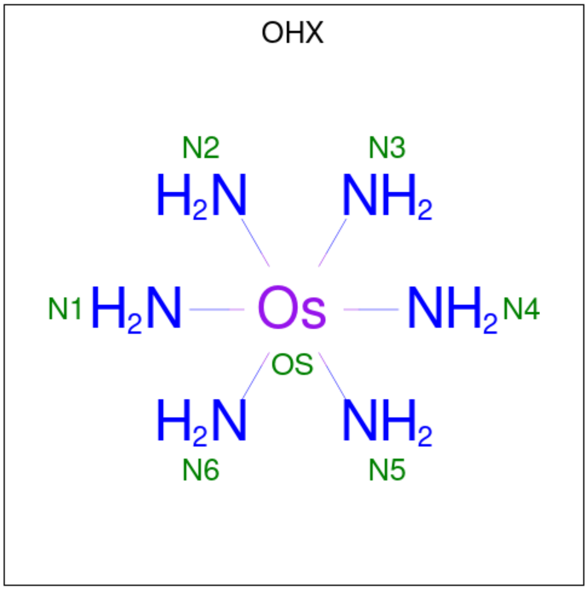
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	o7	3	Total Mg 3 3	0	0
91	o9	1	Total Mg 1 1	0	0
91	q0	1	Total Mg 1 1	0	0
91	q1	1	Total Mg 1 1	0	0
91	q2	1	Total Mg 1 1	0	0
91	q3	2	Total Mg 2 2	0	0
91	p0	1	Total Mg 1 1	0	0

- Molecule 92 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
92	2	1	Total N Os 7 6 1	0	0
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92	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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92	S6	1	Total N Os 7 6 1	0	0
92	S8	1	Total N Os 7 6 1	0	0
92	C3	1	Total N Os 7 6 1	0	0
92	C5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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92	C8	1	Total N Os 7 6 1	0	0
92	D9	1	Total N Os 7 6 1	0	0
92	SR	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
92	1	1	Total N Os 7 6 1	0	0
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92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	3	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
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92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0
92	4	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	L2	1	Total N Os 7 6 1	0	0
92	L3	1	Total N Os 7 6 1	0	0
92	L3	1	Total N Os 7 6 1	0	0
92	L3	1	Total N Os 7 6 1	0	0
92	L4	1	Total N Os 7 6 1	0	0
92	L5	1	Total N Os 7 6 1	0	0
92	M0	1	Total N Os 7 6 1	0	0
92	M0	1	Total N Os 7 6 1	0	0
92	M0	1	Total N Os 7 6 1	0	0
92	M0	1	Total N Os 7 6 1	0	0
92	M5	1	Total N Os 7 6 1	0	0
92	M5	1	Total N Os 7 6 1	0	0
92	M7	1	Total N Os 7 6 1	0	0
92	M9	1	Total N Os 7 6 1	0	0
92	N1	1	Total N Os 7 6 1	0	0
92	N8	1	Total N Os 7 6 1	0	0
92	N9	1	Total N Os 7 6 1	0	0
92	O1	1	Total N Os 7 6 1	0	0
92	O3	1	Total N Os 7 6 1	0	0
92	O7	1	Total N Os 7 6 1	0	0
92	O7	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	O7	1	Total N Os 7 6 1	0	0
92	Q2	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
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92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	6	1	Total N Os 7 6 1	0	0
92	s1	1	Total N Os 7 6 1	0	0
92	s4	1	Total N Os 7 6 1	0	0
92	s8	1	Total N Os 7 6 1	0	0
92	c1	1	Total N Os 7 6 1	0	0
92	c3	1	Total N Os 7 6 1	0	0
92	c5	1	Total N Os 7 6 1	0	0
92	c5	1	Total N Os 7 6 1	0	0
92	c8	1	Total N Os 7 6 1	0	0
92	d4	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	d9	1	Total N Os 7 6 1	0	0
92	sR	1	Total N Os 7 6 1	0	0
92	5	1	Total N Os 7 6 1	0	0
92	5	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	7	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	8	1	Total N Os 7 6 1	0	0
92	l2	1	Total N Os 7 6 1	0	0
92	l3	1	Total N Os 7 6 1	0	0
92	l3	1	Total N Os 7 6 1	0	0
92	l4	1	Total N Os 7 6 1	0	0
92	l4	1	Total N Os 7 6 1	0	0
92	l5	1	Total N Os 7 6 1	0	0
92	l5	1	Total N Os 7 6 1	0	0
92	l5	1	Total N Os 7 6 1	0	0
92	l9	1	Total N Os 7 6 1	0	0
92	m0	1	Total N Os 7 6 1	0	0
92	m0	1	Total N Os 7 6 1	0	0
92	m0	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
92	m0	1	Total N Os 7 6 1	0	0
92	m1	1	Total N Os 7 6 1	0	0
92	m4	1	Total N Os 7 6 1	0	0
92	m5	1	Total N Os 7 6 1	0	0
92	m5	1	Total N Os 7 6 1	0	0
92	m7	1	Total N Os 7 6 1	0	0
92	m9	1	Total N Os 7 6 1	0	0
92	n1	1	Total N Os 7 6 1	0	0
92	n3	1	Total N Os 7 6 1	0	0
92	n9	1	Total N Os 7 6 1	0	0
92	o2	1	Total N Os 7 6 1	0	0
92	o3	1	Total N Os 7 6 1	0	0
92	o7	1	Total N Os 7 6 1	0	0
92	o9	1	Total N Os 7 6 1	0	0
92	q2	1	Total N Os 7 6 1	0	0
92	A	1	Total N Os 7 6 1	0	0
92	A	1	Total N Os 7 6 1	0	0
92	a	1	Total N Os 7 6 1	0	0

- Molecule 93 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
93	D6	1	Total Zn 1 1	0	0

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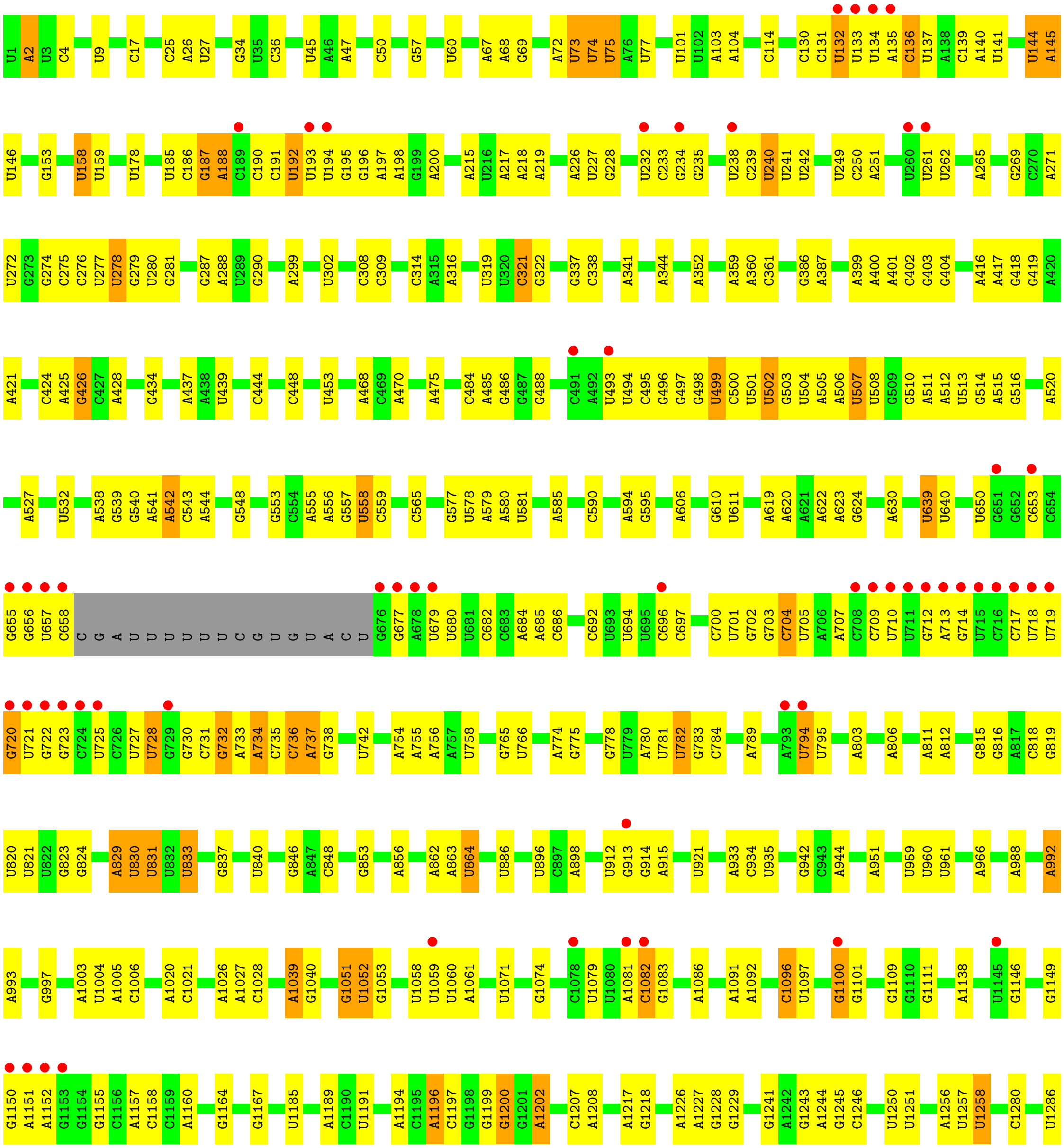
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
93	D7	1	Total Zn 1 1	0	0
93	D9	1	Total Zn 1 1	0	0
93	E1	1	Total Zn 1 1	0	0
93	O7	1	Total Zn 1 1	0	0
93	Q0	1	Total Zn 1 1	0	0
93	Q2	1	Total Zn 1 1	0	0
93	Q3	1	Total Zn 1 1	0	0
93	d6	1	Total Zn 1 1	0	0
93	d7	1	Total Zn 1 1	0	0
93	d9	1	Total Zn 1 1	0	0
93	e1	1	Total Zn 1 1	0	0
93	o7	1	Total Zn 1 1	0	0
93	q0	1	Total Zn 1 1	0	0
93	q2	1	Total Zn 1 1	0	0
93	q3	1	Total Zn 1 1	0	0

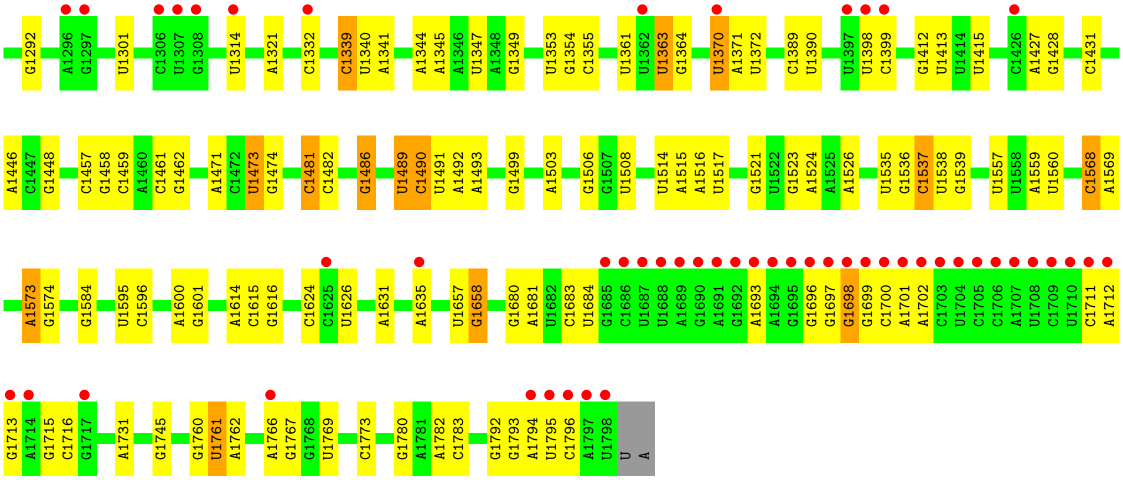
3 Residue-property plots ⓘ

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: 18S rRNA

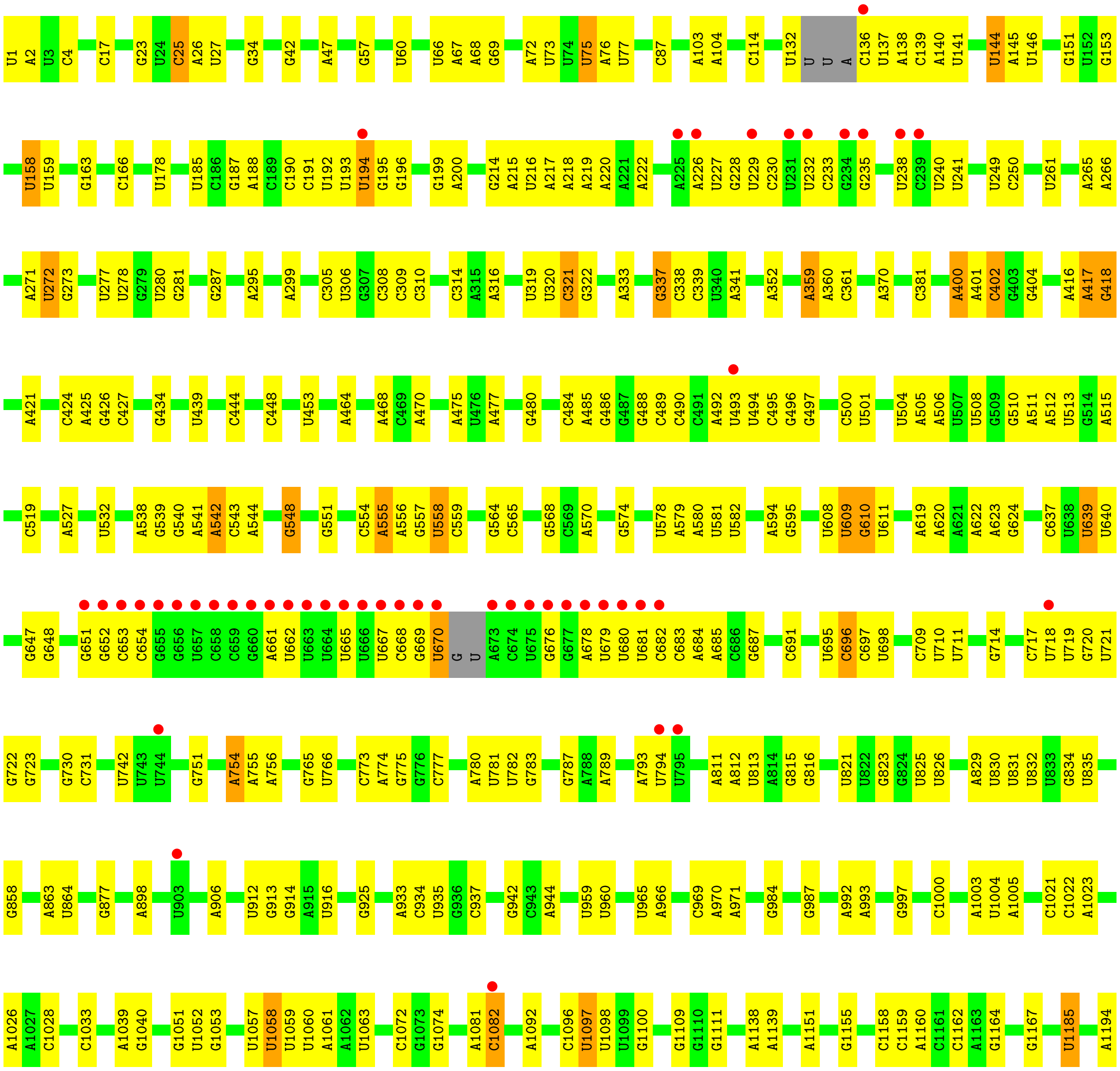
Chain 2:

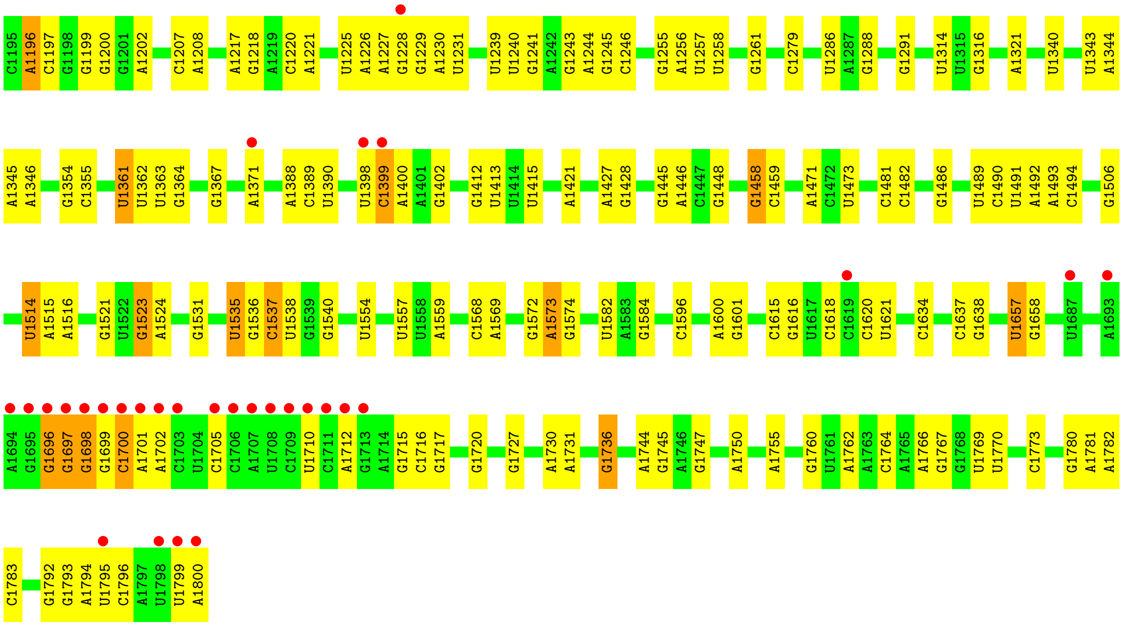




- Molecule 1: 18S rRNA

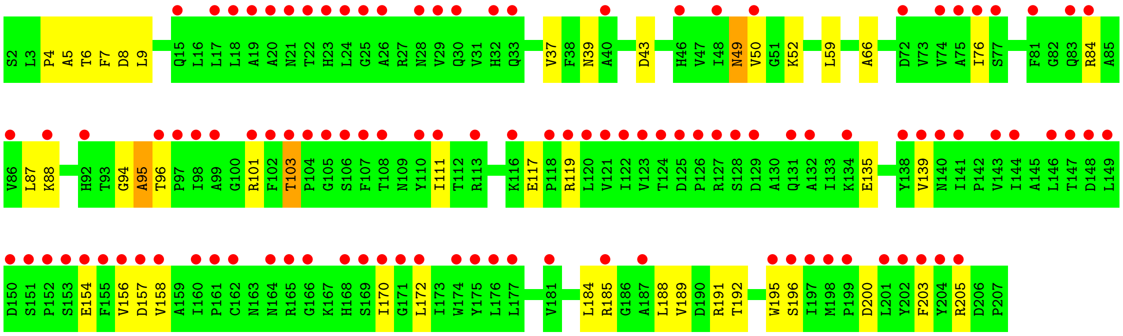
Chain 6:





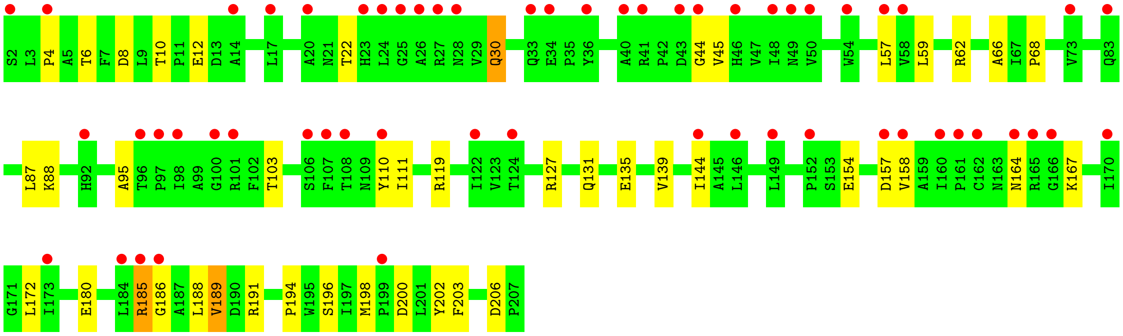
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



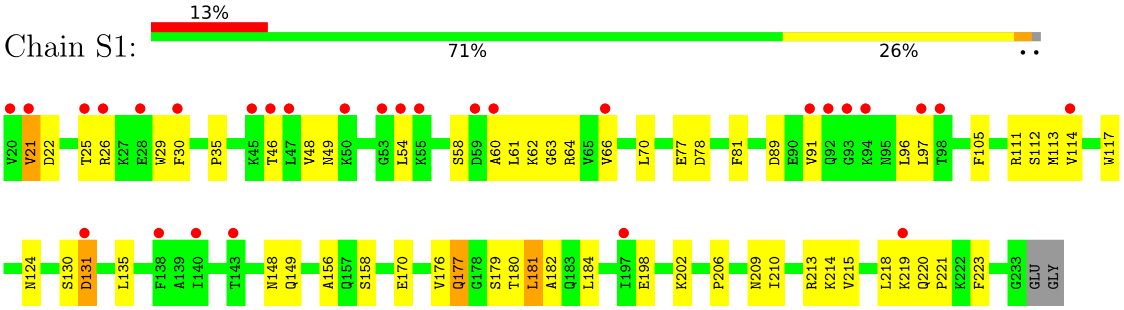
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



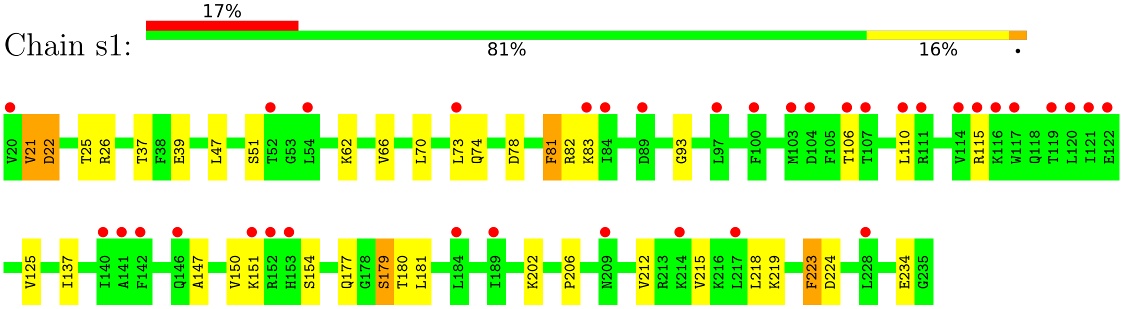
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



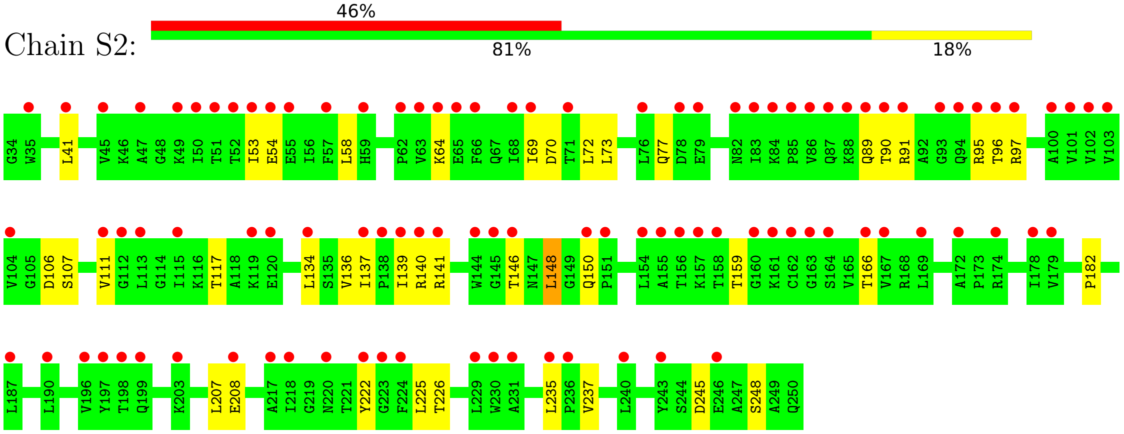
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



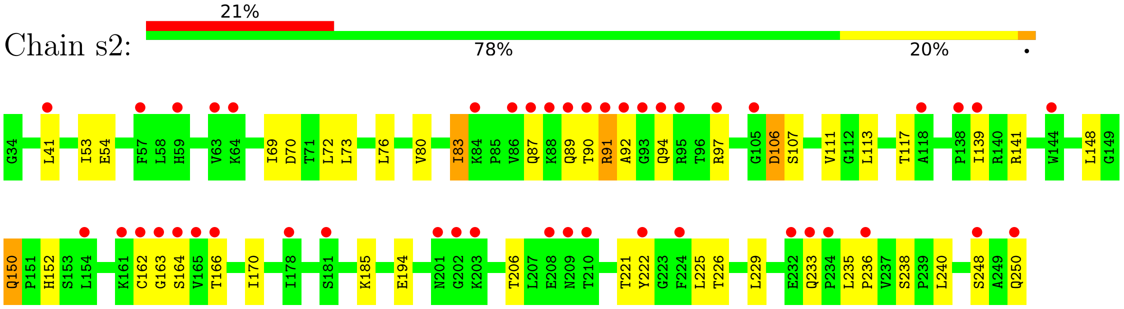
- Molecule 4: 40S ribosomal protein S2

Chain S2:



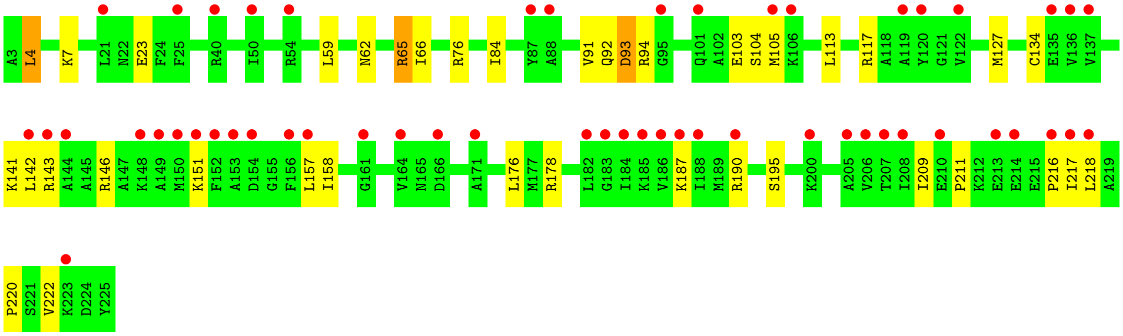
- Molecule 4: 40S ribosomal protein S2

Chain s2:



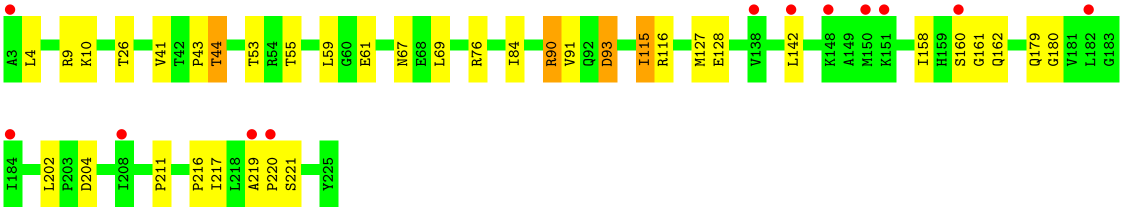
- Molecule 5: 40S ribosomal protein S3

Chain S3:



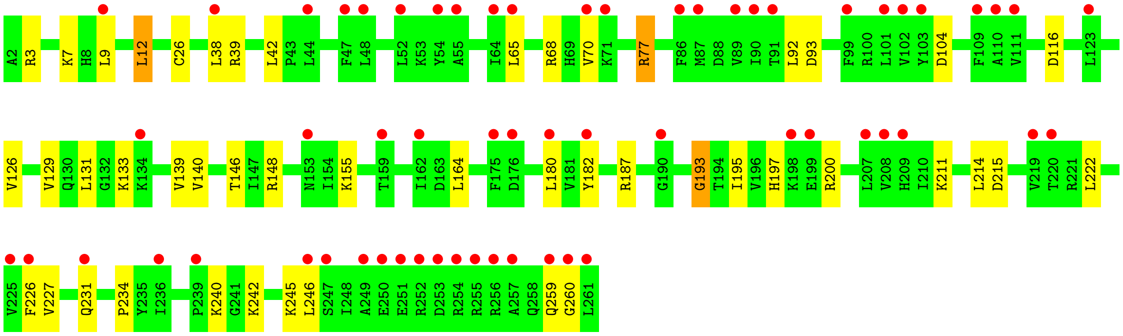
- Molecule 5: 40S ribosomal protein S3

Chain s3:



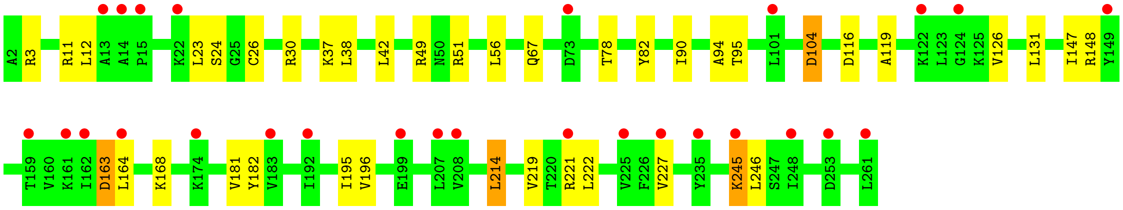
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



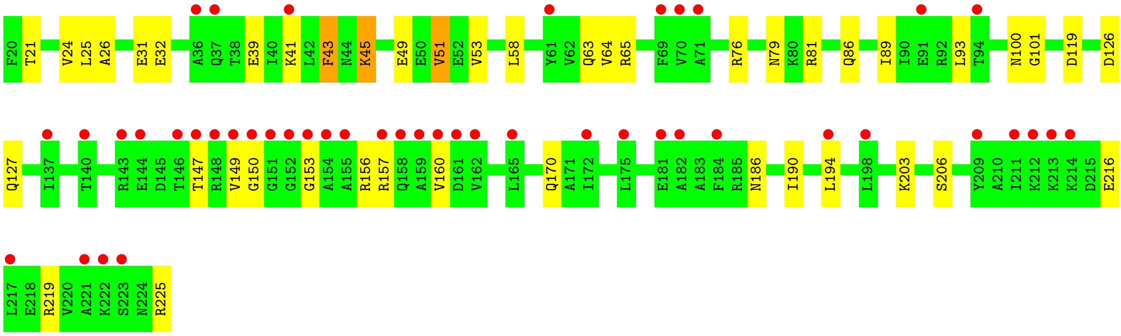
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:



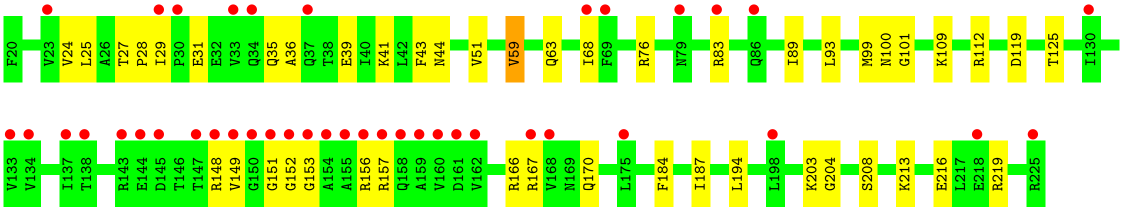
- Molecule 7: 40S ribosomal protein S5

Chain S5:



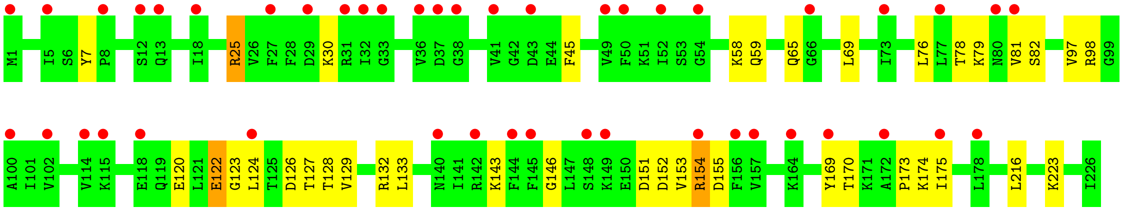
- Molecule 7: 40S ribosomal protein S5

Chain s5:



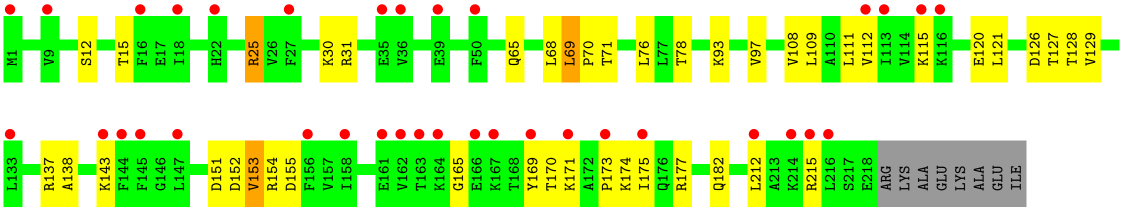
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:



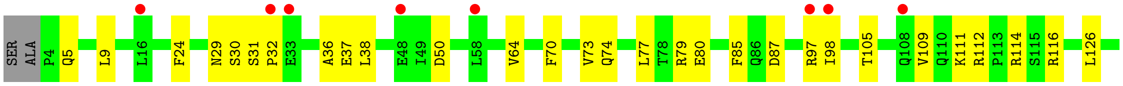
- Molecule 8: 40S ribosomal protein S6-A

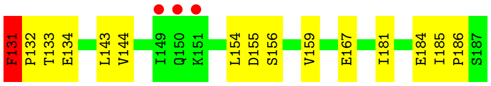
Chain s6:



- Molecule 9: 40S ribosomal protein S7-A

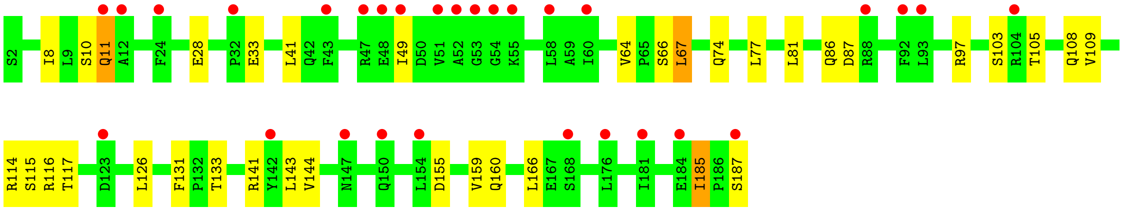
Chain S7:





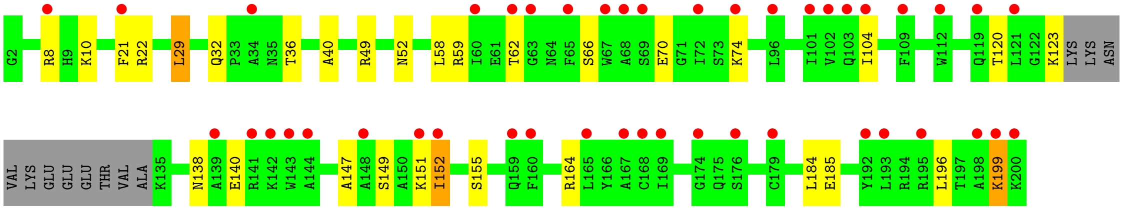
- Molecule 9: 40S ribosomal protein S7-A

Chain s7:



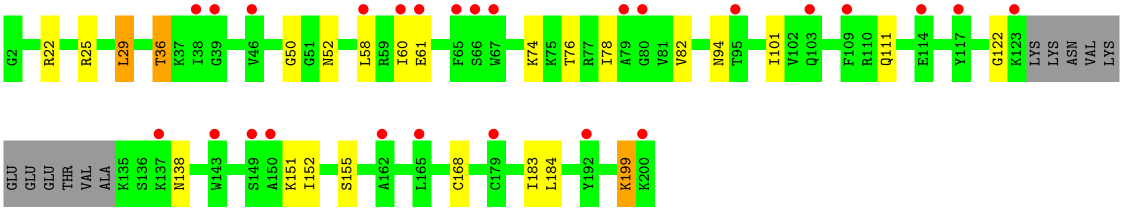
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:



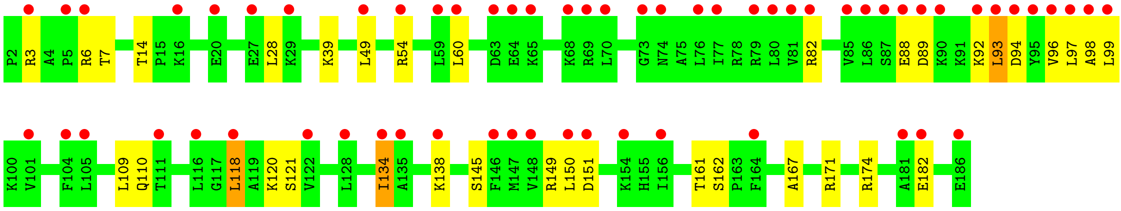
- Molecule 10: 40S ribosomal protein S8-A

Chain s8:



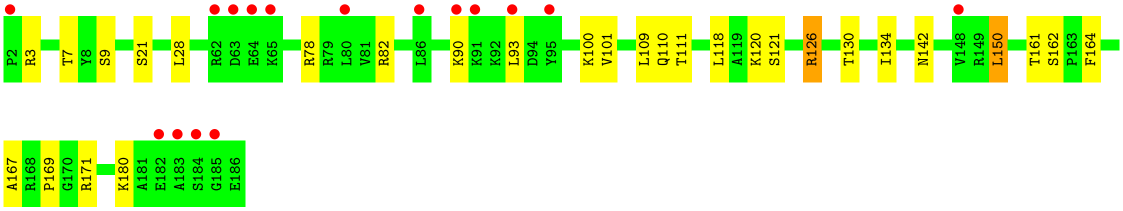
- Molecule 11: 40S ribosomal protein S9-A

Chain S9:



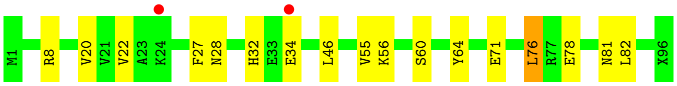
- Molecule 11: 40S ribosomal protein S9-A

Chain s9:



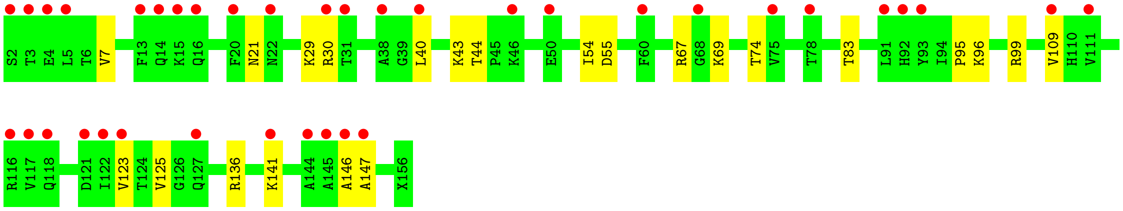
- Molecule 12: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A

Chain C0:



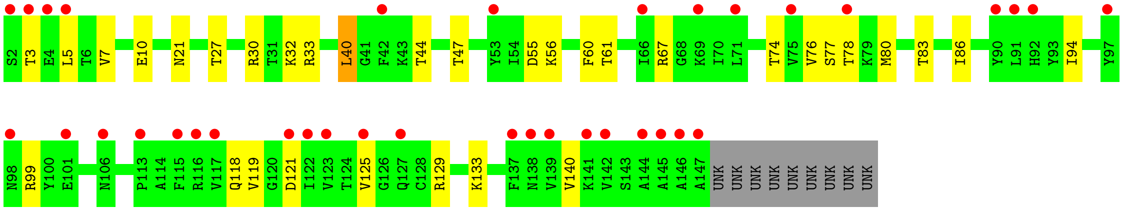
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A

Chain C1:



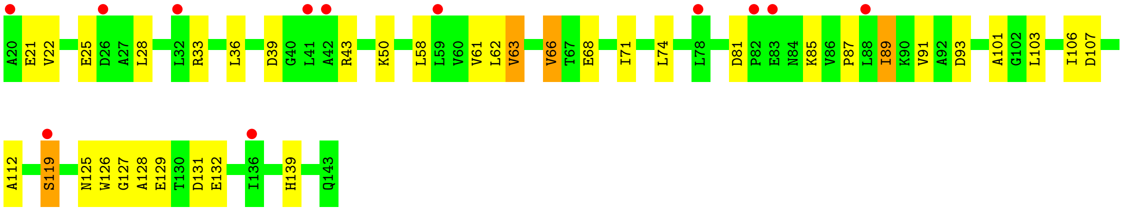
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A

Chain c1:

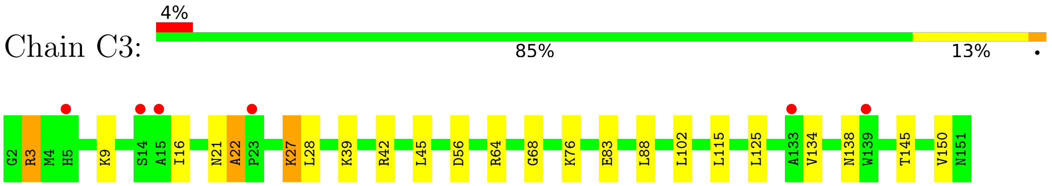


- Molecule 14: 40S Ribosomal Protein S12

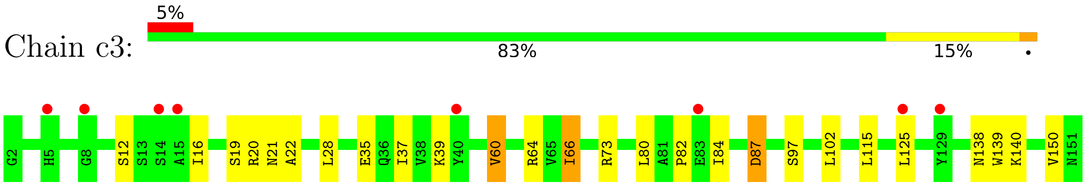
Chain C2:



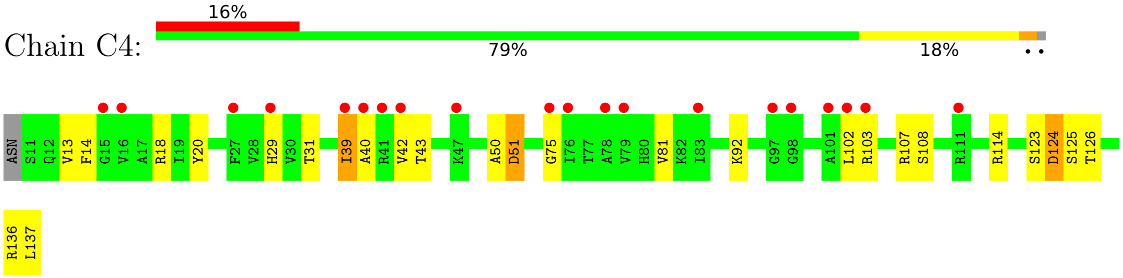
- Molecule 15: 40S ribosomal protein S13



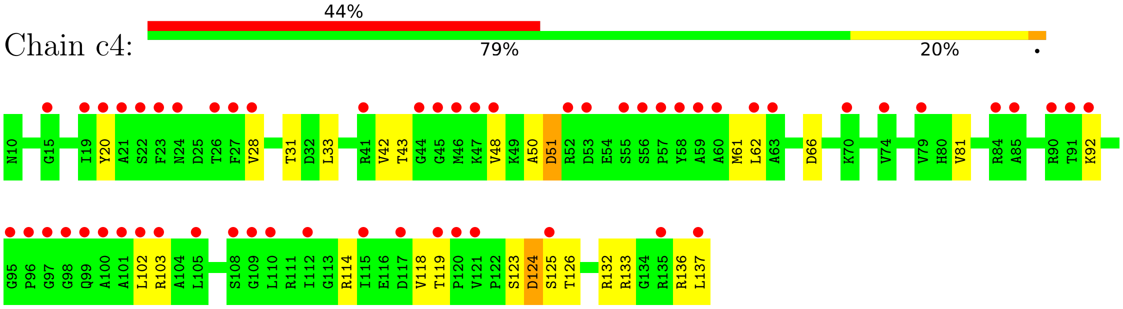
- Molecule 15: 40S ribosomal protein S13



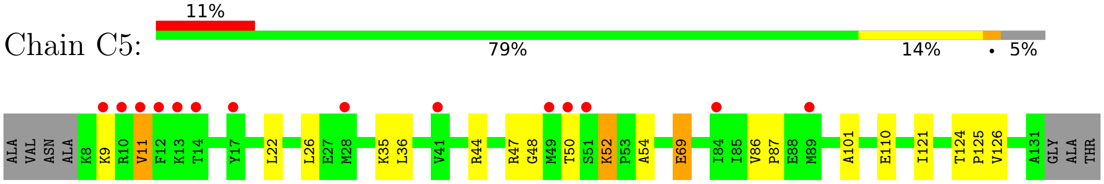
- Molecule 16: 40S Ribosomal Protein S14



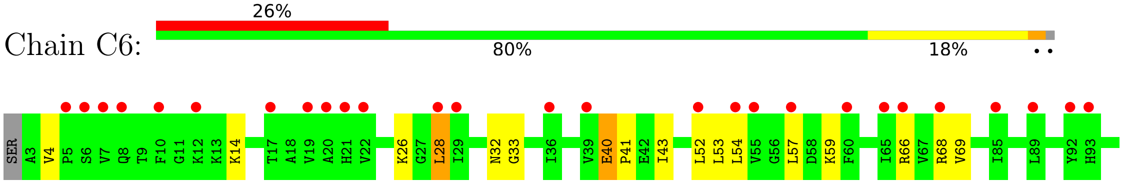
- Molecule 16: 40S Ribosomal Protein S14

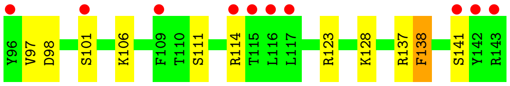


- Molecule 17: 40S ribosomal protein S15



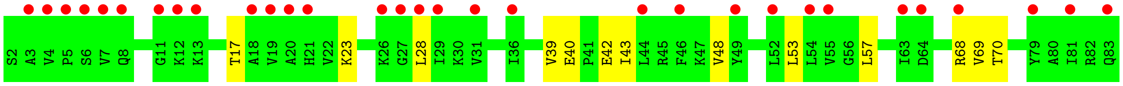
- Molecule 18: 40S ribosomal protein S16-A

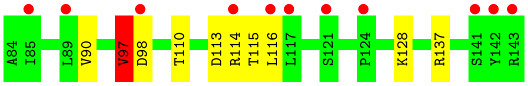




- Molecule 18: 40S ribosomal protein S16-A

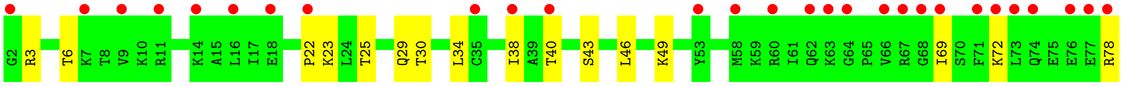
Chain c6:

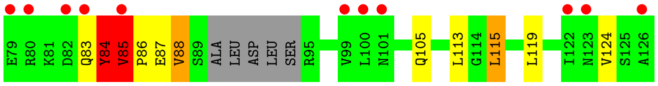




- Molecule 19: 40S ribosomal protein S17-A

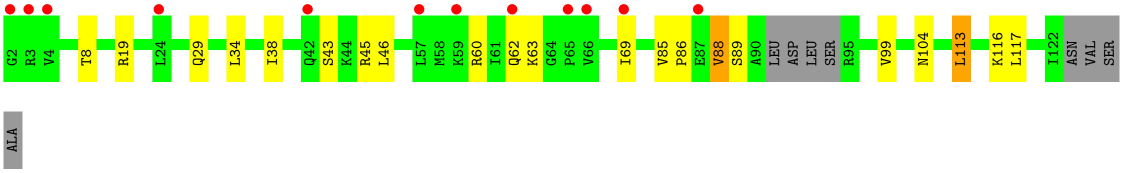
Chain C7:





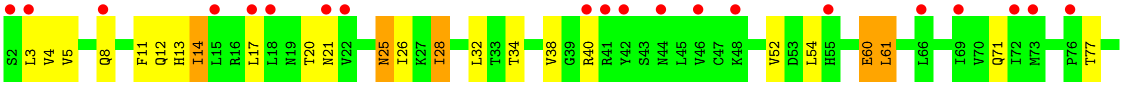
- Molecule 19: 40S ribosomal protein S17-A

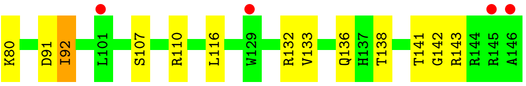
Chain c7:



- Molecule 20: 40S ribosomal protein S18-A

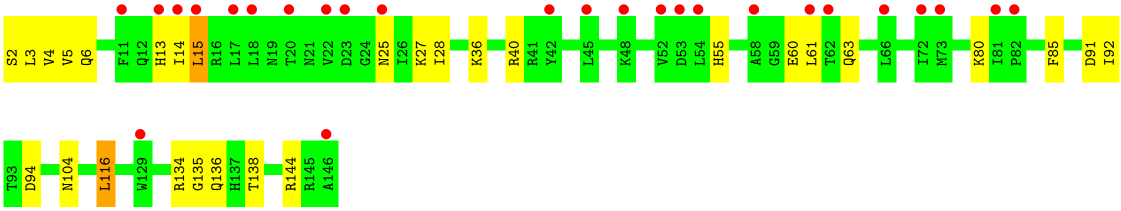
Chain C8:





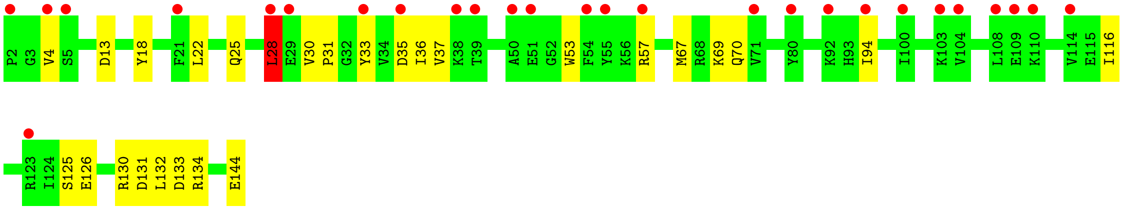
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



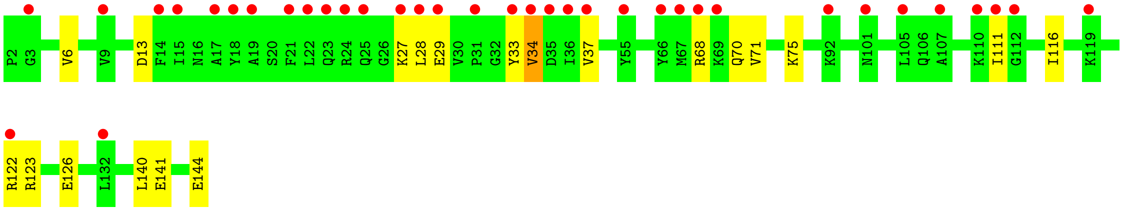
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



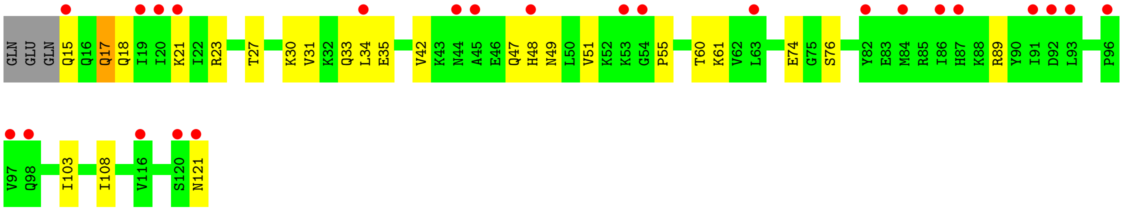
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



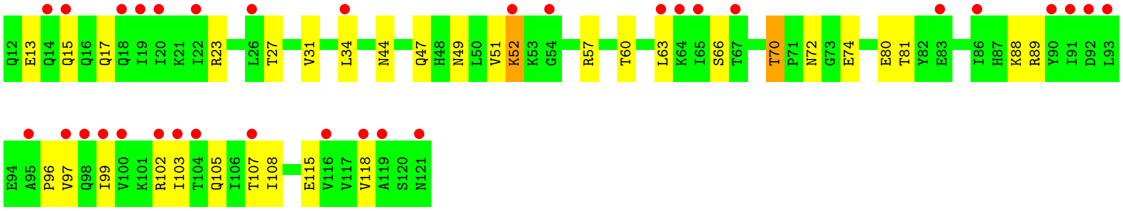
- Molecule 22: 40S ribosomal protein S20

Chain D0:

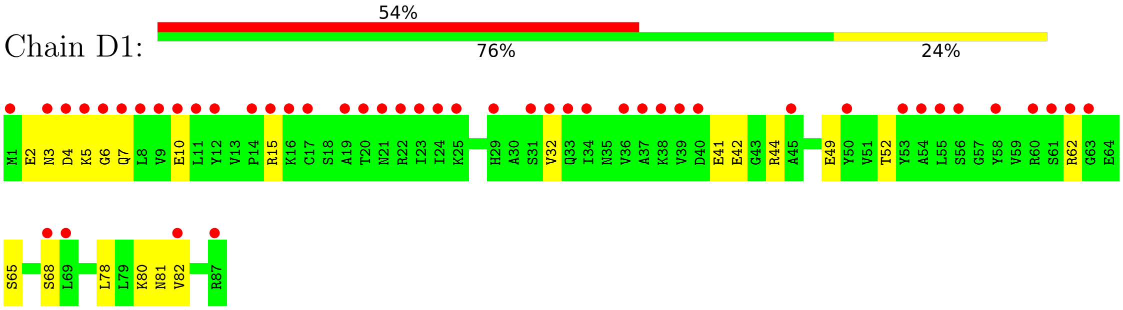


- Molecule 22: 40S ribosomal protein S20

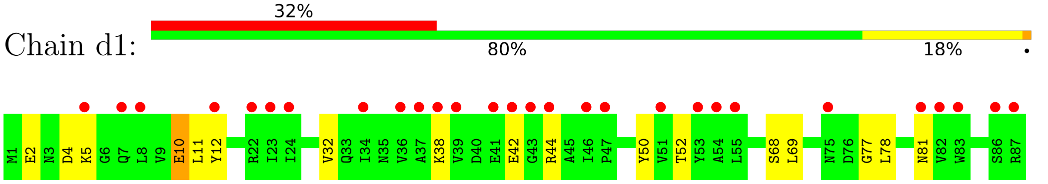
Chain d0:



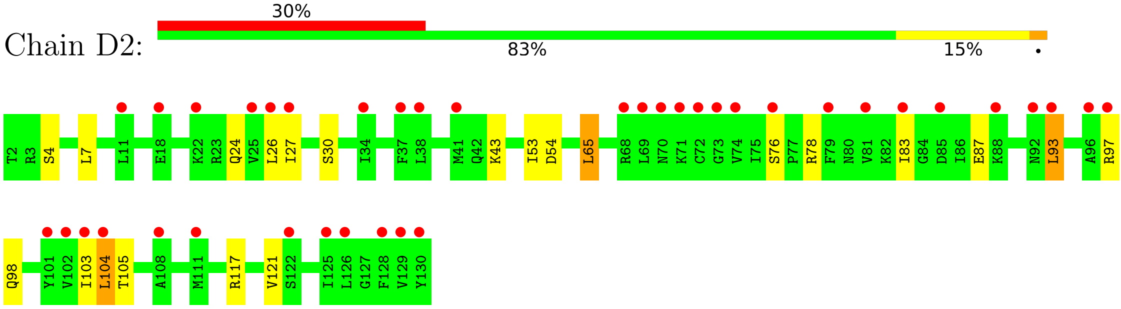
- Molecule 23: 40S ribosomal protein S21-A



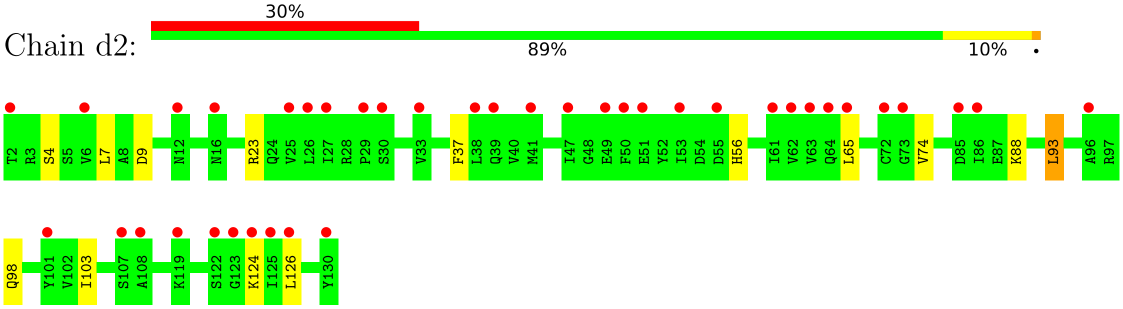
- Molecule 23: 40S ribosomal protein S21-A



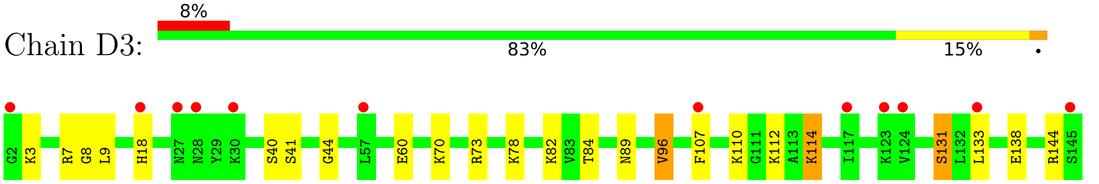
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 24: 40S ribosomal protein S22-A

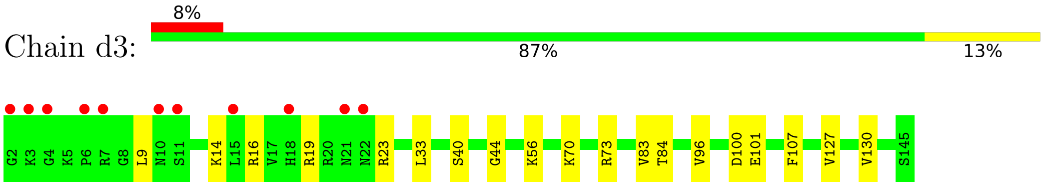


- Molecule 25: 40S ribosomal protein S23-A



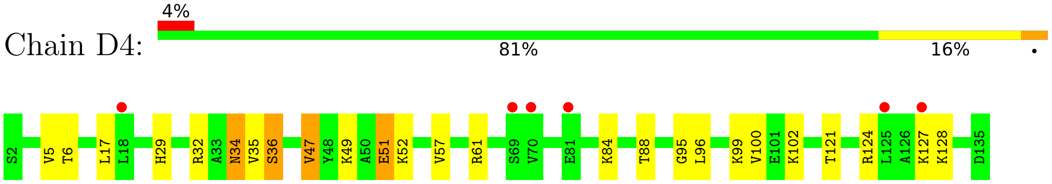
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



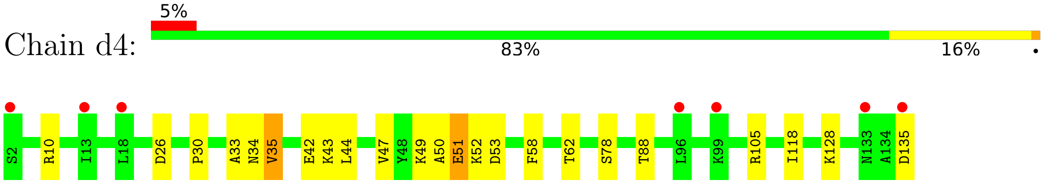
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



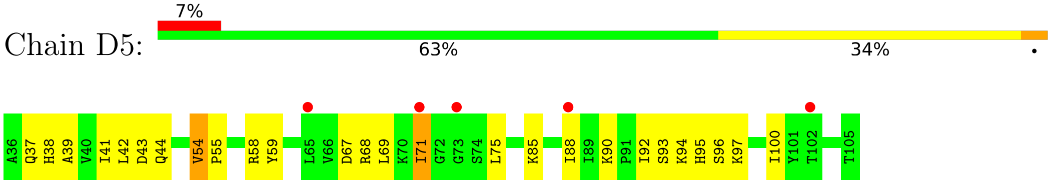
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:



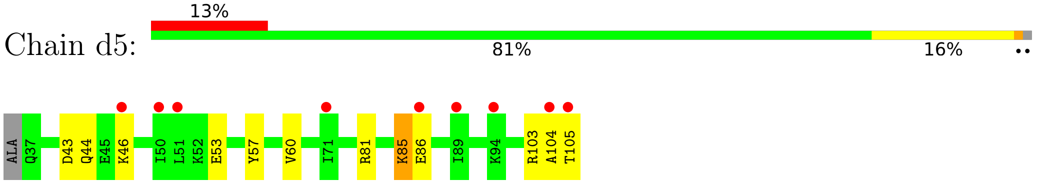
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:



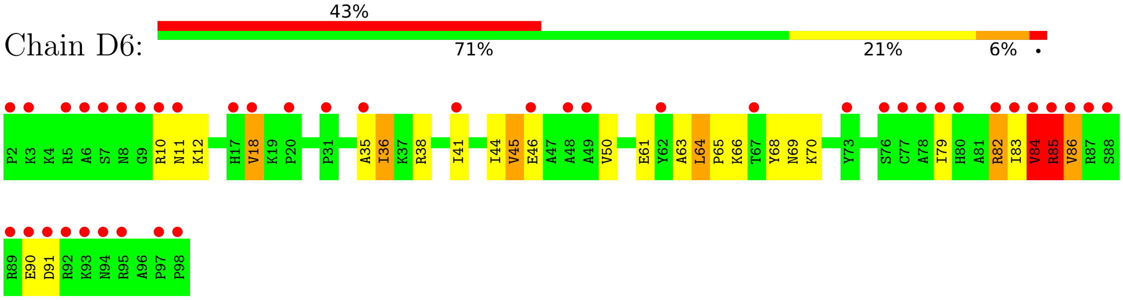
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



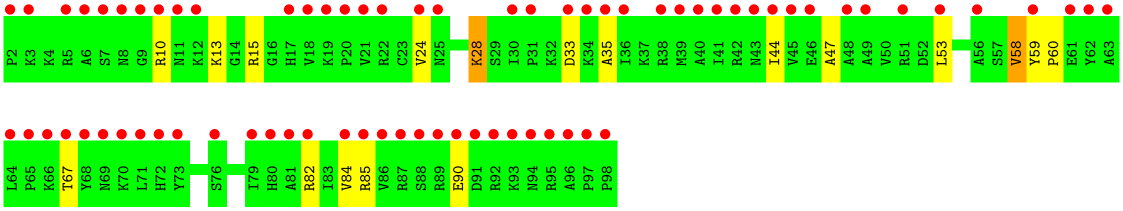
- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



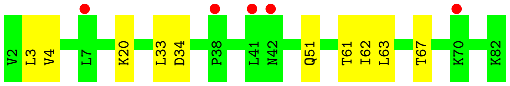
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



- Molecule 29: 40S ribosomal protein S27-A

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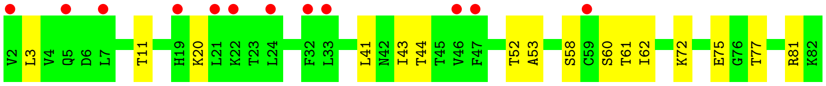
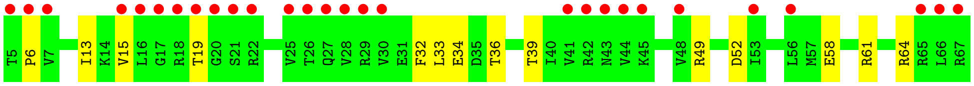


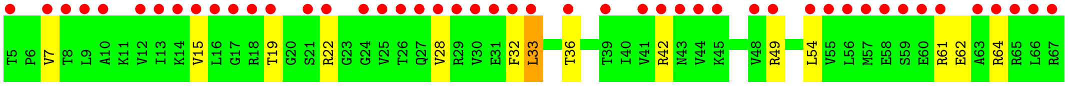
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



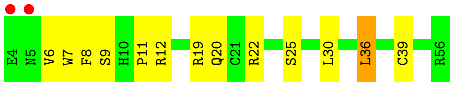
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



- Molecule 31: 40S ribosomal protein S29-A

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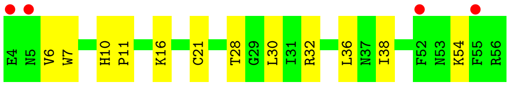
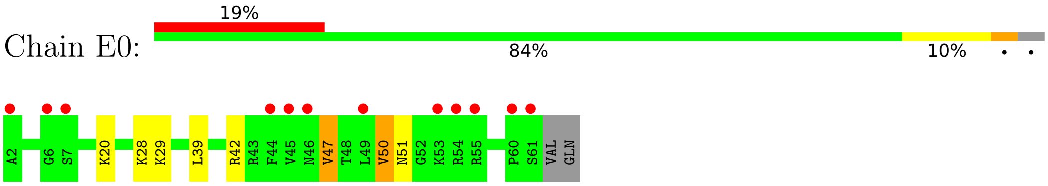
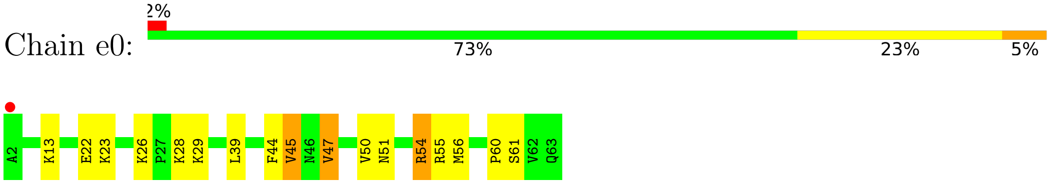


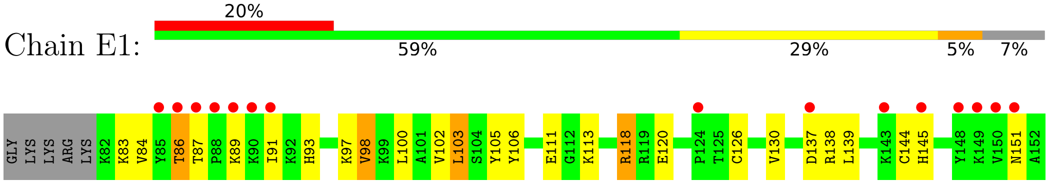
- Molecule 32: 40S ribosomal protein S30-A



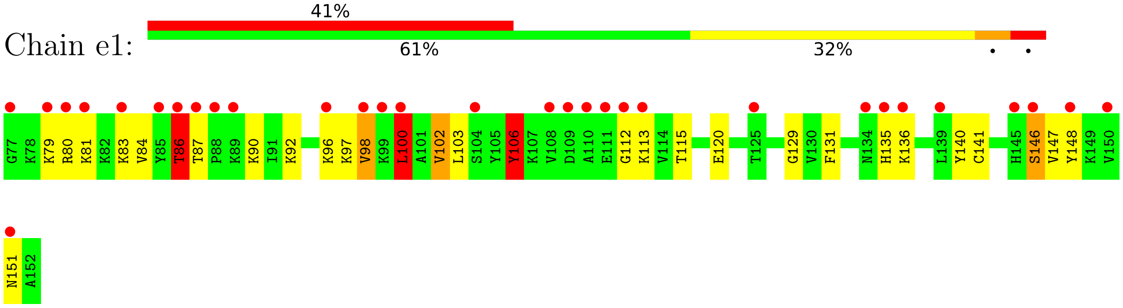
- Molecule 32: 40S ribosomal protein S30-A



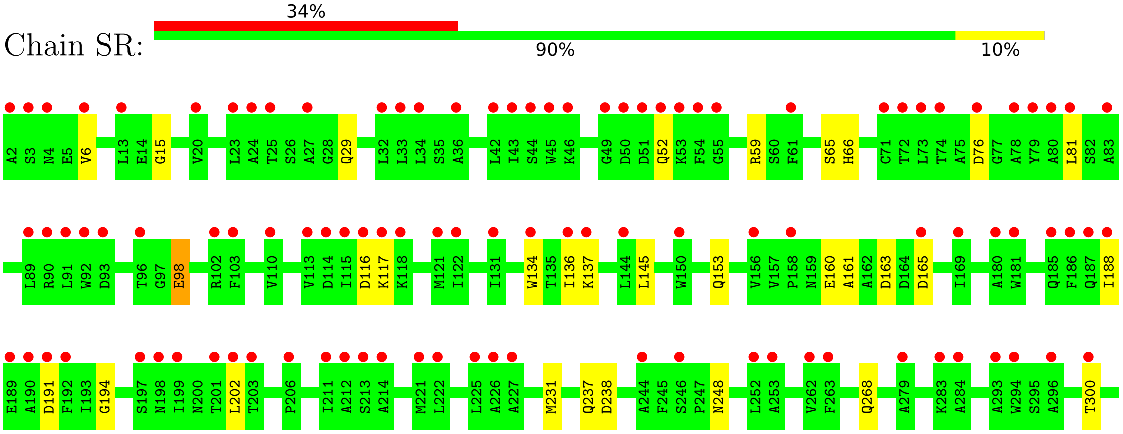
- Molecule 33: Ubiquitin-40S ribosomal protein S31

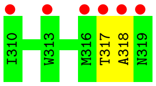


- Molecule 33: Ubiquitin-40S ribosomal protein S31



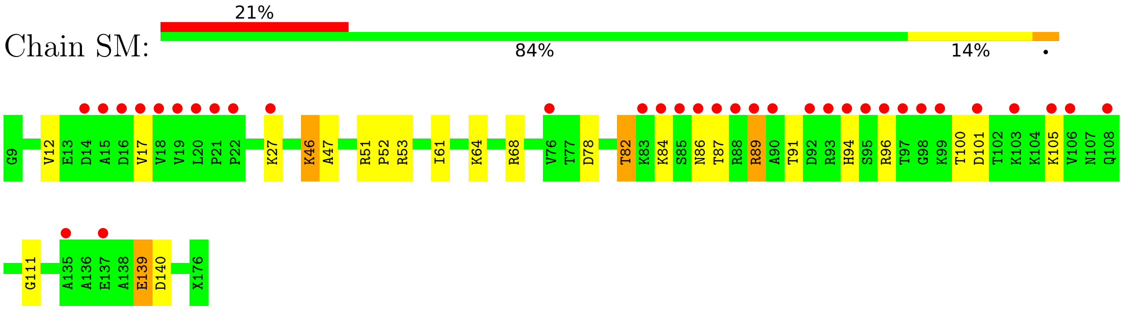
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein





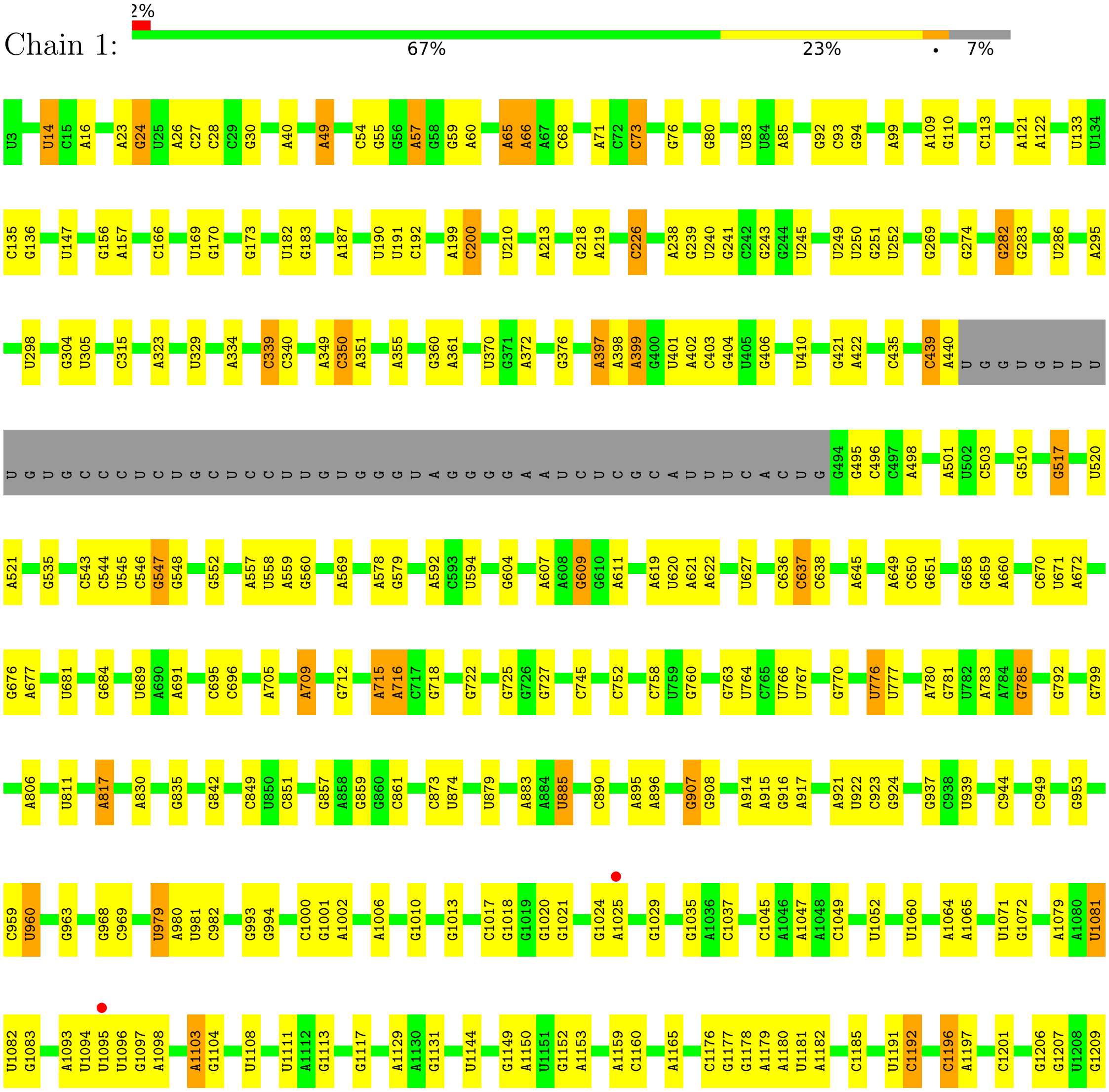
- Molecule 35: Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1

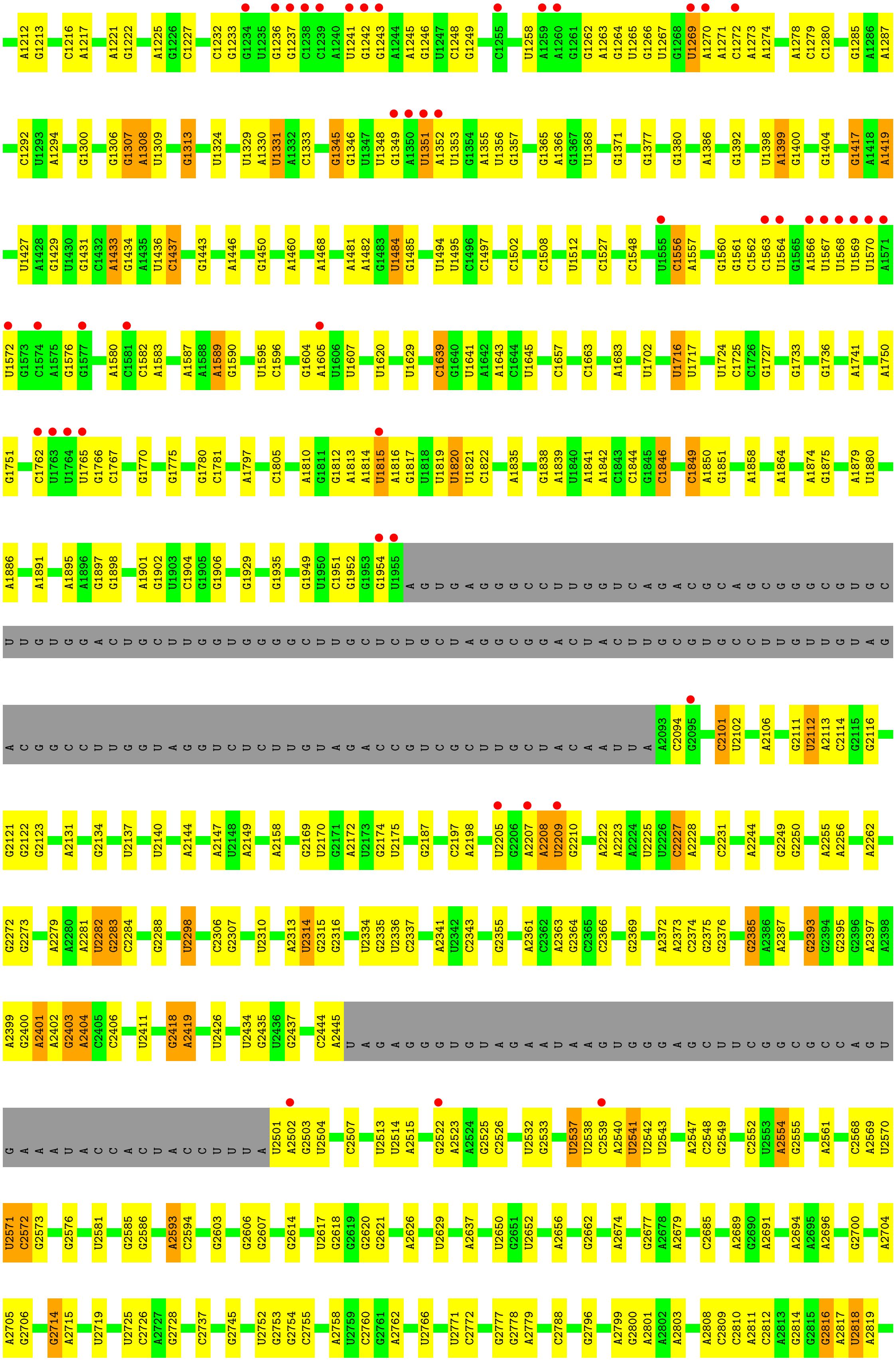
Chain SM:



- Molecule 36: 25S rRNA

Chain 1:

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C1292 U1293 A1294 G1300 G1306 G1307 A1308 U1309 G1313 U1324 U1329 A1330 U1331 A1332 C1333 G1345 G1346 U1347 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 G1365 A1366 G1367 U1368 G1371 G1377 G1380 A1386 G1392 U1398 A1399 G1400 G1404 G1417 A1418 A1419
U1427 A1428 G1429 U1430 G1431 C1432 A1433 G1434 A1435 U1436 C1437 G1443 A1446 G1450 A1460 A1468 A1481 A1482 G1483 U1484 G1485 U1494 U1495 C1496 C1497 C1502 C1508 U1512 C1527 C1548 U1555 C1556 A1557 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571
U1572 G1573 C1574 A1575 G1576 G1577 A1580 C1581 C1582 A1583 A1587 A1588 A1589 G1590 U1595 C1596 G1604 A1605 U1606 U1607 U1620 U1629 C1639 G1640 U1641 A1642 A1643 C1644 U1645 C1657 C1663 A1683 U1702 U1716 U1717 U1724 C1725 C1726 G1727 G1733 G1736 A1741 A1750
G1751 C1762 U1763 U1764 U1765 G1766 C1767 G1770 G1775 G1780 C1781 A1797 C1805 A1810 G1811 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 C1822 A1835 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 C1849 A1850 G1851 A1858 A1864 A1874 G1875 A1879 U1880
A1886 A1891 A1895 A1896 G1897 G1898 A1901 G1902 U1903 C1904 G1905 G1906 G1929 G1935 G1949 U1950 C1951 G1952 G1953 G1954 U1955 A G U G A G G G C C U U G G G U C A G A C G C A G C G G G C C G U G C
U U G U G G A C U G C U U G G U G G G G C U U G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U G U U G U A G
A C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C A A U U A A2093 C2094 G2095 C2101 U2102 A2106 G2111 U2112 A2113 C2114 G2115 G2116
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G2272 G2273 A2279 A2280 A2281 U2282 G2283 C2284 G2288 U2298 C2306 G2307 U2310 A2313 U2314 G2315 G2316 U2334 G2335 U2336 C2337 A2341 U2342 C2343 G2355 A2361 C2362 A2363 G2364 C2365 C2366 G2369 A2372 A2373 C2374 G2375 G2376 G2385 A2386 A2387 G2393 G2394 G2395 G2396 A2397 A2398
A2399 G2400 A2401 A2402 G2403 A2404 C2405 C2406 U2411 G2418 A2419 U2426 U2434 G2435 U2436 G2437 C2444 A2445 U A G A G G G U G U A G A A U A A G U G G G A G C U U C G G C G C C A G U
G A A A U A C C A C U A C C U U U A U2501 A2502 G2503 U2504 C2507 U2513 U2514 A2515 G2522 A2523 A2524 G2525 C2526 U2532 G2533 U2537 U2538 C2539 A2540 U2541 U2542 U2543 A2547 C2548 G2549 C2552 U2553 A2554 G2555 A2561 C2568 A2569 U2570
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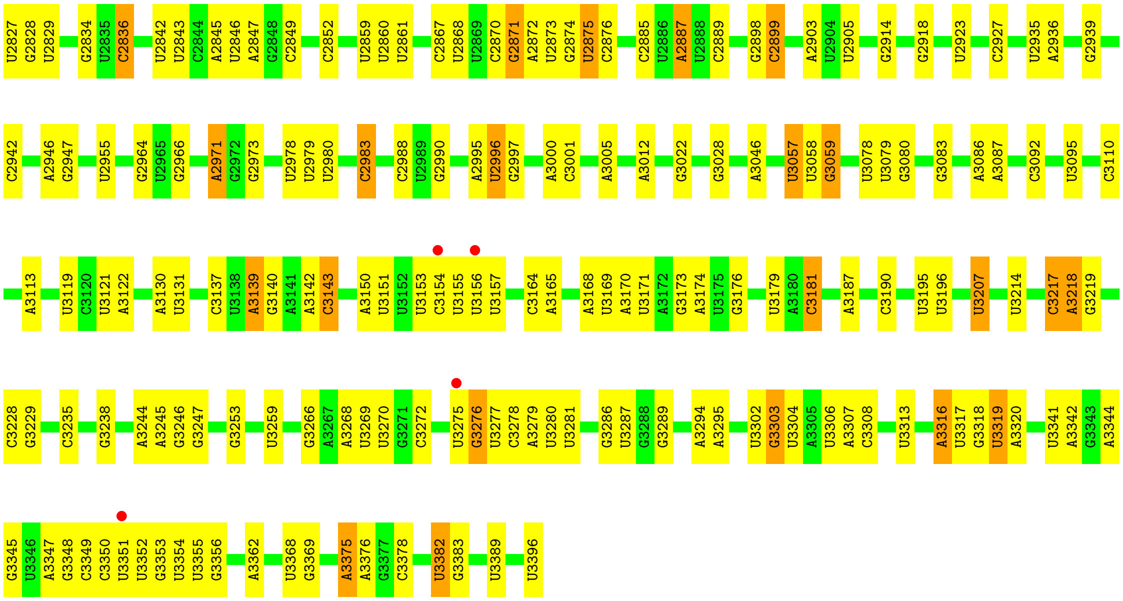
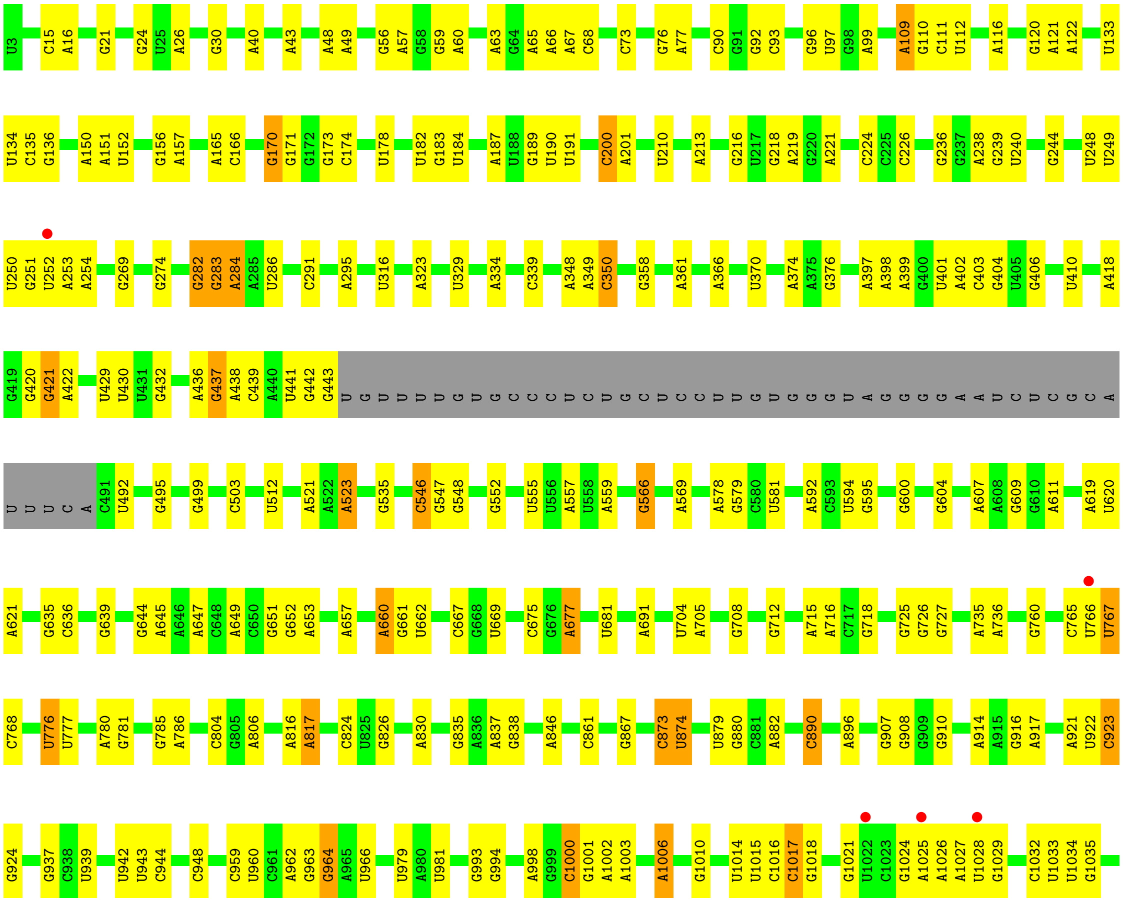
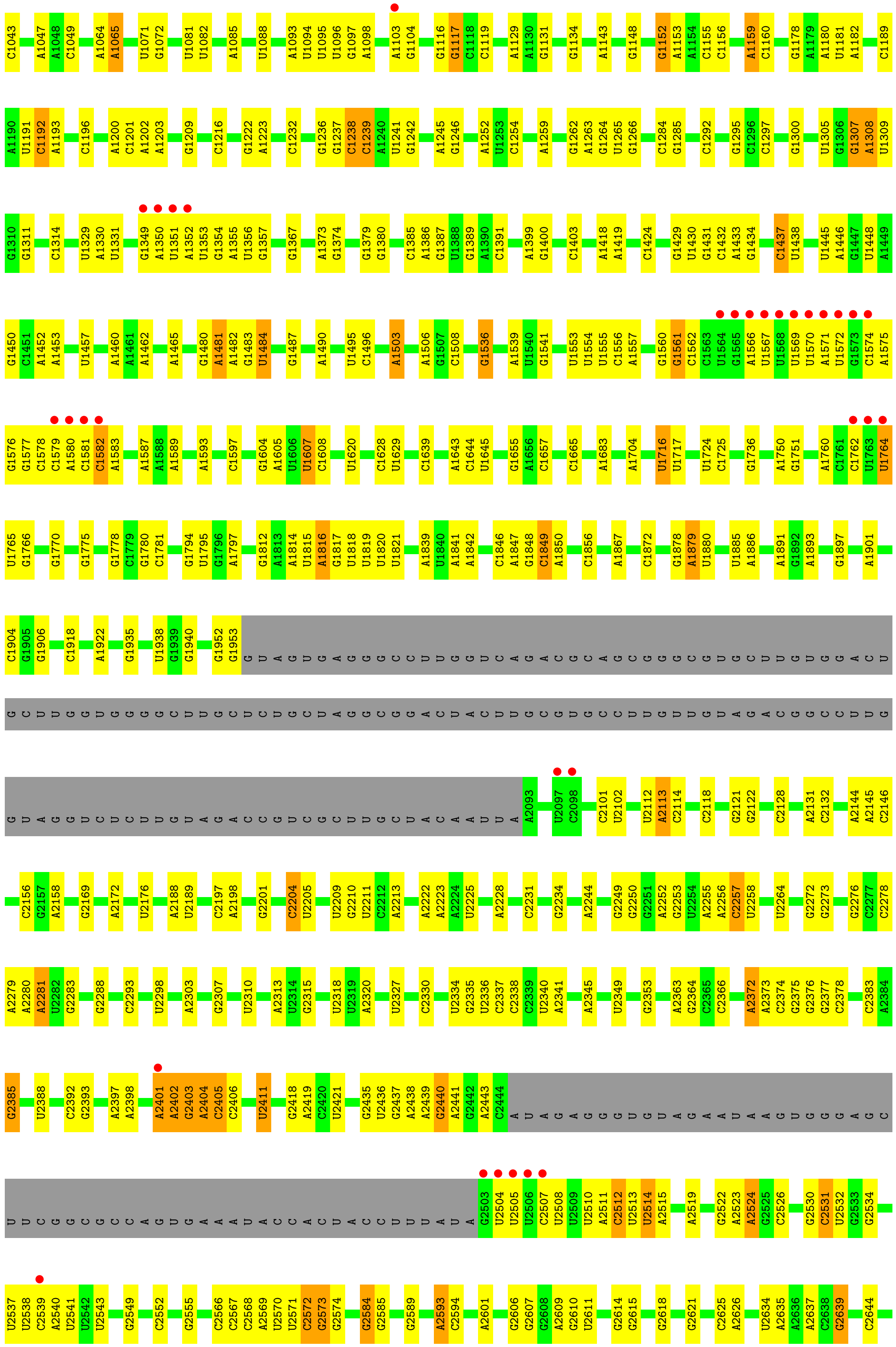


- Molecule 36: 25S rRNA

Chain 5:

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A1190 U1191 C1192 A1193 C1196 A1200 C1201 A1202 A1203 G1209 C1216 G1222 A1223 C1232 G1236 G1237 C1238 C1239 A1240 U1241 G1242 A1245 G1246 A1252 U1253 C1254 A1259 G1262 A1263 G1264 U1265 G1266 C1284 G1285 C1292 G1295 C1296 C1297 G1300 U1305 G1306 G1307 A1308 U1309
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G1450 C1451 A1452 A1453 U1457 A1460 A1461 A1462 A1465 G1480 A1481 A1482 G1483 U1484 G1487 A1490 U1495 C1496 A1503 A1506 G1507 C1508 G1536 A1539 U1540 G1541 U1553 U1554 U1555 C1556 A1557 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1573 C1574 A1575
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U1765 G1766 G1770 G1775 G1778 C1779 G1780 C1781 G1794 U1795 G1796 A1797 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 A1839 U1840 A1841 A1842 C1846 A1847 G1848 C1849 A1850 C1856 A1867 C1872 G1878 A1879 U1880 U1885 A1886 A1891 G1892 A1893 G1897 A1901
C1904 G1905 G1906 C1918 A1922 G1935 U1938 G1939 G1940 G1952 G1953 G U A G U G A G G G C C U U G G U C A G A C G C A G C G G G C G U G C U U G U G G A C U
G C U U G G U G G G G C U U G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U G U U G U A G A C G G C C U U G
G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C A A U U A A2093 U2097 C2098 C2101 U2102 U2112 A2113 C2114 C2118 G2121 G2122 C2128 A2131 C2132 A2144 A2145 C2146
C2156 G2157 A2158 G2169 A2172 U2176 A2188 U2189 C2197 A2198 G2201 C2204 U2205 U2209 G2210 U2211 C2212 A2213 A2222 A2223 A2224 U2225 A2228 C2231 G2234 A2244 G2249 G2250 G2251 A2252 G2253 U2254 A2255 A2256 C2257 U2258 U2264 G2272 G2273 G2276 C2277 C2278
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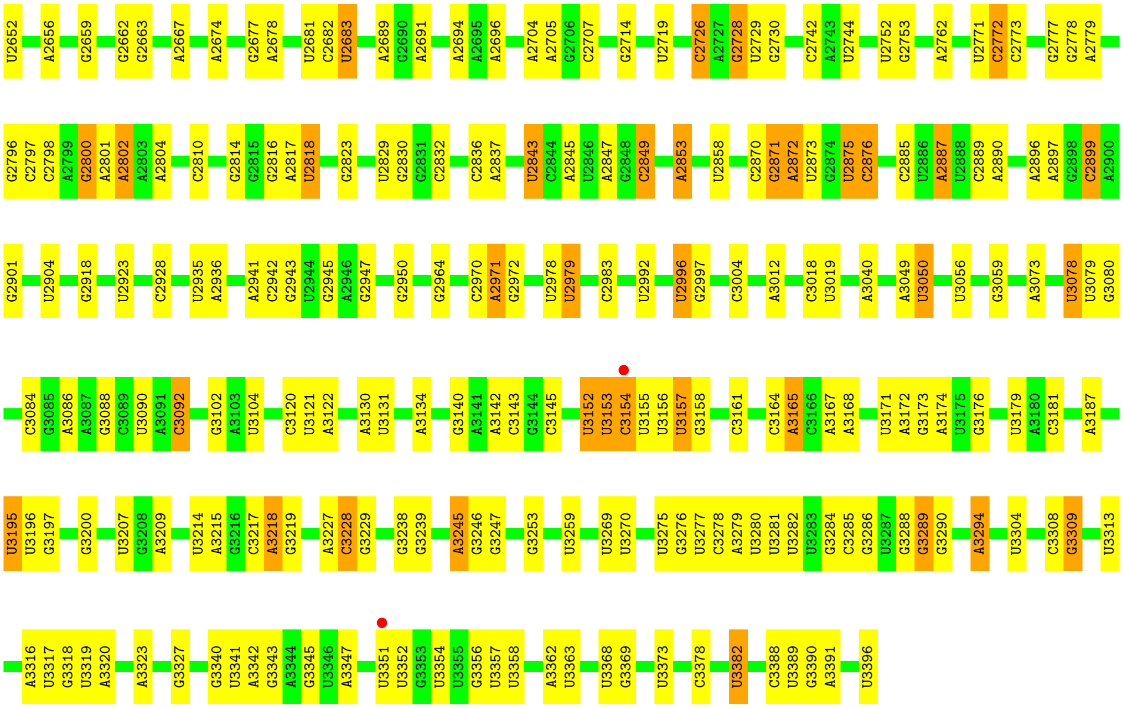
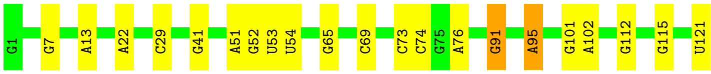
U2537 U2538 C2539 A2540 U2541 U2542 U2543 G2549 C2552 G2555 C2566 C2567 C2568 A2569 U2570 U2571 C2572 G2573 C2574 G2584 G2585 G2589 A2593 C2594 A2601 G2606 G2607 G2608 A2609 G2610 U2611 G2614 G2615 G2618 C2621 C2625 A2626 U2634 A2635 A2636 A2637 C2638 G2639 C2644



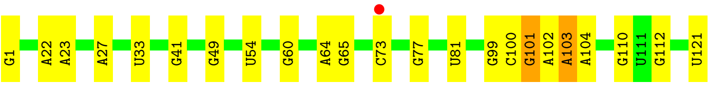
- Molecule 37: 5S rRNA

Chain 3:



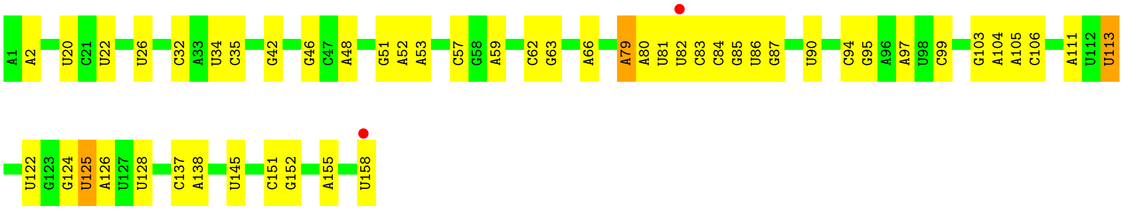
- Molecule 37: 5S rRNA

Chain 7:



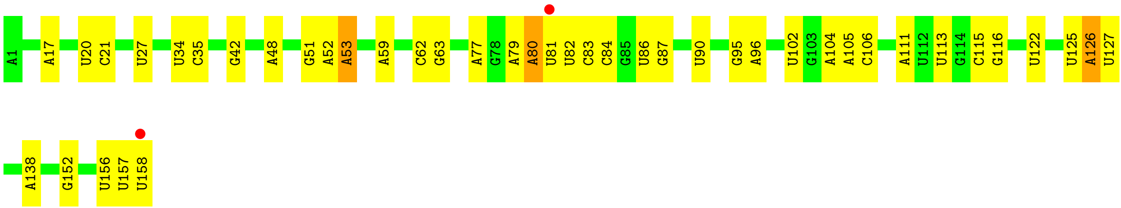
- Molecule 38: 5.8S rRNA

Chain 4:



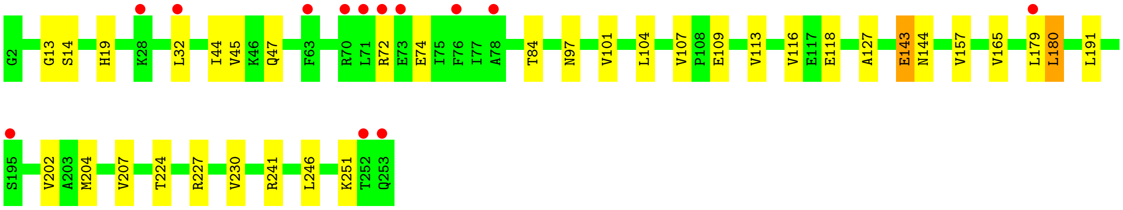
- Molecule 38: 5.8S rRNA

Chain 8:



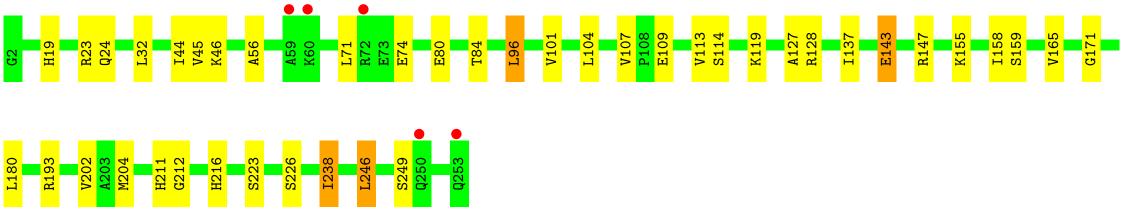
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



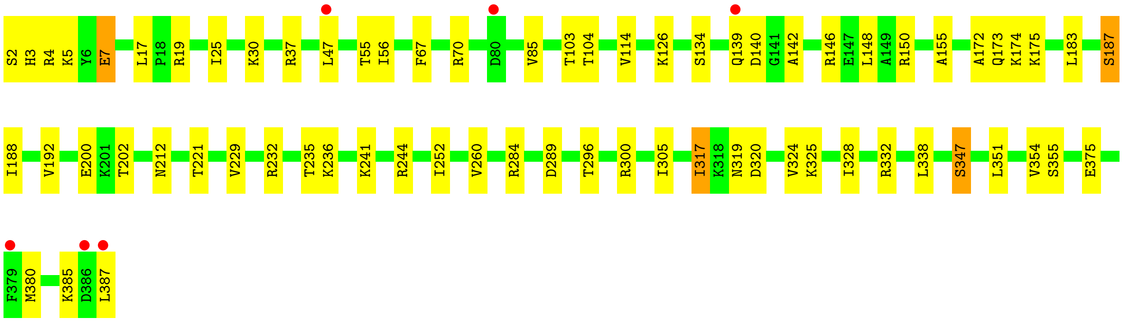
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



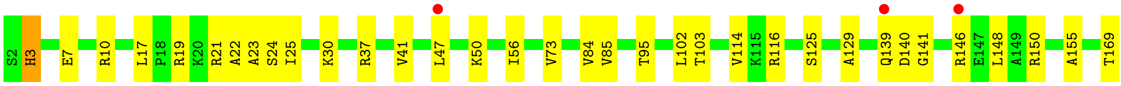
• Molecule 40: 60S ribosomal protein L3

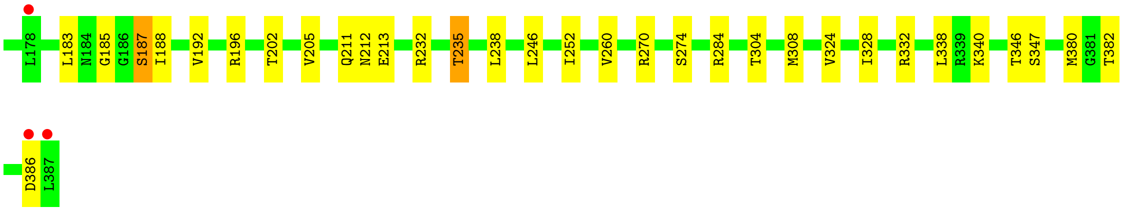
Chain L3:



• Molecule 40: 60S ribosomal protein L3

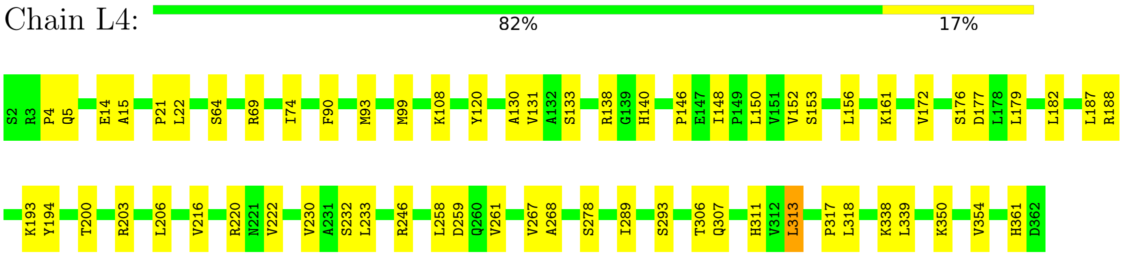
Chain l3:





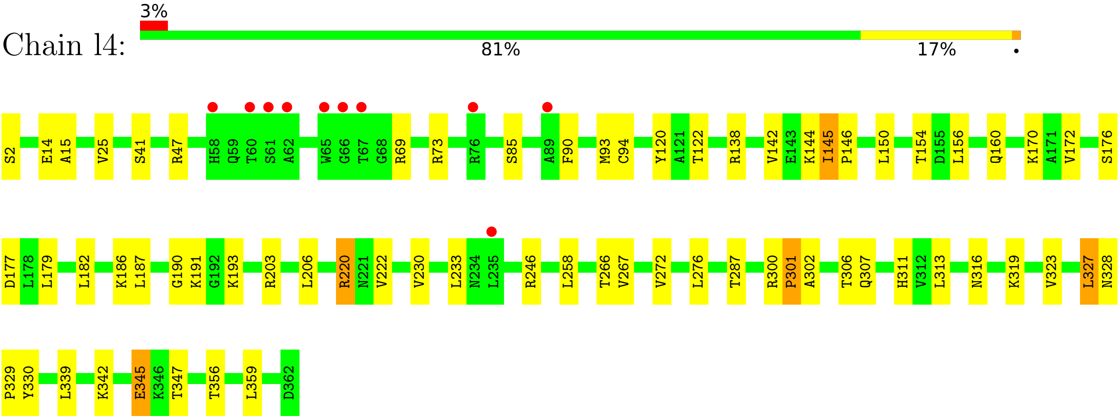
- Molecule 41: 60S ribosomal protein L4-A

Chain L4:



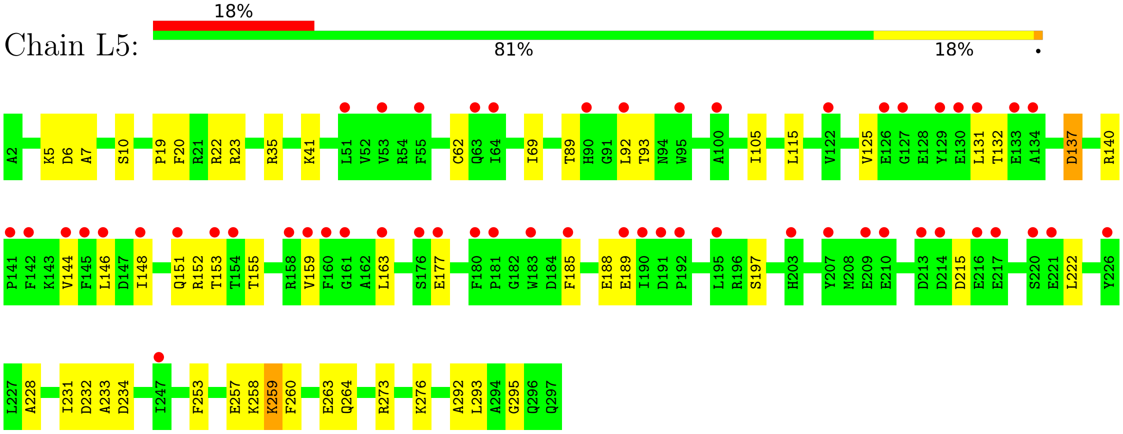
- Molecule 41: 60S ribosomal protein L4-A

Chain l4:



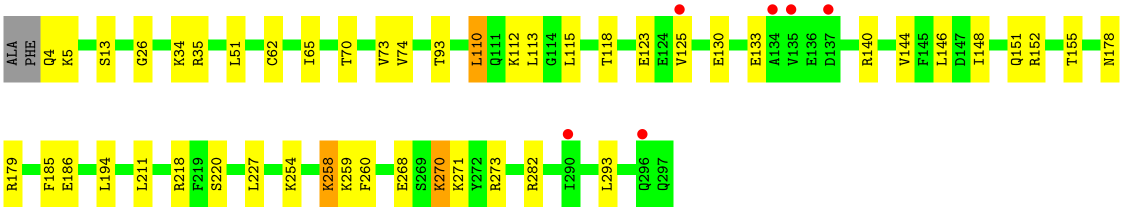
- Molecule 42: 60S ribosomal protein L5

Chain L5:



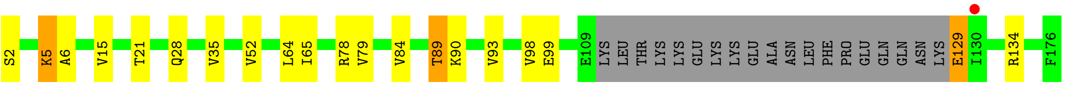
- Molecule 42: 60S ribosomal protein L5

Chain l5:



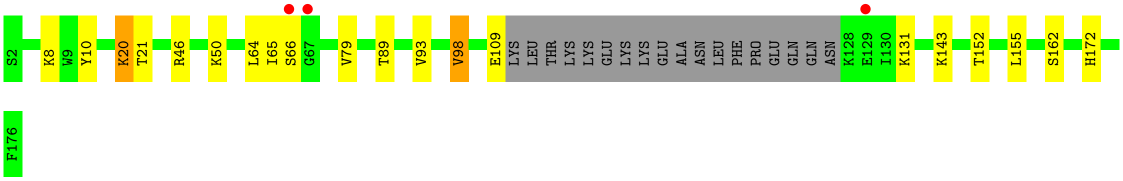
- Molecule 43: 60S ribosomal protein L6-A

Chain L6:



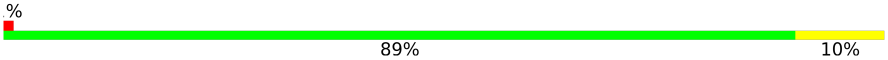
- Molecule 43: 60S ribosomal protein L6-A

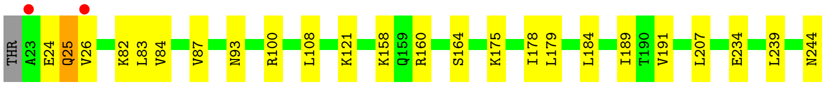
Chain l6:



- Molecule 44: 60S ribosomal protein L7-A

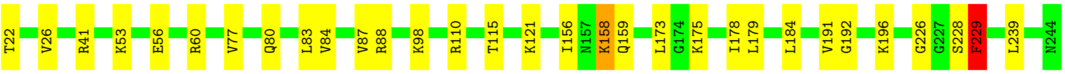
Chain L7:





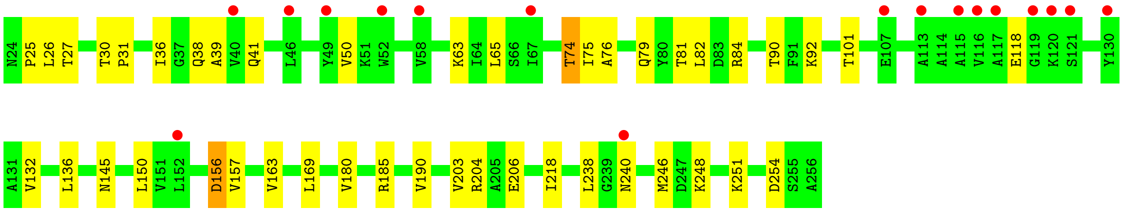
- Molecule 44: 60S ribosomal protein L7-A

Chain l7:

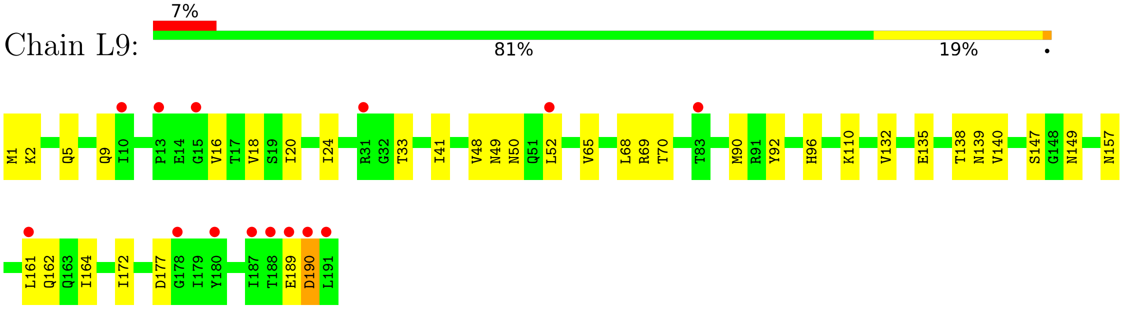


- Molecule 45: 60S ribosomal protein L8-A

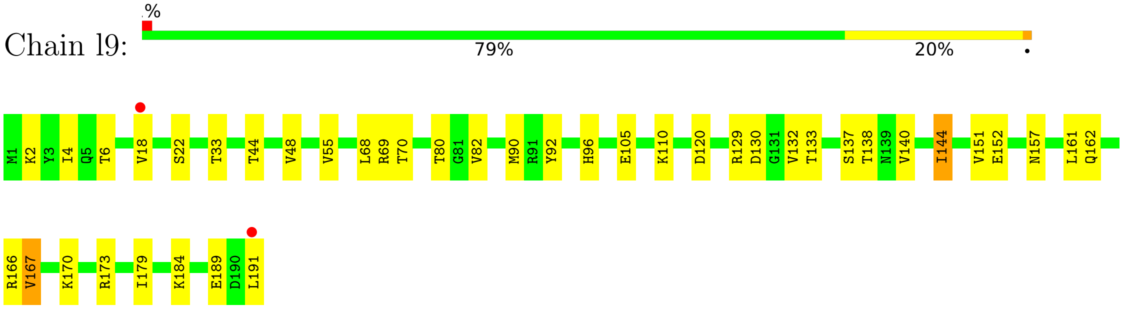
Chain L8:



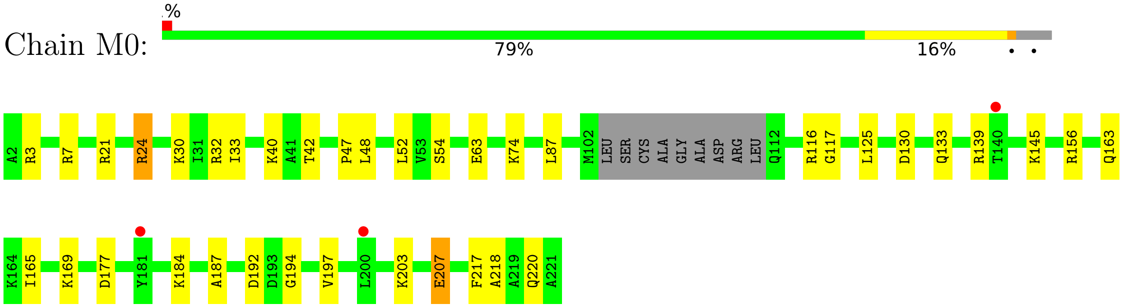
- Molecule 46: 60S ribosomal protein L9-A



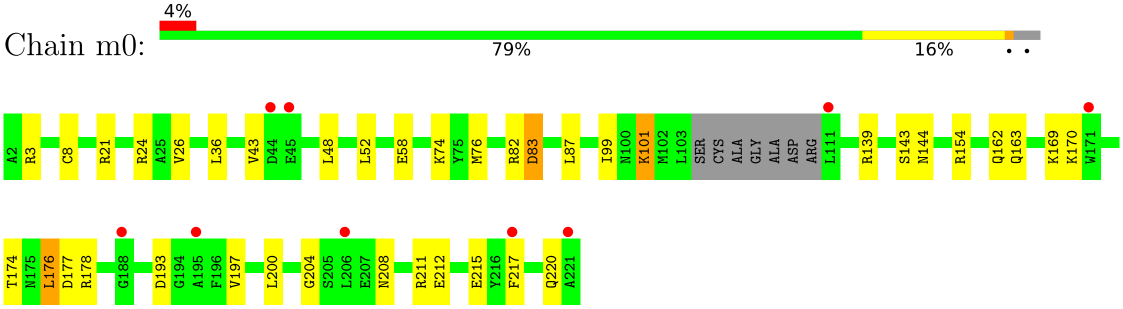
- Molecule 46: 60S ribosomal protein L9-A



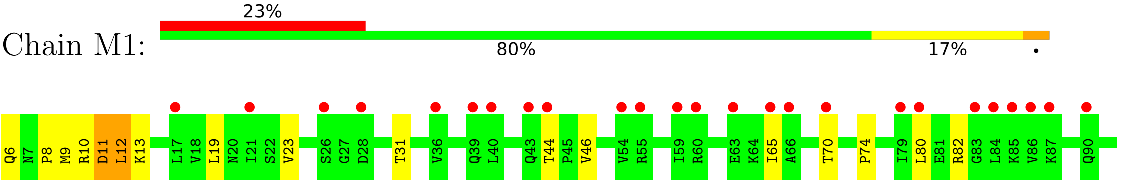
- Molecule 47: 60S ribosomal protein L10

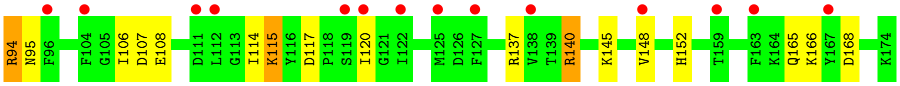


- Molecule 47: 60S ribosomal protein L10



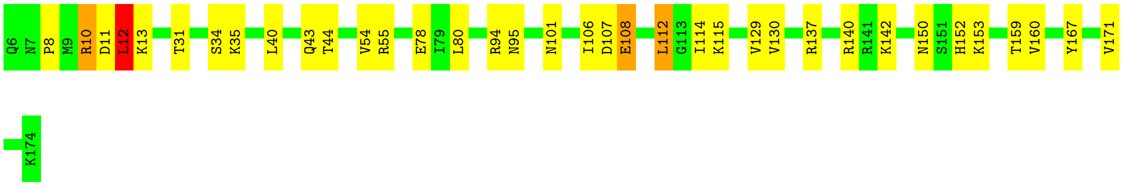
- Molecule 48: 60S ribosomal protein L11-B





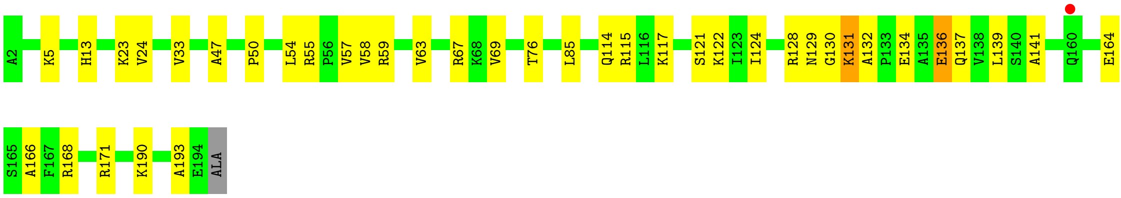
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:



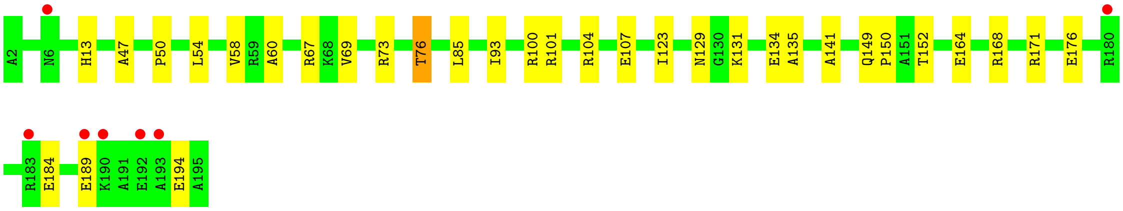
- Molecule 49: 60S ribosomal protein L13-A

Chain M3:



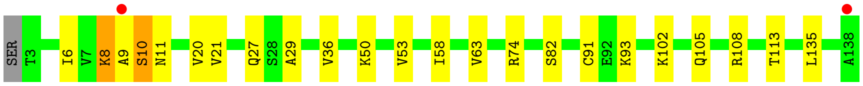
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:



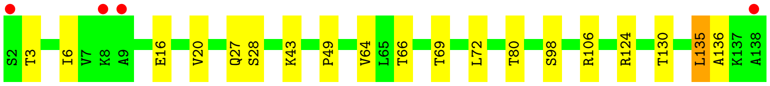
- Molecule 50: 60S ribosomal protein L14-A

Chain M4:

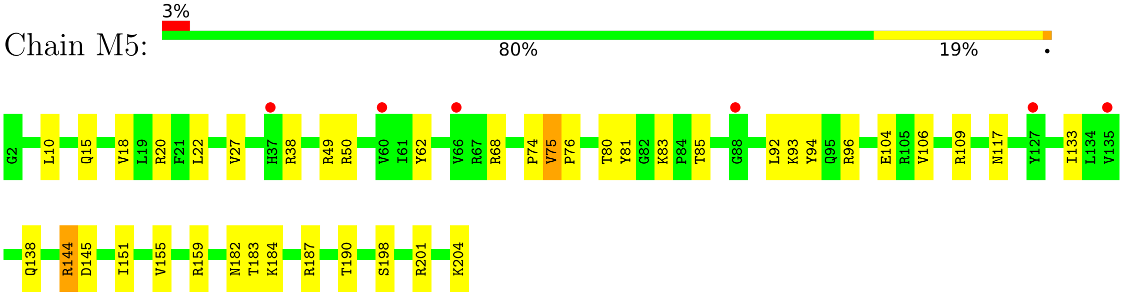


- Molecule 50: 60S ribosomal protein L14-A

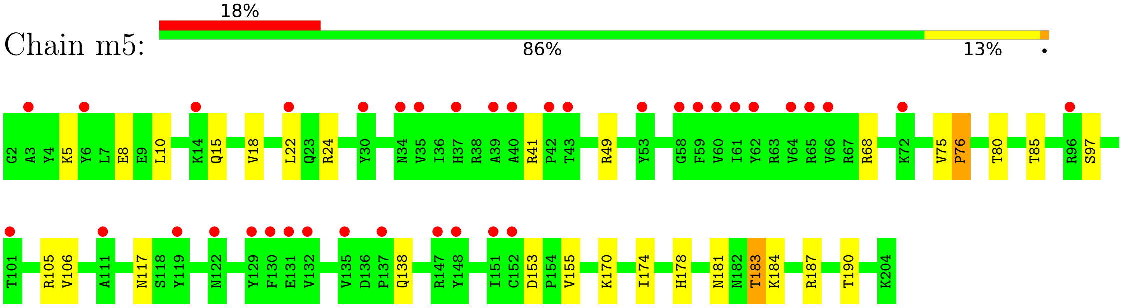
Chain m4:



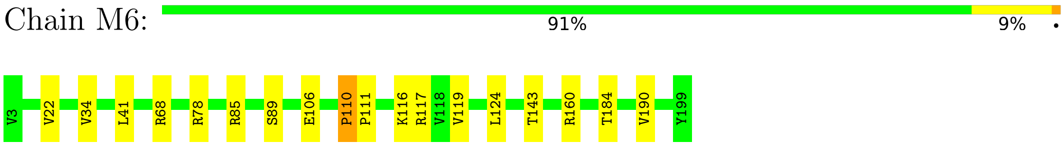
- Molecule 51: 60S ribosomal protein L15-A



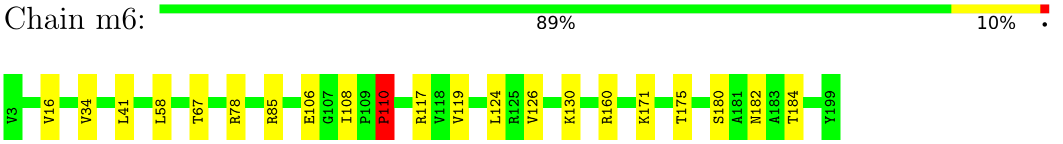
- Molecule 51: 60S ribosomal protein L15-A



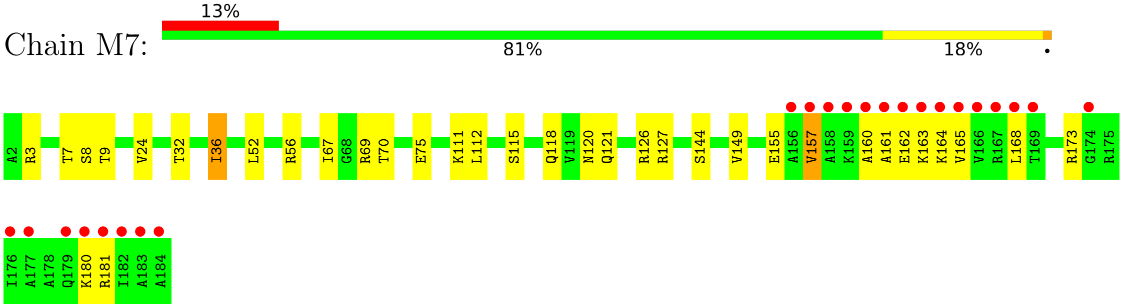
- Molecule 52: 60S ribosomal protein L16-A



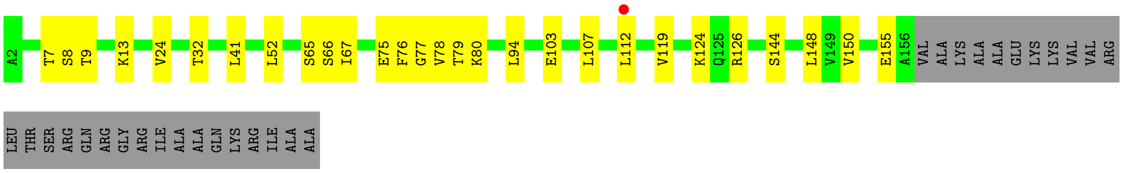
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 53: 60S ribosomal protein L17-A

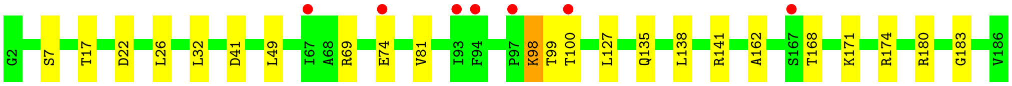


- Molecule 53: 60S ribosomal protein L17-A



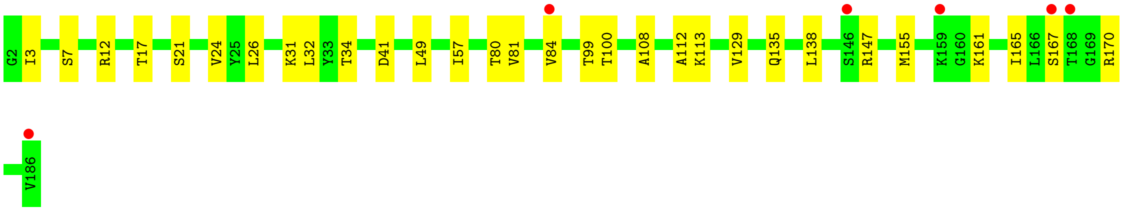
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



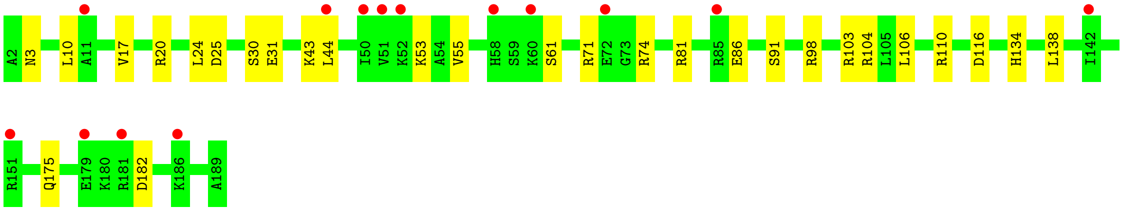
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



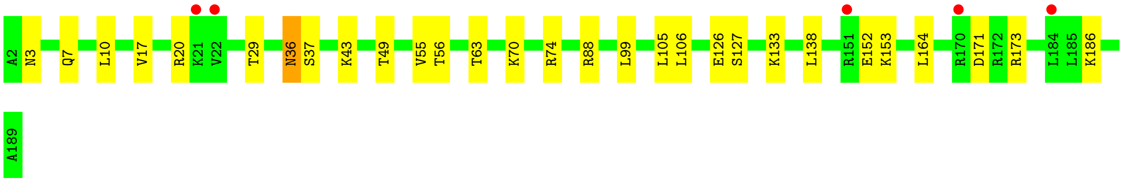
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



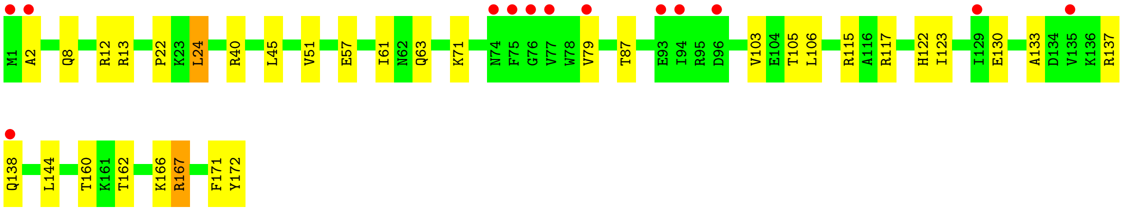
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



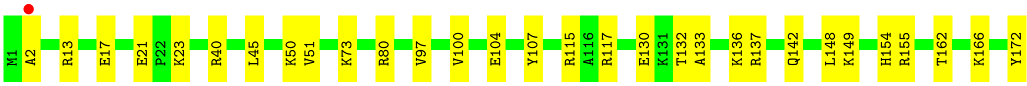
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



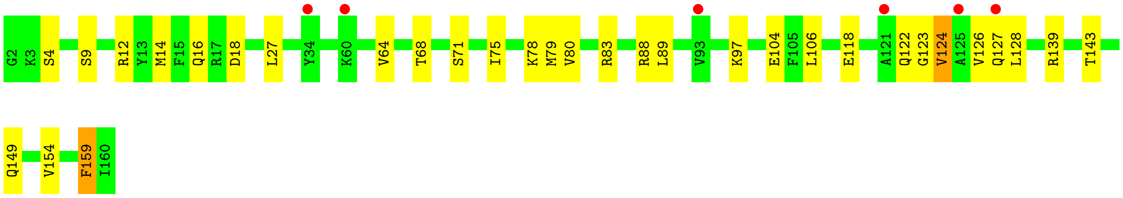
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



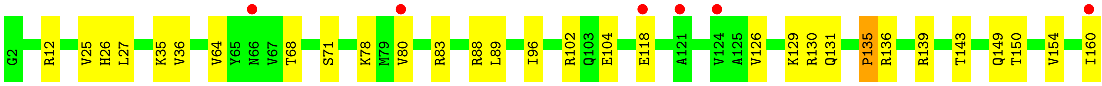
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



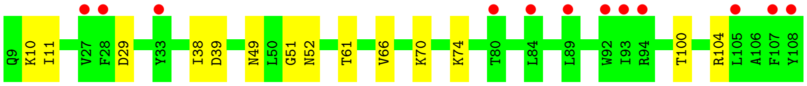
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



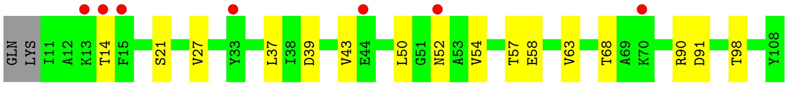
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:



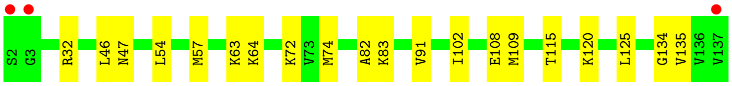
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



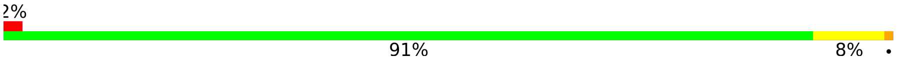
- Molecule 59: 60S ribosomal protein L23-A

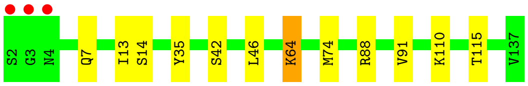
Chain N3:



- Molecule 59: 60S ribosomal protein L23-A

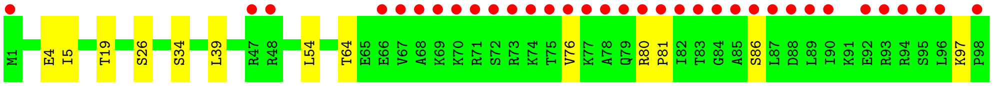
Chain n3:





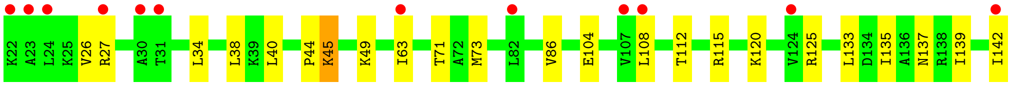
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:



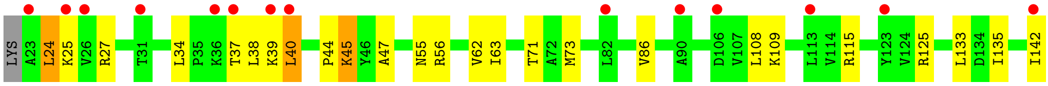
- Molecule 61: 60S ribosomal protein L25

Chain N5:



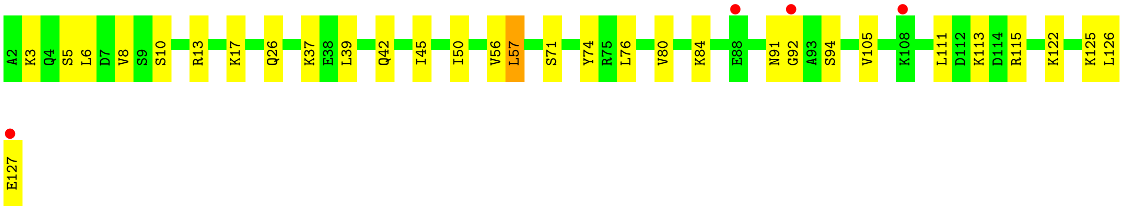
- Molecule 61: 60S ribosomal protein L25

Chain n5:



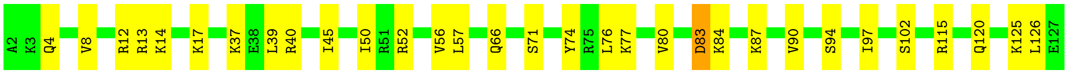
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:

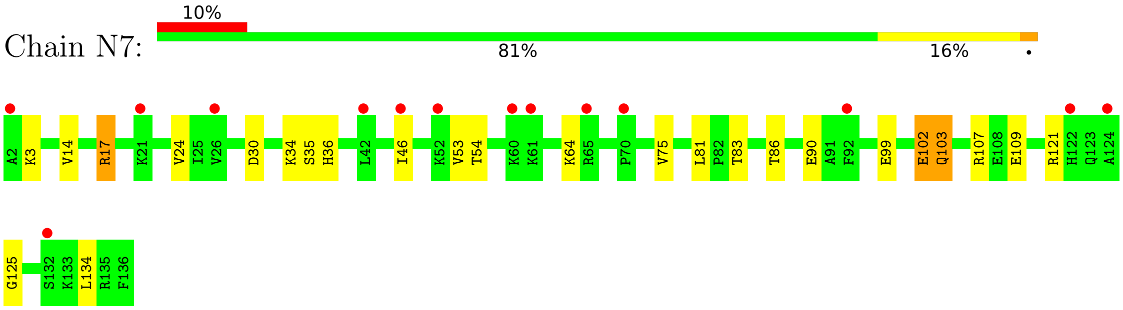


- Molecule 62: 60S ribosomal protein L26-A

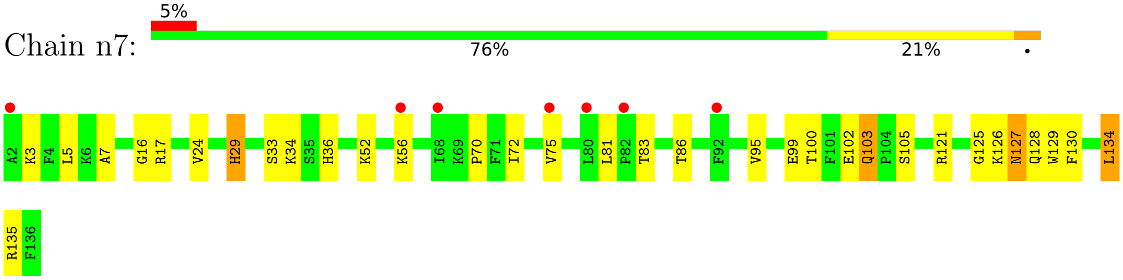
Chain n6:



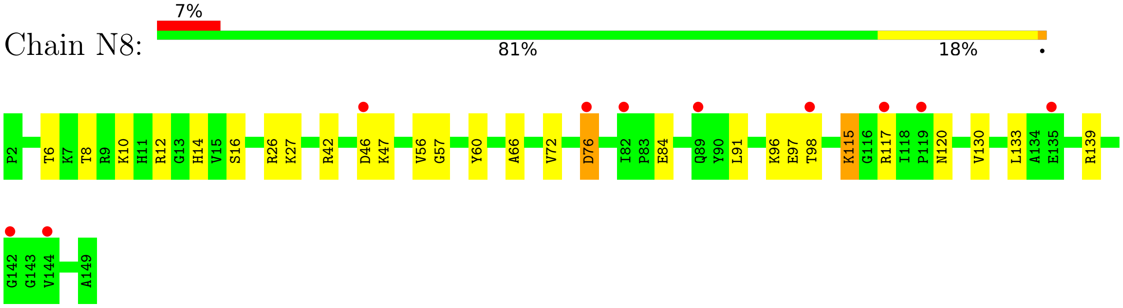
- Molecule 63: 60S ribosomal protein L27-A



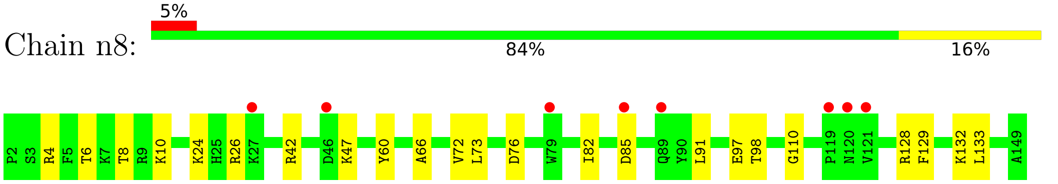
- Molecule 63: 60S ribosomal protein L27-A



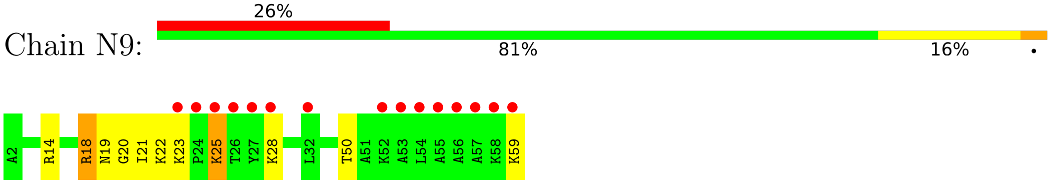
- Molecule 64: 60S ribosomal protein L28



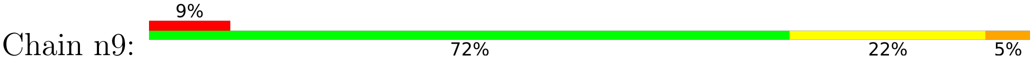
- Molecule 64: 60S ribosomal protein L28

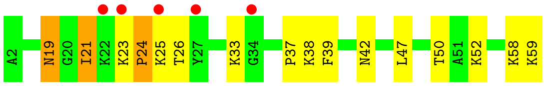


- Molecule 65: 60S ribosomal protein L29



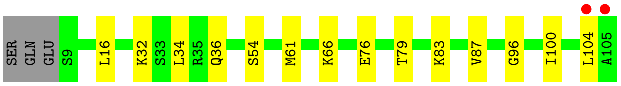
- Molecule 65: 60S ribosomal protein L29





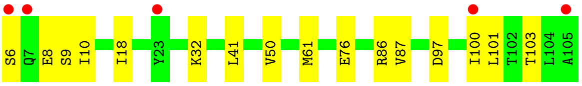
- Molecule 66: 60S ribosomal protein L30

Chain O0:



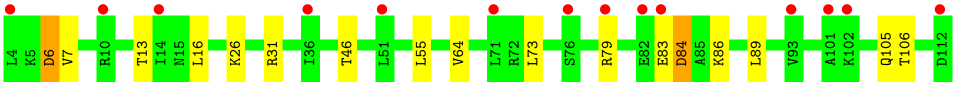
- Molecule 66: 60S ribosomal protein L30

Chain o0:



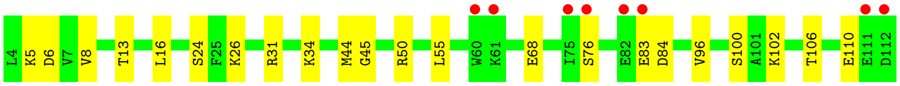
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



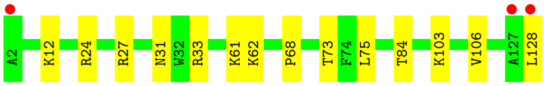
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



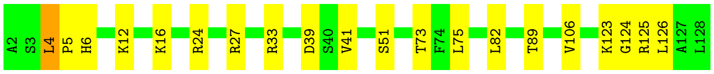
- Molecule 68: 60S ribosomal protein L32

Chain O2:



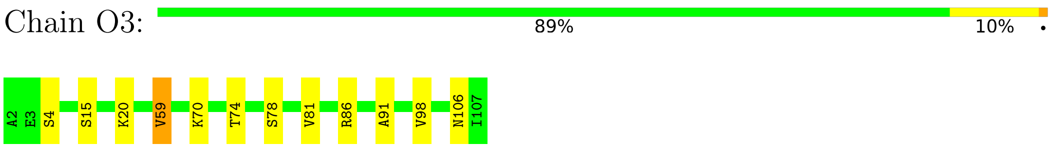
- Molecule 68: 60S ribosomal protein L32

Chain o2:



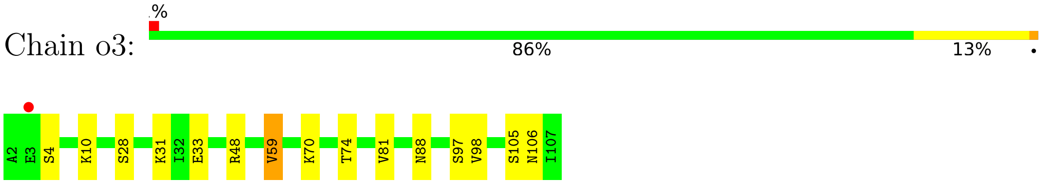
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



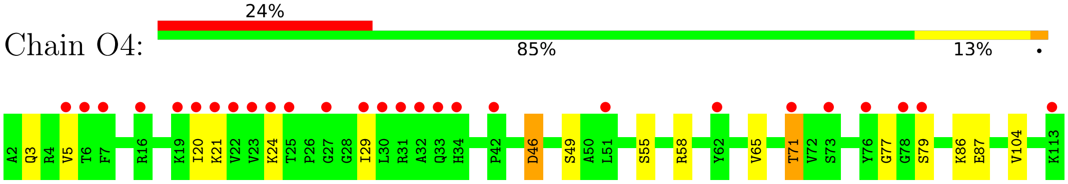
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



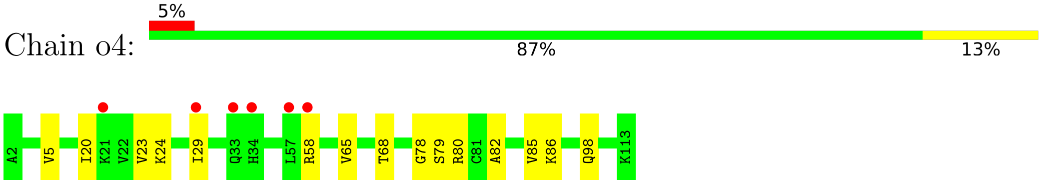
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



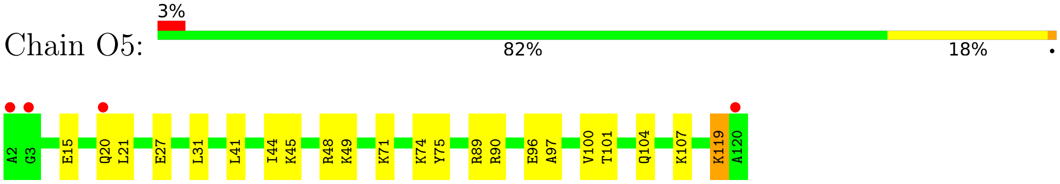
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



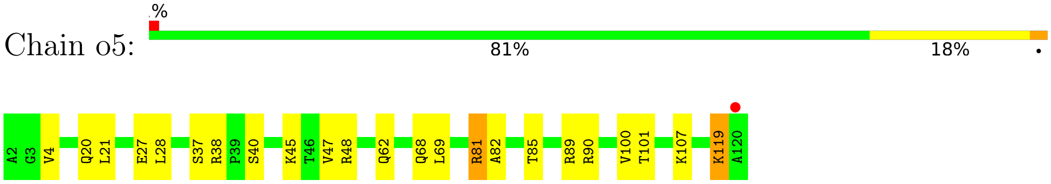
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



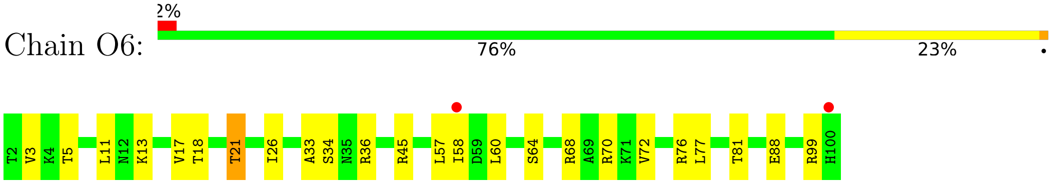
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



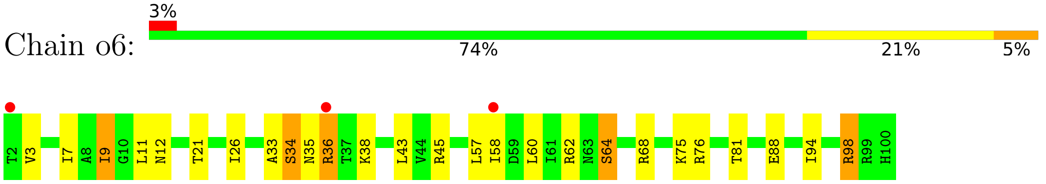
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



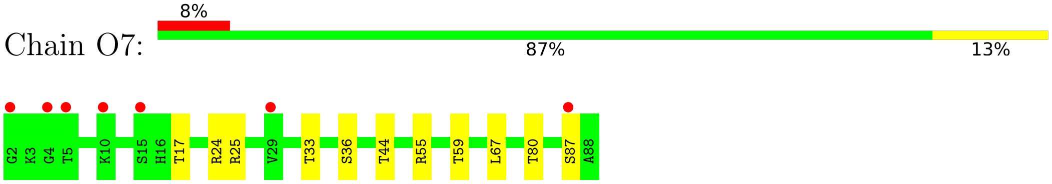
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



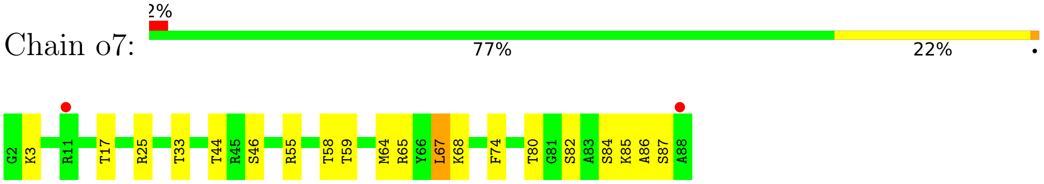
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



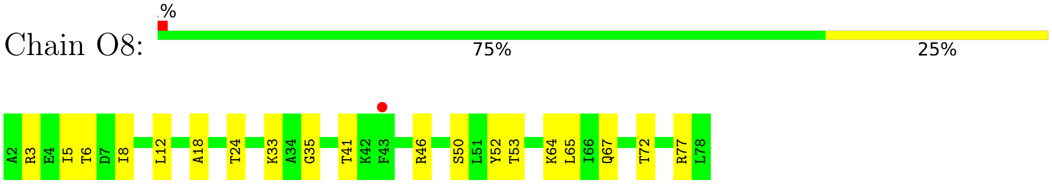
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



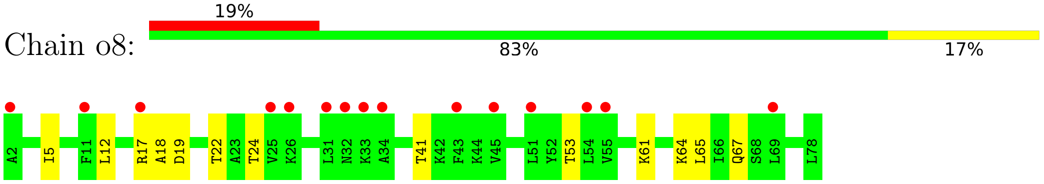
- Molecule 74: 60S ribosomal protein L38

Chain O8:



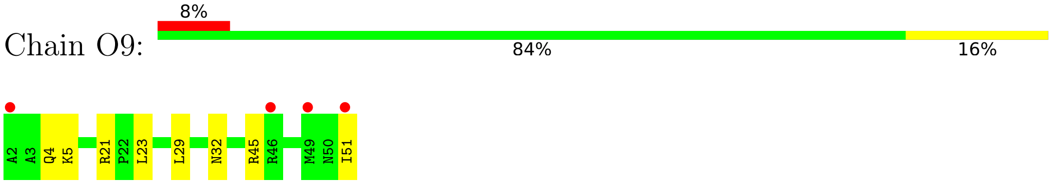
- Molecule 74: 60S ribosomal protein L38

Chain o8:



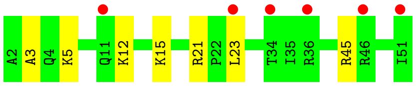
- Molecule 75: 60S ribosomal protein L39

Chain O9:



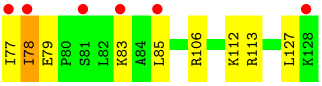
- Molecule 75: 60S ribosomal protein L39

Chain o9:



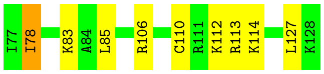
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



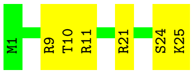
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



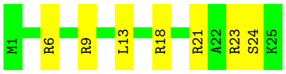
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



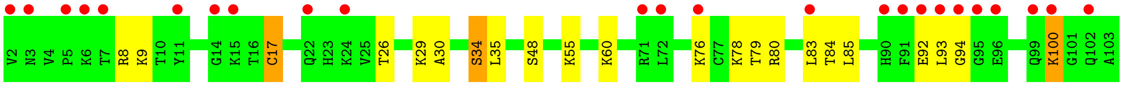
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



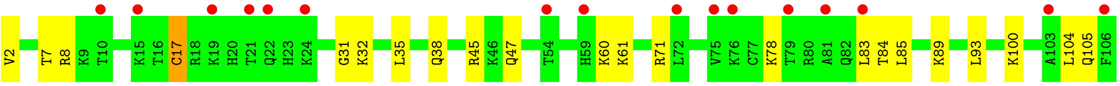
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



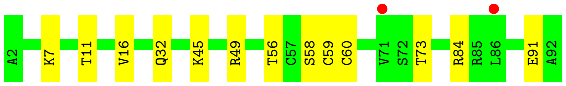
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



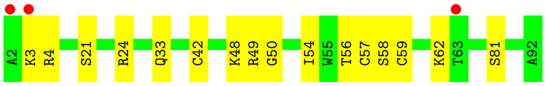
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



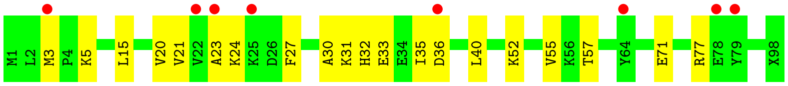
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



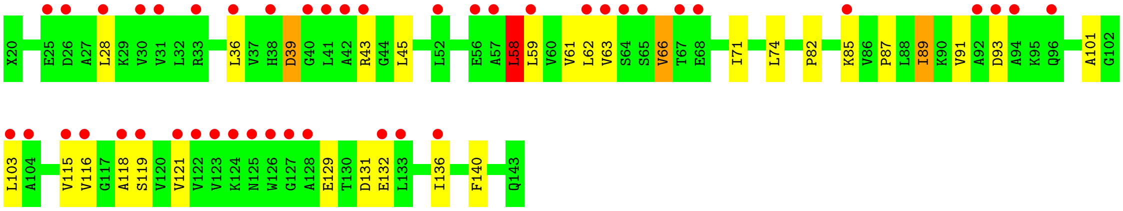
- Molecule 80: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10

Chain c0:



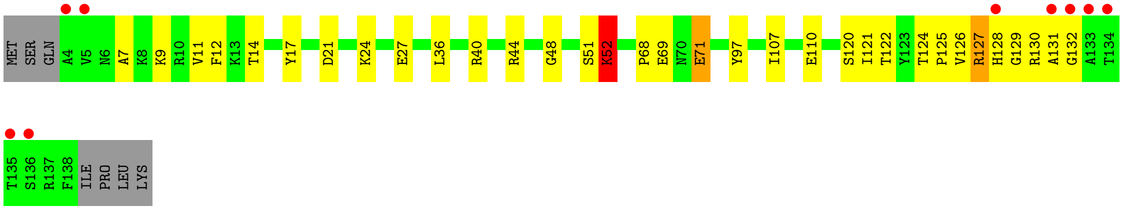
- Molecule 81: 40S Ribosomal Protein S12

Chain c2:



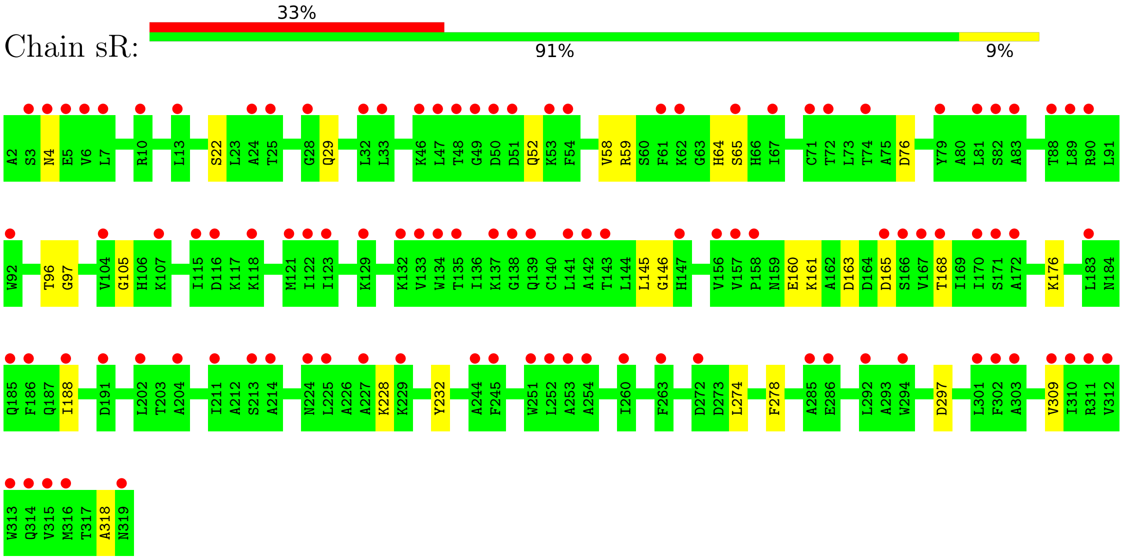
- Molecule 82: 40S ribosomal protein S15

Chain c5:



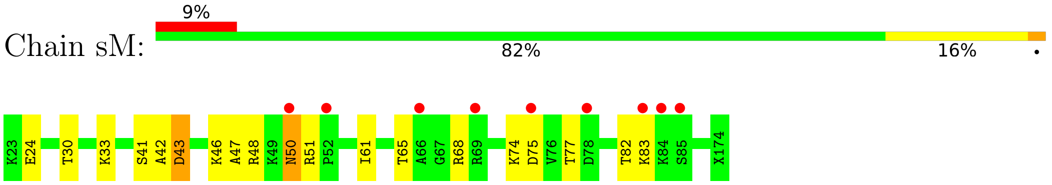
- Molecule 83: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



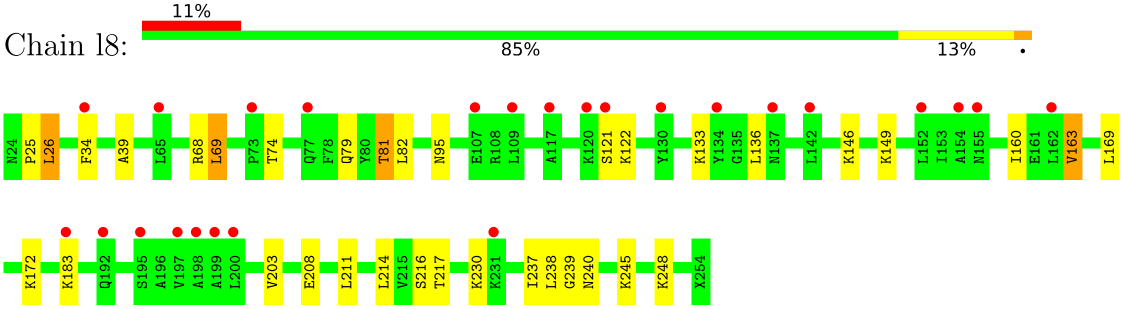
- Molecule 84: Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1

Chain sM:



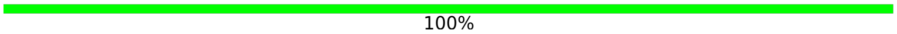
- Molecule 85: 60S ribosomal protein L8-A,60S ribosomal protein L8-A,60S Ribosomal Protein L8

Chain l8:



- Molecule 86: 60S Ribosomal Protein L12

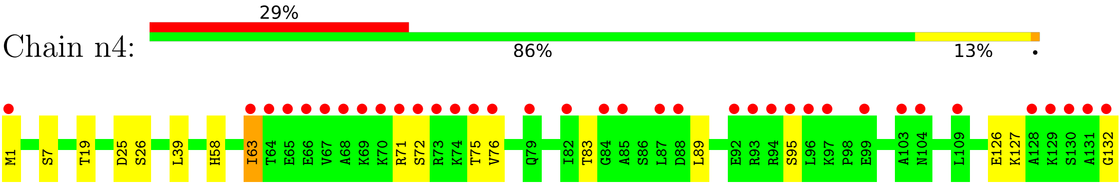
Chain m2:

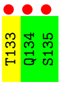


There are no outlier residues recorded for this chain.

- Molecule 87: 60S ribosomal protein L24-A

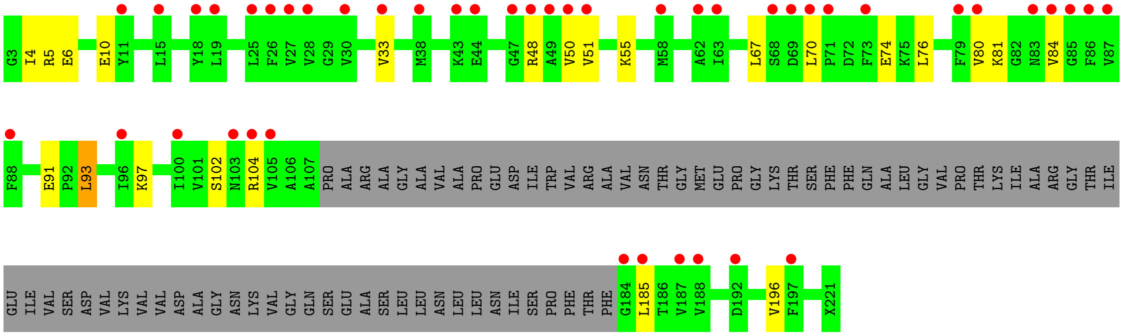
Chain n4:





- Molecule 88: 60S acidic ribosomal protein P0,60S acidic ribosomal protein P0,60S Ribosomal Protein P0

Chain p0:



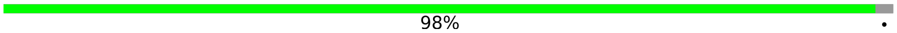
- Molecule 89: 60S Ribosomal Protein P1/2

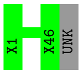
Chain p1:

There are no outlier residues recorded for this chain.

- Molecule 89: 60S Ribosomal Protein P1/2

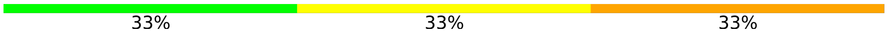
Chain p2:





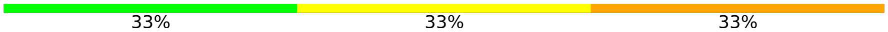
- Molecule 90: aminoacyl-tRNA fragment ACCPmn

Chain A:



- Molecule 90: aminoacyl-tRNA fragment ACCPmn

Chain a:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.18Å 288.24Å 303.58Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	172.59 – 3.25 172.59 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (172.59-3.25) 99.9 (172.59-3.25)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.208 , 0.249 0.210 , 0.251	Depositor DCC
R_{free} test set	23194 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	414290	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: OHX, ZN, PPU, MG

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	2	0.56	1/42468 (0.0%)	1.09	161/66173 (0.2%)
1	6	0.64	3/42790 (0.0%)	1.13	143/66673 (0.2%)
2	S0	0.38	1/1617 (0.1%)	0.54	0/2215
2	s0	0.39	0/1623	0.57	0/2222
3	S1	0.31	0/1735	0.58	2/2335 (0.1%)
3	s1	0.39	0/1748	0.58	0/2352
4	S2	0.36	0/1665	0.56	0/2263
4	s2	0.44	0/1665	0.64	1/2263 (0.0%)
5	S3	0.38	0/1759	0.54	0/2368
5	s3	0.37	0/1759	0.55	0/2368
6	S4	0.38	0/2109	0.61	0/2839
6	s4	0.44	1/2109 (0.0%)	0.62	1/2839 (0.0%)
7	S5	0.34	0/1629	0.55	0/2202
7	s5	0.36	0/1629	0.54	0/2202
8	S6	0.38	0/1823	0.55	0/2439
8	s6	0.43	0/1779	0.62	0/2379
9	S7	0.36	0/1506	0.58	0/2028
9	s7	0.36	0/1516	0.58	0/2043
10	S8	0.41	0/1514	0.59	1/2021 (0.0%)
10	s8	0.46	0/1514	0.63	1/2021 (0.0%)
11	S9	0.36	0/1519	0.55	0/2035
11	s9	0.43	0/1519	0.60	0/2035
12	C0	0.31	0/725	0.54	1/978 (0.1%)
13	C1	0.39	0/1195	0.57	0/1612
13	c1	0.45	0/1194	0.62	0/1610
14	C2	0.33	0/898	0.60	0/1220
15	C3	0.38	0/1215	0.58	1/1638 (0.1%)
15	c3	0.39	0/1215	0.59	0/1638
16	C4	0.35	0/901	0.56	0/1217
16	c4	0.40	0/960	0.59	0/1290
17	C5	0.39	0/998	0.57	0/1341
18	C6	0.36	0/1125	0.64	2/1510 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	c6	0.34	0/1131	0.58	1/1518 (0.1%)
19	C7	0.38	0/935	0.58	1/1254 (0.1%)
19	c7	0.33	0/914	0.56	0/1224
20	C8	0.37	0/1211	0.59	0/1628
20	c8	0.36	0/1211	0.60	2/1628 (0.1%)
21	C9	0.39	1/1130 (0.1%)	0.54	1/1517 (0.1%)
21	c9	0.38	0/1130	0.54	0/1517
22	D0	0.37	0/865	0.56	0/1169
22	d0	0.37	0/892	0.59	0/1205
23	D1	0.36	0/693	0.55	0/935
23	d1	0.43	0/693	0.59	0/935
24	D2	0.37	0/1038	0.63	3/1395 (0.2%)
24	d2	0.42	0/1038	0.62	1/1395 (0.1%)
25	D3	0.43	0/1139	0.61	0/1518
25	d3	0.50	0/1139	0.67	0/1518
26	D4	0.38	0/1087	0.54	0/1449
26	d4	0.42	0/1087	0.61	0/1449
27	D5	0.32	0/571	0.60	0/768
27	d5	0.31	0/566	0.52	0/761
28	D6	0.35	0/782	0.63	0/1047
28	d6	0.42	0/782	0.57	0/1047
29	D7	0.35	0/620	0.55	0/838
29	d7	0.35	0/620	0.55	0/838
30	D8	0.34	0/499	0.54	0/670
30	d8	0.33	0/499	0.56	0/670
31	D9	0.43	0/452	0.65	1/600 (0.2%)
31	d9	0.43	0/452	0.58	0/600
32	E0	0.35	0/483	0.55	0/643
32	e0	0.40	0/499	0.60	0/665
33	E1	0.35	0/577	0.66	0/770
33	e1	0.34	0/619	0.68	2/822 (0.2%)
34	SR	0.32	0/2490	0.54	0/3389
35	SM	0.40	0/984	0.59	0/1323
36	1	0.81	15/75394 (0.0%)	1.28	488/117545 (0.4%)
36	5	0.84	23/75414 (0.0%)	1.31	508/117575 (0.4%)
37	3	0.70	0/2883	1.16	6/4491 (0.1%)
37	7	0.81	0/2883	1.32	19/4491 (0.4%)
38	4	0.77	0/3746	1.27	23/5832 (0.4%)
38	8	0.74	0/3746	1.19	11/5832 (0.2%)
39	L2	0.51	1/1948 (0.1%)	0.66	0/2617
39	l2	0.50	0/1946	0.70	2/2614 (0.1%)
40	L3	0.51	1/3146 (0.0%)	0.65	0/4228
40	l3	0.56	0/3146	0.69	1/4228 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	L4	0.54	0/2800	0.70	0/3790
41	l4	0.51	1/2800 (0.0%)	0.68	2/3790 (0.1%)
42	L5	0.45	1/2425 (0.0%)	0.59	0/3271
42	l5	0.56	1/2408 (0.0%)	0.64	2/3248 (0.1%)
43	L6	0.50	0/1260	0.65	0/1694
43	l6	0.55	0/1269	0.66	0/1705
44	L7	0.54	0/1821	0.67	1/2451 (0.0%)
44	l7	0.57	0/1828	0.65	2/2461 (0.1%)
45	L8	0.42	0/1836	0.58	1/2481 (0.0%)
46	L9	0.47	0/1539	0.63	0/2073
46	l9	0.54	0/1539	0.65	0/2073
47	M0	0.55	0/1741	0.65	1/2335 (0.0%)
47	m0	0.60	1/1758 (0.1%)	0.71	1/2358 (0.0%)
48	M1	0.40	0/1374	0.58	0/1842
48	m1	0.54	0/1374	0.69	3/1842 (0.2%)
49	M3	0.54	1/1568 (0.1%)	0.68	0/2106
49	m3	0.48	0/1573	0.67	0/2113
50	M4	0.49	0/1068	0.64	0/1438
50	m4	0.52	0/1074	0.62	0/1446
51	M5	0.52	0/1757	0.68	0/2354
51	m5	0.47	0/1757	0.63	0/2354
52	M6	0.60	0/1585	0.67	0/2128
52	m6	0.66	0/1585	0.69	0/2128
53	M7	0.54	0/1443	0.67	1/1944 (0.1%)
53	m7	0.62	0/1250	0.69	0/1683
54	M8	0.51	0/1465	0.66	0/1965
54	m8	0.50	0/1465	0.69	0/1965
55	M9	0.41	0/1538	0.57	0/2050
55	m9	0.42	0/1538	0.55	0/2050
56	N0	0.51	0/1481	0.66	1/1990 (0.1%)
56	n0	0.56	0/1481	0.66	0/1990
57	N1	0.51	0/1300	0.64	0/1743
57	n1	0.58	0/1300	0.66	0/1743
58	N2	0.36	0/812	0.53	0/1099
58	n2	0.38	0/794	0.55	0/1076
59	N3	0.51	0/1018	0.70	0/1369
59	n3	0.60	0/1018	0.71	0/1369
60	N4	0.45	0/712	0.57	0/958
61	N5	0.45	0/979	0.65	0/1321
61	n5	0.45	0/974	0.63	0/1314
62	N6	0.51	0/1004	0.72	2/1341 (0.1%)
62	n6	0.48	0/1004	0.70	0/1341
63	N7	0.44	0/1118	0.57	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
63	n7	0.48	1/1118 (0.1%)	0.55	0/1497
64	N8	0.50	0/1204	0.70	1/1612 (0.1%)
64	n8	0.52	1/1204 (0.1%)	0.67	1/1612 (0.1%)
65	N9	0.50	0/473	0.62	0/629
65	n9	0.52	0/473	0.77	0/629
66	O0	0.38	0/751	0.52	0/1008
66	o0	0.39	0/775	0.59	0/1040
67	O1	0.47	0/890	0.58	0/1196
67	o1	0.57	0/897	0.61	0/1205
68	O2	0.54	0/1041	0.67	0/1394
68	o2	0.57	0/1041	0.68	0/1394
69	O3	0.64	0/868	0.65	0/1168
69	o3	0.62	0/868	0.66	0/1168
70	O4	0.47	0/890	0.61	0/1189
70	o4	0.43	0/890	0.59	0/1189
71	O5	0.51	0/978	0.62	0/1301
71	o5	0.44	0/974	0.56	0/1297
72	O6	0.45	0/778	0.64	0/1034
72	o6	0.41	0/777	0.59	0/1033
73	O7	0.49	0/696	0.63	0/923
73	o7	0.49	0/696	0.67	0/923
74	O8	0.39	0/618	0.53	0/826
74	o8	0.38	0/614	0.52	0/822
75	O9	0.52	0/443	0.72	0/588
75	o9	0.52	0/443	0.68	0/588
76	Q0	0.57	0/423	0.65	0/562
76	q0	0.63	0/423	0.72	0/562
77	Q1	0.46	0/234	0.67	0/300
77	q1	0.60	0/234	0.65	0/300
78	Q2	0.72	1/860 (0.1%)	0.67	0/1136
78	q2	0.69	1/860 (0.1%)	0.71	1/1136 (0.1%)
79	Q3	0.50	0/701	0.65	0/934
79	q3	0.56	0/701	0.64	0/934
80	c0	0.33	0/693	0.52	0/933
81	c2	0.30	0/824	0.58	1/1116 (0.1%)
82	c5	0.41	0/1060	0.58	0/1426
83	sR	0.32	0/2495	0.53	0/3395
84	sM	0.44	0/481	0.57	0/644
85	l8	0.41	0/1765	0.59	1/2387 (0.0%)
87	n4	0.47	0/1052	0.58	0/1398
88	p0	0.36	0/977	0.57	0/1313
90	A	0.74	0/43	1.56	1/64 (1.6%)
90	a	0.79	0/43	2.00	2/64 (3.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.65	56/430203 (0.0%)	1.04	1409/631685 (0.2%)

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
3	S1	0	1
6	S4	0	1
7	s5	0	2
9	S7	0	1
10	s8	0	1
11	s9	0	1
13	c1	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
24	D2	0	1
25	D3	0	1
25	d3	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	2
33	E1	0	1
33	e1	0	1
39	L2	0	1
39	l2	0	3
40	L3	0	1
40	l3	0	1
42	l5	0	2
43	L6	0	2
44	l7	0	2
45	L8	0	1
49	M3	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
56	N0	0	2
56	n0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	N1	0	1
61	N5	0	1
63	n7	0	1
64	n8	0	1
65	N9	0	2
65	n9	0	2
68	o2	0	1
70	O4	0	1
82	c5	0	1
87	n4	0	1
All	All	0	56

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	14.16	2.06	1.82
78	q2	17	CYS	CB-SG	11.98	2.02	1.82
36	5	2971	A	N9-C4	11.70	1.44	1.37
63	n7	36	HIS	C-N	9.18	1.51	1.34
36	5	1152	G	N9-C4	-8.42	1.31	1.38
36	5	3019	U	C4-O4	8.39	1.30	1.23
36	5	2971	A	N3-C4	8.28	1.39	1.34
6	s4	82	TYR	C-N	-7.47	1.20	1.34
36	1	2971	A	N9-C4	7.32	1.42	1.37
36	5	430	U	P-OP2	7.17	1.61	1.49
36	5	2875	U	N1-C2	6.81	1.44	1.38
36	1	2401	A	N3-C4	6.80	1.39	1.34
42	l5	179	ARG	C-N	-6.79	1.18	1.34
36	5	2996	U	N1-C2	6.64	1.44	1.38
36	5	2404	A	N7-C5	6.59	1.43	1.39
36	1	2207	A	N9-C4	6.55	1.41	1.37
2	S0	95	ALA	C-N	6.52	1.49	1.34
36	5	2401	A	N3-C4	6.47	1.38	1.34
36	1	2404	A	N3-C4	6.35	1.38	1.34
36	5	2404	A	C5-C6	6.32	1.46	1.41
36	5	566	G	C8-N7	6.22	1.34	1.30
36	1	2714	G	N9-C4	-6.12	1.33	1.38
36	5	1152	G	N3-C4	-6.12	1.31	1.35
36	5	1152	G	N9-C8	6.01	1.42	1.37
49	M3	132	ALA	C-N	5.89	1.45	1.34
36	5	1159	A	N3-C4	-5.84	1.31	1.34
1	6	1720	G	C6-O6	5.83	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1143	A	N9-C4	-5.80	1.34	1.37
36	5	2401	A	N9-C4	5.75	1.41	1.37
41	l4	94	CYS	CB-SG	-5.57	1.72	1.81
36	1	1103	A	N9-C4	5.55	1.41	1.37
39	L2	118	GLU	C-N	-5.53	1.21	1.34
36	5	1192	C	N1-C2	5.45	1.45	1.40
36	1	2208	A	N9-C4	5.45	1.41	1.37
36	5	2372	A	N7-C5	-5.44	1.35	1.39
36	5	1922	A	N9-C4	-5.41	1.34	1.37
36	1	2401	A	N7-C5	5.35	1.42	1.39
40	L3	7	GLU	CG-CD	5.30	1.59	1.51
47	m0	8	CYS	CB-SG	-5.25	1.73	1.81
36	5	523	A	N9-C4	-5.25	1.34	1.37
21	C9	116	ILE	C-N	-5.18	1.22	1.34
36	1	2401	A	C6-N1	5.18	1.39	1.35
64	n8	98	THR	C-N	5.18	1.46	1.34
42	L5	62	CYS	CB-SG	-5.17	1.73	1.81
36	1	2404	A	N7-C5	5.15	1.42	1.39
36	1	361	A	C6-N1	-5.14	1.31	1.35
1	6	754	A	N3-C4	5.12	1.38	1.34
1	2	1508	U	C4-O4	5.11	1.27	1.23
36	5	2404	A	N9-C4	5.09	1.41	1.37
36	5	2941	A	N9-C4	-5.08	1.34	1.37
36	1	2875	U	N1-C2	5.07	1.43	1.38
1	6	359	A	N9-C4	-5.06	1.34	1.37
36	1	1399	A	N9-C4	-5.04	1.34	1.37
36	1	2726	C	N3-C4	-5.04	1.30	1.33
36	1	2147	A	N9-C4	-5.02	1.34	1.37
36	5	2872	A	C6-N1	5.01	1.39	1.35

All (1409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-N9	-18.57	114.86	126.00
36	5	1152	G	N3-C4-C5	17.62	137.41	128.60
36	5	1152	G	C2-N3-C4	-14.18	104.81	111.90
36	1	1495	U	C5-C6-N1	-12.24	116.58	122.70
36	5	2704	A	O5'-P-OP1	-11.99	94.91	105.70
36	1	2714	G	N3-C4-N9	-11.85	118.89	126.00
36	5	1305	U	O5'-P-OP1	-11.66	95.21	105.70
36	1	2714	G	N3-C4-C5	11.50	134.35	128.60
36	1	2704	A	O5'-P-OP1	-11.08	95.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2726	C	C6-N1-C2	-10.14	116.25	120.30
36	1	1177	G	N1-C6-O6	10.07	125.94	119.90
38	8	80	A	C8-N9-C4	-9.97	101.81	105.80
38	8	80	A	N7-C8-N9	9.96	118.78	113.80
1	2	1096	C	N1-C2-O2	9.92	124.85	118.90
36	1	2617	U	C4-C5-C6	9.92	125.65	119.70
36	5	546	C	N1-C2-O2	9.88	124.83	118.90
36	1	2403	G	N1-C6-O6	9.75	125.75	119.90
36	5	2392	C	C6-N1-C2	9.73	124.19	120.30
36	5	2377	G	C8-N9-C4	9.65	110.26	106.40
36	5	2283	G	N1-C6-O6	9.63	125.68	119.90
36	1	609	G	O5'-P-OP2	-9.59	97.07	105.70
37	7	101	G	N1-C6-O6	9.55	125.63	119.90
36	5	2726	C	C5-C4-N4	9.53	126.87	120.20
36	1	3217	C	C2-N1-C1'	9.52	129.27	118.80
1	6	1720	G	C5-C6-N1	-9.52	106.74	111.50
36	5	3245	A	C5-N7-C8	-9.40	99.20	103.90
36	5	2872	A	O5'-P-OP1	-9.38	97.26	105.70
36	1	2572	C	N1-C2-O2	9.27	124.46	118.90
36	5	1152	G	C8-N9-C1'	9.25	139.03	127.00
36	5	2964	G	N1-C6-O6	-9.07	114.45	119.90
36	1	2726	C	C6-N1-C2	-9.04	116.68	120.30
36	1	2816	G	N1-C6-O6	9.01	125.30	119.90
36	5	2971	A	C2-N3-C4	9.01	115.10	110.60
36	5	3245	A	C2-N3-C4	-8.97	106.11	110.60
36	1	645	A	N1-C6-N6	-8.96	113.22	118.60
1	2	73	U	O4'-C1'-N1	8.96	115.37	108.20
36	1	1495	U	C2-N1-C1'	-8.91	107.01	117.70
36	5	546	C	N3-C2-O2	-8.90	115.67	121.90
36	5	2816	G	N1-C6-O6	8.88	125.23	119.90
36	5	1403	C	C6-N1-C2	8.87	123.85	120.30
36	5	2816	G	C5-C6-O6	-8.87	123.28	128.60
36	1	650	C	N1-C2-O2	-8.83	113.60	118.90
90	a	75	C	C6-N1-C2	-8.82	116.77	120.30
36	1	776	U	C4-C5-C6	8.76	124.96	119.70
36	1	372	A	O5'-P-OP2	-8.74	97.83	105.70
36	5	2871	G	O5'-P-OP2	-8.74	97.83	105.70
36	1	2726	C	C5-C4-N4	8.72	126.31	120.20
36	5	2572	C	N1-C2-O2	8.67	124.10	118.90
36	5	3245	A	N7-C8-N9	8.67	118.13	113.80
36	1	2617	U	N1-C2-N3	8.63	120.08	114.90
36	5	1481	A	C8-N9-C4	-8.56	102.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	2524	A	O4'-C1'-N9	8.55	115.04	108.20
36	1	2827	U	C2-N1-C1'	-8.54	107.45	117.70
36	1	2726	C	N3-C4-N4	-8.54	112.03	118.00
36	1	716	A	O5'-P-OP1	-8.52	98.03	105.70
1	6	144	U	N3-C2-O2	-8.50	116.25	122.20
36	1	2406	C	C6-N1-C2	8.50	123.70	120.30
36	5	1192	C	N1-C2-O2	8.49	124.00	118.90
36	5	3154	C	N1-C2-O2	8.47	123.98	118.90
1	2	74	U	O4'-C1'-N1	8.40	114.92	108.20
36	1	3238	G	N1-C6-O6	8.38	124.93	119.90
36	1	2355	G	N1-C6-O6	8.37	124.92	119.90
36	5	3245	A	N1-C6-N6	8.34	123.61	118.60
36	1	65	A	P-O3'-C3'	8.33	129.70	119.70
36	5	922	U	C5-C6-N1	-8.33	118.54	122.70
36	1	1177	G	C5-C6-O6	-8.31	123.61	128.60
36	5	776	U	C5-C6-N1	-8.29	118.56	122.70
36	1	2816	G	C5-C6-O6	-8.29	123.63	128.60
38	4	94	C	C6-N1-C2	8.28	123.61	120.30
36	1	2871	G	O5'-P-OP2	-8.28	98.25	105.70
36	5	2376	G	C5-C6-O6	-8.27	123.64	128.60
36	5	645	A	N1-C6-N6	-8.26	113.64	118.60
36	5	3004	C	C6-N1-C2	8.26	123.60	120.30
36	5	2996	U	N1-C2-O2	8.25	128.57	122.80
1	2	1096	C	C2-N1-C1'	8.25	127.87	118.80
36	1	406	G	O4'-C1'-N9	8.24	114.79	108.20
36	5	566	G	C5-N7-C8	-8.23	100.18	104.30
36	5	2964	G	C5-C6-O6	8.20	133.52	128.60
36	1	2868	U	N1-C2-O2	8.18	128.53	122.80
36	1	2314	U	C2-N1-C1'	8.17	127.50	117.70
36	5	1152	G	C5-N7-C8	-8.16	100.22	104.30
36	1	406	G	N3-C4-N9	-8.15	121.11	126.00
36	1	637	C	P-O3'-C3'	8.14	129.47	119.70
36	1	1949	G	O5'-P-OP1	-8.14	98.38	105.70
1	2	453	U	C2-N1-C1'	8.14	127.46	117.70
36	1	3306	U	N3-C2-O2	-8.12	116.51	122.20
36	5	1152	G	C4-N9-C1'	-8.10	115.97	126.50
1	6	453	U	C2-N1-C1'	8.08	127.39	117.70
36	1	2973	G	N1-C6-O6	8.07	124.74	119.90
37	7	101	G	C5-C6-O6	-8.04	123.77	128.60
36	5	1897	G	C4-C5-N7	8.03	114.01	110.80
36	5	2372	A	N1-C6-N6	8.01	123.41	118.60
36	1	2572	C	N3-C2-O2	-8.00	116.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	l7	229	PHE	CB-CG-CD1	7.98	126.39	120.80
36	1	2715	A	O5'-P-OP1	-7.96	98.54	105.70
36	5	1308	A	OP1-P-OP2	-7.94	107.69	119.60
36	1	3217	C	N1-C2-O2	7.94	123.66	118.90
1	6	194	U	C2-N1-C1'	7.94	127.22	117.70
1	2	453	U	N3-C2-O2	-7.92	116.66	122.20
36	1	885	U	C5-C6-N1	-7.89	118.75	122.70
36	1	517	G	N3-C4-C5	-7.87	124.67	128.60
36	5	2978	U	O4'-C1'-N1	7.87	114.49	108.20
36	5	2726	C	N3-C2-O2	-7.86	116.40	121.90
36	5	1307	G	P-O3'-C3'	7.83	129.09	119.70
36	5	2572	C	C2-N1-C1'	7.79	127.38	118.80
36	5	776	U	C4-C5-C6	7.79	124.38	119.70
36	5	1607	U	P-O3'-C3'	7.79	129.05	119.70
36	5	1879	A	O5'-P-OP1	7.79	120.05	110.70
36	1	3139	A	O5'-P-OP1	-7.78	98.70	105.70
36	1	1904	C	C6-N1-C2	-7.75	117.20	120.30
36	5	552	G	N1-C6-O6	7.74	124.55	119.90
1	6	1730	A	N1-C6-N6	7.74	123.25	118.60
36	1	1150	A	O5'-P-OP2	-7.73	98.74	105.70
36	1	2572	C	C2-N1-C1'	7.73	127.30	118.80
36	1	2827	U	C5-C6-N1	-7.70	118.85	122.70
36	5	1116	G	O5'-P-OP1	-7.69	98.78	105.70
36	5	2392	C	N3-C4-C5	7.69	124.98	121.90
36	1	1495	U	C4-C5-C6	7.67	124.30	119.70
1	2	558	U	N1-C2-O2	7.67	128.16	122.80
1	2	1389	C	N1-C2-O2	7.66	123.50	118.90
1	2	830	U	N3-C2-O2	-7.64	116.85	122.20
36	5	1604	G	C4-N9-C1'	7.64	136.44	126.50
36	1	439	C	N1-C2-O2	7.62	123.47	118.90
36	1	2868	U	N3-C2-O2	-7.61	116.87	122.20
36	5	1200	A	N1-C6-N6	7.58	123.15	118.60
1	2	1596	C	N3-C2-O2	-7.55	116.62	121.90
36	5	2683	U	N1-C2-O2	7.55	128.08	122.80
36	1	1365	G	C8-N9-C4	-7.54	103.39	106.40
1	2	145	A	C8-N9-C4	-7.52	102.79	105.80
1	2	321	C	C6-N1-C2	-7.51	117.30	120.30
1	2	639	U	N3-C2-O2	-7.50	116.95	122.20
36	5	2978	U	C5-C6-N1	-7.50	118.95	122.70
1	2	934	C	C2-N1-C1'	7.50	127.05	118.80
36	5	3154	C	C2-N1-C1'	7.49	127.04	118.80
36	5	3019	U	N3-C4-C5	-7.49	110.11	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2621	G	N1-C6-O6	7.49	124.39	119.90
1	2	1096	C	N3-C2-O2	-7.47	116.67	121.90
31	D9	36	LEU	CA-CB-CG	7.46	132.47	115.30
36	5	880	G	C4-N9-C1'	-7.45	116.82	126.50
36	1	650	C	N3-C2-O2	7.43	127.10	121.90
1	6	163	G	N3-C4-N9	-7.43	121.54	126.00
36	1	2978	U	O4'-C1'-N1	7.42	114.14	108.20
36	5	3152	U	N1-C2-N3	-7.42	110.45	114.90
36	1	835	G	O4'-C1'-N9	7.42	114.13	108.20
36	5	2385	G	N3-C4-C5	7.41	132.31	128.60
36	1	3319	U	P-O3'-C3'	7.39	128.57	119.70
36	5	635	G	C5-C6-O6	-7.39	124.17	128.60
1	2	831	U	C5-C6-N1	7.37	126.39	122.70
36	1	3344	A	O4'-C1'-N9	7.36	114.09	108.20
36	1	2819	A	O5'-P-OP2	-7.35	99.08	105.70
36	5	2327	U	C5-C6-N1	-7.35	119.03	122.70
36	5	3019	U	N3-C4-O4	7.30	124.51	119.40
36	1	3217	C	C6-N1-C1'	-7.29	112.05	120.80
36	1	645	A	N9-C4-C5	7.29	108.72	105.80
36	5	546	C	C6-N1-C2	-7.29	117.39	120.30
1	2	1537	C	C5-C4-N4	-7.27	115.11	120.20
1	2	558	U	N3-C2-O2	-7.27	117.11	122.20
37	7	101	G	C4-C5-N7	7.26	113.70	110.80
36	1	2714	G	C2-N3-C4	-7.25	108.27	111.90
36	5	437	G	C5-C6-O6	-7.25	124.25	128.60
36	1	1111	U	C6-N1-C2	7.22	125.33	121.00
36	5	2644	C	O5'-P-OP1	-7.21	99.21	105.70
36	1	2973	G	C5-C6-O6	-7.21	124.28	128.60
36	5	1879	A	C4-C5-N7	7.21	114.30	110.70
1	6	639	U	C2-N1-C1'	7.20	126.34	117.70
37	7	49	G	N1-C6-O6	7.20	124.22	119.90
36	1	3306	U	N3-C4-O4	-7.20	114.36	119.40
36	1	2996	U	N1-C2-O2	7.19	127.84	122.80
36	5	429	U	OP2-P-O3'	7.19	121.02	105.20
1	6	163	G	C2-N3-C4	-7.18	108.31	111.90
36	5	1006	A	O5'-P-OP2	-7.18	99.23	105.70
36	1	1308	A	N7-C8-N9	7.17	117.39	113.80
36	5	2531	C	N1-C2-O2	7.17	123.20	118.90
36	5	1308	A	N7-C8-N9	7.17	117.38	113.80
1	2	453	U	N1-C2-O2	7.16	127.81	122.80
1	2	1389	C	N3-C2-O2	-7.16	116.89	121.90
36	1	2719	U	C5-C6-N1	-7.15	119.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3275	U	C5-C6-N1	7.15	126.27	122.70
36	1	410	U	N3-C4-C5	-7.13	110.32	114.60
36	1	2617	U	C5-C4-O4	7.13	130.18	125.90
36	1	745	C	C6-N1-C2	7.12	123.15	120.30
1	2	507	U	N1-C2-O2	7.11	127.78	122.80
36	5	3197	G	N3-C4-N9	-7.10	121.74	126.00
1	2	577	G	C4-C5-N7	7.09	113.64	110.80
1	2	1200	G	N1-C6-O6	7.09	124.16	119.90
36	5	2728	G	O5’-P-OP2	-7.09	99.32	105.70
36	1	1897	G	OP2-P-O3’	7.09	120.80	105.20
36	1	3344	A	C8-N9-C4	-7.09	102.96	105.80
36	5	2377	G	N7-C8-N9	-7.09	109.55	113.10
36	5	607	A	N1-C6-N6	-7.09	114.35	118.60
36	1	3217	C	N3-C2-O2	-7.08	116.94	121.90
36	1	3306	U	C5-C4-O4	7.08	130.15	125.90
36	5	1879	A	N1-C6-N6	7.06	122.84	118.60
36	1	3022	G	O4’-C1’-N9	7.06	113.84	108.20
36	5	1879	A	C6-C5-N7	-7.06	127.36	132.30
36	5	3245	A	C6-C5-N7	-7.06	127.36	132.30
36	1	406	G	C5-C6-O6	7.05	132.83	128.60
36	1	2827	U	C5-C4-O4	7.05	130.13	125.90
36	1	718	G	N3-C4-C5	7.05	132.12	128.60
36	5	2283	G	C5-C6-O6	-7.05	124.37	128.60
36	5	3152	U	N1-C2-O2	7.05	127.73	122.80
78	q2	17	CYS	CA-CB-SG	7.03	126.65	114.00
1	6	1361	U	C2-N1-C1’	7.02	126.13	117.70
36	1	2706	G	C5-C6-O6	-7.02	124.39	128.60
36	5	2943	G	C6-C5-N7	-7.01	126.19	130.40
36	5	2531	C	C2-N1-C1’	7.00	126.50	118.80
1	2	736	C	C2-N1-C1’	7.00	126.50	118.80
38	4	32	C	N3-C4-C5	6.99	124.70	121.90
36	1	3382	U	N1-C2-O2	6.98	127.69	122.80
1	6	1747	G	C8-N9-C4	6.98	109.19	106.40
36	5	3140	G	C4-C5-N7	6.96	113.59	110.80
38	4	125	U	C2-N1-C1’	6.95	126.04	117.70
36	5	2272	G	O4’-C1’-N9	6.95	113.76	108.20
36	1	435	C	C6-N1-C2	6.95	123.08	120.30
1	2	507	U	N3-C2-O2	-6.94	117.34	122.20
36	1	1838	G	N1-C6-O6	6.94	124.06	119.90
36	5	406	G	N3-C4-N9	-6.94	121.84	126.00
36	1	2418	G	OP1-P-O3’	6.93	120.45	105.20
37	3	101	G	C8-N9-C4	6.92	109.17	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	880	G	C8-N9-C1'	6.92	135.99	127.00
36	5	948	C	C6-N1-C2	6.91	123.06	120.30
1	6	1700	C	C2-N1-C1'	6.90	126.39	118.80
36	5	358	G	N1-C6-O6	6.89	124.04	119.90
1	6	144	U	C2-N1-C1'	6.88	125.96	117.70
36	1	3344	A	N7-C8-N9	6.87	117.23	113.80
36	1	2355	G	C5-C6-O6	-6.87	124.48	128.60
36	5	3368	U	C2-N1-C1'	-6.86	109.47	117.70
36	5	1879	A	C5-N7-C8	-6.85	100.47	103.90
36	1	3362	A	O4'-C1'-N9	6.84	113.67	108.20
36	1	282	G	C8-N9-C4	-6.84	103.67	106.40
36	5	2404	A	N1-C6-N6	-6.83	114.50	118.60
1	2	1039	A	O4'-C1'-N9	6.82	113.66	108.20
36	5	2943	G	N1-C6-O6	6.82	123.99	119.90
1	2	1481	C	C6-N1-C2	-6.81	117.58	120.30
36	5	1192	C	C2-N1-C1'	6.81	126.29	118.80
1	2	590	C	C6-N1-C2	-6.81	117.58	120.30
1	2	1560	U	N3-C2-O2	-6.81	117.44	122.20
36	1	2818	U	C5-C6-N1	6.81	126.10	122.70
36	5	3078	U	N3-C2-O2	-6.80	117.44	122.20
36	5	3245	A	C4-C5-N7	6.80	114.10	110.70
1	6	1745	G	N3-C4-N9	6.80	130.08	126.00
36	1	410	U	N3-C4-O4	6.80	124.16	119.40
36	5	2872	A	C4-C5-C6	-6.80	113.60	117.00
36	5	420	G	C8-N9-C4	6.79	109.12	106.40
37	7	1	G	N3-C4-N9	6.79	130.08	126.00
1	2	639	U	N1-C2-O2	6.79	127.55	122.80
36	5	404	G	O5'-P-OP2	-6.78	99.60	105.70
36	1	355	A	C8-N9-C4	6.78	108.51	105.80
36	1	1437	C	C6-N1-C2	-6.77	117.59	120.30
36	5	1582	C	C6-N1-C2	-6.75	117.60	120.30
1	6	158	U	P-O3'-C3'	6.74	127.79	119.70
36	1	2983	C	N3-C4-N4	-6.74	113.28	118.00
38	8	115	C	C6-N1-C2	6.73	122.99	120.30
36	1	2760	C	N1-C2-O2	-6.73	114.86	118.90
36	1	1308	A	C8-N9-C4	-6.71	103.12	105.80
36	1	1495	U	N1-C2-O2	-6.71	118.10	122.80
36	1	1741	A	C2-N3-C4	-6.71	107.25	110.60
1	6	1473	U	N3-C2-O2	-6.71	117.50	122.20
36	1	3207	U	C5-C4-O4	6.71	129.92	125.90
36	5	2376	G	N1-C6-O6	6.70	123.92	119.90
37	7	100	C	C6-N1-C2	6.69	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	103	G	N3-C4-C5	-6.68	125.26	128.60
1	2	732	G	C5-C6-O6	-6.68	124.59	128.60
36	5	2372	A	C6-C5-N7	-6.67	127.63	132.30
36	5	3214	U	N3-C2-O2	-6.67	117.53	122.20
36	5	645	A	N9-C4-C5	6.67	108.47	105.80
36	5	1148	G	C5-C6-O6	-6.66	124.60	128.60
36	5	3245	A	C8-N9-C4	-6.66	103.13	105.80
36	1	23	A	N1-C6-N6	-6.66	114.61	118.60
36	1	1306	G	N9-C4-C5	-6.66	102.74	105.40
36	5	3153	U	N3-C2-O2	-6.65	117.54	122.20
36	1	2209	U	C5-C6-N1	6.65	126.02	122.70
1	6	1389	C	N1-C2-O2	6.65	122.89	118.90
36	1	2946	A	N1-C6-N6	6.62	122.57	118.60
36	1	2617	U	N3-C4-C5	-6.62	110.63	114.60
24	d2	93	LEU	CA-CB-CG	6.62	130.53	115.30
36	1	1306	G	N1-C6-O6	6.62	123.87	119.90
36	1	2827	U	N3-C4-O4	-6.62	114.77	119.40
36	1	3278	C	N1-C2-O2	6.62	122.87	118.90
36	5	1604	G	C8-N9-C1’	-6.62	118.40	127.00
36	1	2979	U	N1-C2-O2	6.61	127.43	122.80
36	1	2617	U	C5-C6-N1	-6.61	119.39	122.70
1	6	1	U	N1-C2-O2	6.61	127.43	122.80
37	7	101	G	C6-C5-N7	-6.61	126.43	130.40
36	5	3084	C	O5’-P-OP1	-6.61	99.75	105.70
36	5	2572	C	N3-C2-O2	-6.61	117.27	121.90
1	2	558	U	C2-N1-C1’	6.60	125.62	117.70
36	5	2875	U	N3-C2-O2	-6.60	117.58	122.20
36	5	350	C	N1-C2-O2	6.59	122.86	118.90
36	5	1897	G	C5-N7-C8	-6.59	101.00	104.30
36	1	2726	C	N3-C2-O2	-6.59	117.29	121.90
36	1	24	G	C8-N9-C4	6.59	109.03	106.40
1	2	507	U	C2-N1-C1’	6.58	125.60	117.70
1	6	1033	C	C6-N1-C2	6.58	122.93	120.30
1	6	1	U	C2-N1-C1’	6.58	125.60	117.70
38	8	17	A	N1-C6-N6	6.58	122.55	118.60
1	6	1473	U	N1-C2-O2	6.57	127.40	122.80
36	5	2858	U	N3-C2-O2	-6.57	117.60	122.20
90	A	75	C	C6-N1-C2	-6.57	117.67	120.30
1	2	704	C	C2-N1-C1’	6.56	126.02	118.80
1	2	132	U	P-O3’-C3’	6.55	127.56	119.70
36	1	3278	C	N3-C2-O2	-6.55	117.31	121.90
36	1	406	G	C4-N9-C1’	-6.55	117.99	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1311	G	O5'-P-OP2	-6.54	99.81	105.70
36	5	2573	G	N1-C6-O6	6.54	123.83	119.90
18	C6	40	GLU	C-N-CD	-6.54	106.20	120.60
36	5	284	A	O5'-P-OP1	-6.54	99.81	105.70
85	l8	69	LEU	CA-CB-CG	6.54	130.35	115.30
38	4	125	U	N1-C2-O2	6.54	127.38	122.80
1	6	194	U	N1-C2-O2	6.54	127.38	122.80
36	5	1481	A	N7-C8-N9	6.53	117.07	113.80
36	1	2123	G	C8-N9-C4	6.53	109.01	106.40
1	2	1537	C	N3-C4-N4	6.53	122.57	118.00
36	5	1189	C	N1-C2-O2	-6.53	114.98	118.90
36	5	1604	G	N3-C4-C5	-6.53	125.33	128.60
36	1	969	C	N1-C2-O2	-6.53	114.98	118.90
1	6	1097	U	P-O3'-C3'	6.53	127.53	119.70
36	1	2314	U	C5-C6-N1	6.52	125.96	122.70
1	6	1473	U	C2-N1-C1'	6.52	125.53	117.70
36	1	817	A	N9-C4-C5	-6.52	103.19	105.80
1	6	1596	C	C6-N1-C2	-6.52	117.69	120.30
36	1	85	A	C2-N3-C4	-6.51	107.34	110.60
36	5	1152	G	N3-C2-N2	-6.51	115.34	119.90
36	1	2874	G	C5-C6-O6	6.51	132.50	128.60
36	5	3197	G	N3-C2-N2	-6.51	115.34	119.90
1	2	9	U	O5'-P-OP1	-6.50	99.85	105.70
36	1	2571	U	N3-C2-O2	-6.49	117.66	122.20
36	5	3154	C	N3-C2-O2	-6.49	117.35	121.90
1	2	1347	U	N1-C2-O2	-6.48	118.26	122.80
1	2	1773	C	C6-N1-C2	-6.48	117.71	120.30
36	5	3209	A	O4'-C1'-N9	6.48	113.38	108.20
36	1	1368	U	C5-C4-O4	-6.48	122.01	125.90
36	5	3197	G	N3-C4-C5	6.47	131.84	128.60
36	1	2719	U	C2-N3-C4	-6.47	123.12	127.00
36	1	2400	G	C8-N9-C4	6.46	108.98	106.40
36	1	979	U	N3-C2-O2	-6.46	117.68	122.20
53	M7	3	ARG	NE-CZ-NH2	-6.46	117.07	120.30
39	l2	246	LEU	CA-CB-CG	6.45	130.15	115.30
36	1	350	C	N3-C2-O2	-6.44	117.39	121.90
1	6	453	U	N3-C2-O2	-6.44	117.69	122.20
36	5	406	G	O4'-C1'-N9	6.44	113.35	108.20
36	5	2281	A	N1-C6-N6	6.44	122.46	118.60
36	5	1367	G	N1-C6-O6	6.43	123.76	119.90
36	1	3214	U	N1-C2-O2	6.43	127.30	122.80
1	2	830	U	N1-C2-O2	6.43	127.30	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D2	93	LEU	CA-CB-CG	6.43	130.08	115.30
36	5	2363	A	C8-N9-C4	-6.43	103.23	105.80
36	1	1351	U	N1-C2-O2	6.42	127.30	122.80
36	1	2988	C	C6-N1-C2	6.42	122.87	120.30
36	5	361	A	N1-C6-N6	-6.42	114.75	118.60
36	1	1149	G	C4-N9-C1'	-6.42	118.16	126.50
36	5	566	G	C4-C5-N7	6.42	113.37	110.80
36	5	1847	A	O5'-P-OP2	-6.41	99.93	105.70
36	5	3228	C	N1-C2-O2	6.41	122.75	118.90
36	5	2996	U	N3-C2-O2	-6.41	117.71	122.20
1	6	1657	U	O5'-P-OP2	-6.41	99.93	105.70
36	5	552	G	C5-C6-N1	-6.40	108.30	111.50
36	1	2758	A	N1-C6-N6	-6.40	114.76	118.60
10	s8	29	LEU	CA-CB-CG	6.40	130.02	115.30
36	5	2524	A	N7-C8-N9	6.40	117.00	113.80
1	6	1	U	N3-C2-O2	-6.40	117.72	122.20
36	1	3277	U	N3-C2-O2	-6.40	117.72	122.20
1	2	1339	C	OP2-P-O3'	6.39	119.27	105.20
36	1	406	G	C6-C5-N7	6.38	134.23	130.40
62	N6	57	LEU	CA-CB-CG	6.38	129.98	115.30
36	1	2363	A	N1-C6-N6	-6.38	114.77	118.60
36	1	1495	U	C2-N3-C4	-6.37	123.18	127.00
37	7	110	G	C8-N9-C4	6.37	108.95	106.40
36	1	2812	C	O5'-P-OP1	-6.37	99.97	105.70
36	1	1891	A	C8-N9-C4	6.36	108.35	105.80
36	5	776	U	N1-C2-N3	6.36	118.72	114.90
36	1	2306	C	N1-C2-O2	6.36	122.72	118.90
36	1	2870	C	C6-N1-C1'	6.35	128.42	120.80
36	5	1904	C	N1-C2-O2	6.35	122.71	118.90
36	5	1152	G	C5-C6-N1	-6.35	108.33	111.50
1	2	1508	U	N3-C4-C5	-6.34	110.79	114.60
1	6	321	C	N3-C2-O2	-6.34	117.46	121.90
1	2	1370	U	P-O3'-C3'	6.34	127.31	119.70
1	2	1246	C	C6-N1-C2	-6.34	117.76	120.30
1	2	1745	G	N3-C4-N9	6.33	129.80	126.00
1	6	542	A	O4'-C1'-N9	6.33	113.26	108.20
36	1	439	C	C2-N1-C1'	6.33	125.76	118.80
36	5	1481	A	P-O3'-C3'	6.32	127.28	119.70
36	5	2726	C	N3-C4-N4	-6.32	113.58	118.00
36	5	3308	C	N1-C2-O2	-6.32	115.11	118.90
1	6	1700	C	N1-C2-O2	6.32	122.69	118.90
1	2	1389	C	C2-N1-C1'	6.32	125.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2887	A	C2-N3-C4	6.32	113.76	110.60
36	5	1483	G	O4'-C1'-N9	6.32	113.25	108.20
36	5	2411	U	C5-C6-N1	-6.32	119.54	122.70
37	7	49	G	C5-C6-O6	-6.31	124.81	128.60
1	2	75	U	C2-N1-C1'	6.31	125.27	117.70
36	5	2349	U	OP1-P-O3'	6.31	119.08	105.20
36	1	1060	U	C5-C6-N1	-6.31	119.55	122.70
1	6	272	U	C2-N1-C1'	6.30	125.27	117.70
1	6	609	U	C5-C4-O4	6.30	129.68	125.90
4	s2	113	LEU	CA-CB-CG	6.30	129.79	115.30
1	6	75	U	P-O3'-C3'	6.30	127.26	119.70
1	6	1000	C	C2-N1-C1'	6.30	125.73	118.80
1	2	1761	U	C5-C4-O4	6.29	129.67	125.90
36	5	1196	C	C6-N1-C2	6.28	122.81	120.30
36	1	3375	A	C8-N9-C4	-6.28	103.29	105.80
36	5	2376	G	N3-C4-N9	6.28	129.76	126.00
36	1	496	C	C6-N1-C2	-6.27	117.79	120.30
1	2	1258	U	N3-C2-O2	-6.27	117.81	122.20
36	5	2327	U	C6-N1-C2	6.27	124.76	121.00
36	5	2830	G	N1-C2-N3	6.26	127.66	123.90
36	5	2971	A	N1-C2-N3	-6.26	126.17	129.30
36	1	2875	U	N3-C2-O2	-6.25	117.83	122.20
1	2	1389	C	C6-N1-C2	-6.24	117.80	120.30
36	1	960	U	C6-N1-C2	6.24	124.75	121.00
36	1	2827	U	C6-N1-C1'	6.24	129.93	121.20
36	1	1196	C	C6-N1-C2	6.24	122.79	120.30
36	5	3215	A	N1-C6-N6	6.24	122.34	118.60
36	1	2816	G	C6-C5-N7	-6.23	126.66	130.40
36	5	966	U	N3-C2-O2	-6.23	117.84	122.20
1	6	687	G	N3-C4-N9	-6.23	122.26	126.00
36	5	1452	A	C5-C6-N6	-6.22	118.72	123.70
36	1	1192	C	N1-C2-O2	6.22	122.63	118.90
36	1	895	A	C5-N7-C8	-6.22	100.79	103.90
36	5	1129	A	O5'-P-OP2	-6.21	100.11	105.70
36	1	3000	A	C8-N9-C4	6.21	108.28	105.80
36	1	2282	U	O5'-P-OP2	-6.20	100.12	105.70
1	6	610	G	C8-N9-C1'	-6.20	118.94	127.00
36	1	857	G	N1-C6-O6	6.20	123.62	119.90
36	1	3382	U	N3-C2-O2	-6.20	117.86	122.20
36	5	2211	U	C4-C5-C6	6.20	123.42	119.70
36	1	3110	C	C6-N1-C2	-6.19	117.82	120.30
36	1	979	U	C6-N1-C2	-6.19	117.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	882	A	N1-C2-N3	6.19	132.40	129.30
36	1	2899	C	C2-N1-C1'	6.19	125.61	118.80
36	5	224	C	C6-N1-C2	-6.18	117.83	120.30
1	2	287	G	O4'-C1'-N9	6.18	113.15	108.20
36	5	1495	U	C2-N1-C1'	6.18	125.12	117.70
36	5	1437	C	C2-N1-C1'	6.18	125.60	118.80
1	6	1745	G	N9-C4-C5	-6.17	102.93	105.40
36	1	2621	G	O5'-P-OP2	-6.17	100.14	105.70
36	1	3095	U	O5'-P-OP1	-6.17	100.15	105.70
36	5	1389	G	N9-C4-C5	-6.17	102.93	105.40
36	1	2719	U	N1-C2-O2	-6.16	118.49	122.80
36	5	1849	C	C6-N1-C2	6.16	122.77	120.30
36	5	923	C	C6-N1-C2	6.16	122.77	120.30
1	6	934	C	N1-C2-O2	6.16	122.60	118.90
36	5	2372	A	C5-C6-N6	-6.16	118.77	123.70
36	5	3152	U	C6-N1-C1'	-6.16	112.58	121.20
36	5	2601	A	C8-N9-C4	6.15	108.26	105.80
36	5	3120	C	O5'-P-OP1	-6.15	100.16	105.70
36	1	1820	U	P-O3'-C3'	6.15	127.08	119.70
36	1	3266	G	N9-C4-C5	6.15	107.86	105.40
37	7	101	G	N9-C4-C5	-6.13	102.95	105.40
38	8	80	A	C5-N7-C8	-6.13	100.84	103.90
36	5	2197	C	C6-N1-C2	6.13	122.75	120.30
36	5	3245	A	N1-C2-N3	6.13	132.36	129.30
36	1	3057	U	N3-C2-O2	-6.12	117.91	122.20
37	7	103	A	C5-C6-N6	-6.12	118.80	123.70
36	1	3375	A	N7-C8-N9	6.12	116.86	113.80
36	5	2330	C	O5'-P-OP2	-6.11	100.20	105.70
1	2	934	C	C6-N1-C1'	-6.11	113.47	120.80
36	1	1351	U	C2-N1-C1'	6.11	125.03	117.70
36	5	3323	A	N1-C6-N6	-6.11	114.94	118.60
36	1	1306	G	C8-N9-C4	6.10	108.84	106.40
36	5	1940	G	C8-N9-C4	6.10	108.84	106.40
1	2	1698	G	P-O3'-C3'	6.10	127.02	119.70
1	6	308	C	C5-C6-N1	-6.10	117.95	121.00
37	3	115	G	C8-N9-C4	6.10	108.84	106.40
36	1	1727	G	C8-N9-C4	-6.09	103.96	106.40
36	5	3382	U	C2-N1-C1'	6.09	125.01	117.70
36	5	2726	C	N1-C2-N3	6.09	123.46	119.20
36	5	3040	A	C8-N9-C4	6.08	108.23	105.80
36	5	2403	G	O5'-P-OP2	-6.08	100.22	105.70
1	6	558	U	P-O3'-C3'	6.08	127.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	610	G	C4-N9-C1'	6.07	134.40	126.50
36	5	1014	U	C2-N1-C1'	6.07	124.99	117.70
36	5	1484	U	C5-C6-N1	-6.07	119.67	122.70
36	5	1604	G	N3-C4-N9	6.07	129.64	126.00
1	2	1006	C	C6-N1-C2	-6.07	117.87	120.30
36	5	2719	U	C2-N1-C1'	-6.06	110.43	117.70
1	2	732	G	N3-C4-N9	6.06	129.63	126.00
36	1	1333	C	C6-N1-C2	-6.06	117.88	120.30
36	1	2679	A	O4'-C1'-N9	6.06	113.05	108.20
36	5	63	A	N1-C6-N6	6.06	122.24	118.60
36	5	1597	C	C6-N1-C2	-6.06	117.88	120.30
36	1	1206	G	O5'-P-OP2	-6.06	100.25	105.70
36	5	3018	C	O5'-P-OP2	-6.05	100.26	105.70
36	1	2714	G	C8-N9-C1'	6.04	134.86	127.00
1	6	858	G	O4'-C1'-N9	6.04	113.03	108.20
36	5	1239	C	C5-C6-N1	6.04	124.02	121.00
1	2	704	C	N1-C2-O2	6.04	122.52	118.90
1	6	359	A	C4-N9-C1'	-6.04	115.43	126.30
41	l4	339	LEU	CA-CB-CG	6.04	129.19	115.30
1	6	1745	G	C8-N9-C1'	-6.04	119.16	127.00
36	5	2541	U	C2-N1-C1'	6.04	124.94	117.70
36	1	406	G	N9-C4-C5	6.03	107.81	105.40
36	1	2836	C	C5-C4-N4	6.03	124.42	120.20
36	1	2403	G	O5'-P-OP2	-6.03	100.27	105.70
1	2	577	G	C5-C6-O6	-6.03	124.98	128.60
1	2	1096	C	C6-N1-C1'	-6.03	113.57	120.80
10	S8	29	LEU	CA-CB-CG	6.02	129.15	115.30
36	5	1006	A	O5'-P-OP1	6.02	117.92	110.70
36	5	2320	A	C2-N3-C4	-6.02	107.59	110.60
48	m1	12	LEU	CA-CB-CG	6.02	129.14	115.30
36	1	2174	G	C8-N9-C4	-6.01	104.00	106.40
36	1	282	G	C2'-C3'-O3'	6.01	123.31	113.70
36	1	340	C	N3-C4-C5	6.01	124.30	121.90
36	1	2618	G	N1-C6-O6	-6.01	116.30	119.90
36	1	2316	G	N1-C6-O6	6.01	123.50	119.90
36	1	715	A	C8-N9-C4	-6.00	103.40	105.80
1	6	42	G	O4'-C1'-N9	6.00	113.00	108.20
36	5	2231	C	C2-N1-C1'	6.00	125.40	118.80
36	5	2847	A	C8-N9-C4	6.00	108.20	105.80
36	1	907	G	O4'-C1'-N9	6.00	113.00	108.20
36	1	2620	G	N1-C6-O6	6.00	123.50	119.90
1	6	1389	C	C2-N1-C1'	6.00	125.39	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2707	C	C5-C4-N4	-6.00	116.00	120.20
36	5	2340	U	C5-C6-N1	5.99	125.70	122.70
40	l3	102	LEU	CA-CB-CG	5.99	129.08	115.30
1	6	427	C	C6-N1-C2	5.99	122.70	120.30
1	6	542	A	P-O3'-C3'	5.99	126.89	119.70
36	5	669	U	N3-C2-O2	-5.99	118.01	122.20
36	5	2211	U	N3-C2-O2	-5.99	118.01	122.20
36	5	2853	A	C8-N9-C4	5.99	108.19	105.80
36	1	1556	C	N1-C2-O2	5.98	122.49	118.90
36	5	1148	G	N1-C6-O6	5.98	123.49	119.90
36	1	1427	U	C6-N1-C2	5.98	124.59	121.00
36	5	2798	C	C2-N1-C1'	-5.98	112.22	118.80
36	5	3153	U	N1-C2-O2	5.98	126.98	122.80
1	2	75	U	N1-C2-O2	5.97	126.98	122.80
36	5	350	C	N3-C2-O2	-5.97	117.72	121.90
36	1	55	G	C8-N9-C4	5.97	108.79	106.40
36	1	1346	G	O5'-P-OP2	-5.97	100.33	105.70
1	2	728	U	C2-N1-C1'	5.97	124.86	117.70
1	6	1537	C	C5-C4-N4	-5.96	116.03	120.20
36	1	2979	U	C2-N3-C4	5.96	130.58	127.00
36	1	3382	U	C2-N1-C1'	5.96	124.85	117.70
36	1	922	U	N1-C2-O2	5.96	126.97	122.80
36	1	2364	G	N1-C6-O6	-5.96	116.33	119.90
36	5	1885	U	C6-N1-C2	5.96	124.57	121.00
1	6	610	G	N3-C4-N9	5.95	129.57	126.00
36	5	3200	G	N1-C6-O6	5.95	123.47	119.90
36	1	2706	G	N1-C6-O6	5.95	123.47	119.90
36	5	2659	G	C5-C6-O6	-5.95	125.03	128.60
47	M0	24	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	2	499	U	C2-N1-C1'	5.94	124.83	117.70
36	5	1938	U	C6-N1-C2	5.94	124.56	121.00
1	2	1241	G	O4'-C1'-N9	5.94	112.95	108.20
36	5	652	G	OP2-P-O3'	5.94	118.27	105.20
36	5	2730	G	N1-C6-O6	5.94	123.46	119.90
36	1	979	U	P-O3'-C3'	5.94	126.83	119.70
36	5	667	C	OP1-P-O3'	5.94	118.26	105.20
36	5	2872	A	C4-N9-C1'	-5.93	115.62	126.30
36	1	2364	G	C6-C5-N7	5.93	133.96	130.40
36	1	2227	C	P-O3'-C3'	5.93	126.81	119.70
36	5	406	G	C4-N9-C1'	-5.92	118.80	126.50
1	2	864	U	C6-N1-C2	-5.92	117.45	121.00
1	6	609	U	C5-C6-N1	-5.92	119.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1332	C	C6-N1-C2	-5.92	117.93	120.30
36	1	1404	G	C8-N9-C4	5.91	108.76	106.40
36	1	2808	A	N9-C4-C5	-5.91	103.44	105.80
36	5	826	G	C5-C6-O6	-5.91	125.06	128.60
36	5	2593	A	P-O3'-C3'	5.91	126.79	119.70
36	5	1496	C	O5'-P-OP1	5.91	117.79	110.70
36	5	48	A	N1-C6-N6	-5.91	115.06	118.60
36	5	2189	U	O5'-P-OP1	-5.91	100.39	105.70
36	5	2197	C	N3-C2-O2	5.91	126.03	121.90
42	l5	110	LEU	CA-CB-CG	5.91	128.88	115.30
36	1	696	C	C6-N1-C2	5.90	122.66	120.30
1	2	1761	U	P-O3'-C3'	5.89	126.77	119.70
36	1	1604	G	C4-N9-C1'	5.89	134.16	126.50
36	5	1433	A	C8-N9-C4	-5.89	103.44	105.80
36	1	28	C	C6-N1-C2	5.89	122.66	120.30
36	1	510	G	N1-C6-O6	5.89	123.43	119.90
36	1	2314	U	N3-C4-O4	5.89	123.52	119.40
1	2	934	C	N1-C2-O2	5.88	122.43	118.90
36	1	2112	U	P-O3'-C3'	5.88	126.76	119.70
36	1	3059	G	OP1-P-O3'	5.88	118.14	105.20
36	5	3368	U	C5-C6-N1	-5.88	119.76	122.70
1	2	1490	C	C6-N1-C2	-5.88	117.95	120.30
36	1	895	A	C4-C5-N7	5.88	113.64	110.70
36	5	1452	A	N1-C6-N6	5.88	122.12	118.60
1	6	1458	G	C4-N9-C1'	5.87	134.13	126.50
36	5	2524	A	N9-C1'-C2'	5.87	121.64	114.00
36	1	439	C	C6-N1-C1'	-5.87	113.75	120.80
36	1	1152	G	O4'-C1'-N9	5.87	112.90	108.20
36	5	1816	A	OP1-P-O3'	5.87	118.12	105.20
36	1	1308	A	C2-N3-C4	-5.87	107.67	110.60
36	5	2726	C	N3-C4-C5	-5.87	119.55	121.90
1	2	833	U	O5'-P-OP2	5.87	117.74	110.70
36	1	1149	G	C8-N9-C4	5.87	108.75	106.40
36	1	2873	U	O4'-C1'-N1	5.87	112.89	108.20
1	6	25	C	C2-N1-C1'	5.87	125.25	118.80
36	5	1437	C	C6-N1-C2	-5.86	117.95	120.30
1	2	736	C	C5-C6-N1	5.86	123.93	121.00
36	1	1324	U	O5'-P-OP2	-5.86	100.43	105.70
1	2	734	A	P-O3'-C3'	5.86	126.73	119.70
20	c8	116	LEU	CA-CB-CG	5.86	128.78	115.30
36	1	671	U	O5'-P-OP2	-5.86	100.43	105.70
1	2	720	G	P-O3'-C3'	5.86	126.73	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	406	G	N1-C6-O6	-5.85	116.39	119.90
36	5	1901	A	C8-N9-C4	-5.85	103.46	105.80
15	C3	22	ALA	C-N-CD	-5.85	107.73	120.60
36	5	282	G	P-O3'-C3'	5.85	126.72	119.70
41	l4	327	LEU	CA-CB-CG	5.85	128.75	115.30
36	5	1308	A	C8-N9-C4	-5.85	103.46	105.80
36	5	2625	C	C6-N1-C2	5.84	122.64	120.30
1	6	144	U	C6-N1-C2	-5.84	117.49	121.00
36	5	2406	C	N3-C2-O2	5.84	125.99	121.90
36	1	1313	G	C5-C6-O6	-5.84	125.10	128.60
36	1	2885	C	C6-N1-C2	5.84	122.64	120.30
36	5	1017	C	C2-N1-C1'	5.84	125.22	118.80
1	6	548	G	N1-C6-O6	5.83	123.40	119.90
36	5	943	U	O5'-P-OP1	-5.83	100.45	105.70
36	1	1377	G	C5-C6-O6	-5.83	125.10	128.60
36	1	517	G	N3-C4-N9	5.83	129.50	126.00
36	1	410	U	C6-N1-C2	-5.82	117.51	121.00
36	5	804	C	N3-C4-C5	-5.82	119.57	121.90
36	1	1494	U	C2-N1-C1'	-5.82	110.71	117.70
36	5	1203	A	N1-C6-N6	5.82	122.09	118.60
36	5	2341	A	C8-N9-C4	5.82	108.13	105.80
36	5	2843	U	N3-C2-O2	-5.81	118.13	122.20
36	1	695	C	C6-N1-C2	5.81	122.62	120.30
36	1	1846	C	N1-C2-O2	-5.81	115.41	118.90
36	1	1371	G	C8-N9-C4	5.81	108.72	106.40
20	c8	15	LEU	CA-CB-CG	5.81	128.66	115.30
36	5	1716	U	P-O3'-C3'	5.81	126.67	119.70
36	1	406	G	C8-N9-C1'	5.81	134.55	127.00
36	5	56	G	O5'-P-OP2	-5.81	100.47	105.70
36	1	1548	C	N1-C2-O2	-5.80	115.42	118.90
36	1	2918	G	C8-N9-C4	-5.80	104.08	106.40
1	6	151	G	N3-C4-N9	-5.80	122.52	126.00
36	5	1152	G	N9-C4-C5	5.80	107.72	105.40
36	5	2872	A	C6-C5-N7	5.80	136.36	132.30
36	5	1350	A	N1-C6-N6	-5.80	115.12	118.60
36	5	437	G	C4-C5-N7	5.80	113.12	110.80
1	6	163	G	N3-C4-C5	5.80	131.50	128.60
36	5	1379	G	N9-C4-C5	-5.80	103.08	105.40
1	6	1764	C	C6-N1-C2	5.79	122.62	120.30
36	5	2899	C	N3-C2-O2	-5.79	117.84	121.90
1	2	1339	C	P-O3'-C3'	5.79	126.65	119.70
36	1	949	C	N1-C2-O2	-5.79	115.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	785	G	N3-C4-C5	-5.79	125.71	128.60
36	1	2571	U	N1-C2-O2	5.79	126.85	122.80
36	1	1838	G	C6-C5-N7	-5.79	126.93	130.40
36	1	3143	C	N3-C2-O2	5.79	125.95	121.90
1	6	647	G	N3-C4-N9	-5.79	122.53	126.00
36	5	3294	A	N1-C6-N6	-5.79	115.13	118.60
1	2	1189	A	C8-N9-C4	5.78	108.11	105.80
36	5	1495	U	C5-C6-N1	5.78	125.59	122.70
36	5	3161	C	C6-N1-C2	-5.78	117.99	120.30
1	2	1332	C	C5-C6-N1	5.78	123.89	121.00
36	1	627	U	C2-N1-C1’	-5.78	110.77	117.70
1	6	453	U	N1-C2-O2	5.77	126.84	122.80
1	2	1052	U	C2-N1-C1’	5.77	124.62	117.70
36	1	2355	G	C6-C5-N7	-5.77	126.94	130.40
36	1	979	U	N1-C2-N3	5.77	118.36	114.90
36	1	3218	A	P-O3’-C3’	5.77	126.62	119.70
36	5	406	G	C6-C5-N7	5.77	133.86	130.40
37	3	95	A	C8-N9-C4	-5.76	103.50	105.80
36	5	1433	A	C2-N3-C4	5.76	113.48	110.60
36	5	2897	A	C5-C6-N6	-5.76	119.09	123.70
36	1	2873	U	N3-C2-O2	-5.76	118.17	122.20
36	1	1417	G	C8-N9-C4	5.76	108.70	106.40
36	1	517	G	C4-N9-C1’	5.76	133.98	126.50
36	1	1177	G	N3-C2-N2	-5.76	115.87	119.90
37	7	77	G	C8-N9-C4	5.76	108.70	106.40
36	1	2873	U	C5-C4-O4	5.75	129.35	125.90
36	5	1503	A	C8-N9-C4	5.75	108.10	105.80
36	5	2364	G	N1-C6-O6	-5.75	116.45	119.90
36	5	2870	C	C2-N3-C4	-5.75	117.02	119.90
36	5	2876	C	O5’-P-OP1	-5.75	100.52	105.70
36	1	2996	U	C2-N1-C1’	5.74	124.59	117.70
36	1	645	A	C8-N9-C4	-5.74	103.50	105.80
36	5	2113	A	C8-N9-C4	5.74	108.09	105.80
36	5	1379	G	N3-C4-N9	5.73	129.44	126.00
36	5	1119	C	C6-N1-C2	5.73	122.59	120.30
36	5	1437	C	C5-C6-N1	5.73	123.87	121.00
1	2	1761	U	C6-N1-C2	-5.73	117.56	121.00
36	5	661	G	O5’-P-OP1	-5.73	100.54	105.70
1	2	145	A	N9-C4-C5	5.73	108.09	105.80
36	1	2364	G	N3-C4-N9	-5.73	122.56	126.00
36	5	1373	A	N1-C6-N6	5.73	122.04	118.60
36	5	2797	C	N3-C4-C5	-5.73	119.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2832	C	C6-N1-C2	5.73	122.59	120.30
36	5	2943	G	C5-C6-O6	-5.73	125.16	128.60
36	1	2818	U	C6-N1-C2	-5.72	117.57	121.00
36	5	3050	U	C5-C4-O4	5.71	129.33	125.90
36	1	2197	C	C6-N1-C2	5.71	122.58	120.30
36	1	1604	G	N3-C4-N9	5.71	129.42	126.00
38	4	125	U	C6-N1-C1'	-5.71	113.21	121.20
36	1	73	C	N1-C2-O2	-5.70	115.48	118.90
36	1	3214	U	N3-C2-O2	-5.70	118.21	122.20
36	5	942	U	N3-C4-O4	5.70	123.39	119.40
36	1	1081	U	C2-N1-C1'	5.70	124.54	117.70
36	1	1663	C	C6-N1-C2	5.70	122.58	120.30
36	5	3218	A	P-O3'-C3'	5.70	126.53	119.70
36	1	2725	U	C5-C6-N1	-5.69	119.85	122.70
36	1	360	G	N3-C4-C5	-5.69	125.75	128.60
36	1	1365	G	N3-C4-C5	-5.69	125.75	128.60
1	6	144	U	N1-C2-O2	5.69	126.78	122.80
1	6	310	C	N3-C4-C5	-5.69	119.62	121.90
36	5	1429	G	N9-C4-C5	-5.69	103.12	105.40
36	5	3140	G	C6-C5-N7	-5.69	126.99	130.40
36	5	437	G	C5-N7-C8	-5.68	101.46	104.30
36	5	3228	C	C2-N1-C1'	5.68	125.05	118.80
33	e1	100	LEU	CA-CB-CG	5.68	128.36	115.30
36	5	1462	A	N1-C6-N6	5.68	122.01	118.60
36	5	890	C	O5'-P-OP2	-5.67	100.59	105.70
1	6	1000	C	N3-C2-O2	-5.67	117.93	121.90
1	6	1399	C	C6-N1-C2	-5.67	118.03	120.30
36	5	48	A	N9-C4-C5	5.67	108.07	105.80
36	5	835	G	O4'-C1'-N9	5.67	112.74	108.20
36	1	2572	C	C6-N1-C2	-5.67	118.03	120.30
36	5	2875	U	C6-N1-C2	-5.67	117.60	121.00
1	2	782	U	P-O3'-C3'	5.67	126.50	119.70
37	3	91	G	C8-N9-C4	-5.66	104.14	106.40
36	5	2943	G	O5'-P-OP2	-5.66	100.61	105.70
36	5	112	U	O5'-P-OP1	-5.65	100.61	105.70
36	5	718	G	C4-N9-C1'	5.65	133.85	126.50
36	5	2901	G	C5-C6-O6	-5.65	125.21	128.60
36	1	2434	U	C5-C4-O4	5.65	129.29	125.90
36	5	2440	G	C8-N9-C4	-5.65	104.14	106.40
36	5	2897	A	N1-C6-N6	5.65	121.99	118.60
36	1	1874	A	O5'-P-OP1	-5.65	100.62	105.70
1	2	959	U	N3-C2-O2	-5.65	118.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	1	3238	G	C5-C6-O6	-5.65	125.21	128.60
36	5	2366	C	C6-N1-C2	-5.65	118.04	120.30
36	1	709	A	C8-N9-C4	5.64	108.06	105.80
36	1	2418	G	C2-N3-C4	5.64	114.72	111.90
36	1	2385	G	C8-N9-C4	5.64	108.66	106.40
36	5	1885	U	C5-C6-N1	-5.64	119.88	122.70
36	1	2231	C	C6-N1-C2	5.63	122.55	120.30
36	5	374	A	N9-C4-C5	5.63	108.05	105.80
36	1	2836	C	N3-C2-O2	-5.63	117.96	121.90
36	5	274	G	C8-N9-C4	5.63	108.65	106.40
36	5	2531	C	N3-C2-O2	-5.63	117.96	121.90
36	1	2355	G	N9-C4-C5	-5.62	103.15	105.40
36	1	1351	U	N3-C2-O2	-5.62	118.27	122.20
36	5	432	G	C8-N9-C4	5.62	108.65	106.40
36	5	998	A	OP2-P-O3'	5.62	117.57	105.20
36	5	1374	G	C8-N9-C4	5.62	108.65	106.40
36	5	2573	G	C5-C6-O6	-5.62	125.23	128.60
1	2	829	A	P-O3'-C3'	5.62	126.44	119.70
36	5	366	A	OP1-P-O3'	5.62	117.56	105.20
36	5	499	G	O5'-P-OP1	-5.62	100.64	105.70
36	5	170	G	C4-N9-C1'	5.61	133.80	126.50
36	5	3347	A	C8-N9-C4	5.61	108.05	105.80
36	5	2146	C	C6-N1-C2	-5.61	118.06	120.30
36	5	1429	G	C8-N9-C4	5.61	108.64	106.40
1	2	734	A	OP1-P-O3'	5.61	117.54	105.20
36	5	358	G	C5-C6-O6	-5.61	125.24	128.60
36	5	2353	G	C5-C6-O6	-5.61	125.24	128.60
36	5	2378	C	C6-N1-C2	-5.61	118.06	120.30
37	7	77	G	O5'-P-OP1	5.61	117.43	110.70
1	2	831	U	C6-N1-C2	-5.61	117.64	121.00
1	2	426	G	C4-N9-C1'	5.60	133.78	126.50
36	1	1294	A	O4'-C1'-N9	5.60	112.68	108.20
36	5	2406	C	C5-C4-N4	-5.60	116.28	120.20
1	2	17	C	C6-N1-C2	-5.60	118.06	120.30
36	5	817	A	C5-C6-N1	5.60	120.50	117.70
36	5	1014	U	C6-N1-C1'	-5.60	113.36	121.20
1	2	1100	G	N9-C4-C5	-5.59	103.16	105.40
36	5	410	U	N3-C4-C5	-5.59	111.24	114.60
36	5	677	A	N1-C6-N6	5.59	121.95	118.60
36	5	2376	G	O5'-P-OP2	-5.59	100.67	105.70
1	2	1363	U	N1-C2-O2	5.59	126.71	122.80
36	5	2283	G	N3-C4-C5	5.59	131.39	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1494	U	C5-C4-O4	5.58	129.25	125.90
36	5	1704	A	C8-N9-C4	5.58	108.03	105.80
36	1	1595	U	C2-N1-C1'	-5.58	111.00	117.70
36	1	1849	C	N1-C2-O2	-5.58	115.55	118.90
1	2	581	U	C2-N1-C1'	5.58	124.40	117.70
1	2	1596	C	N1-C2-O2	5.58	122.25	118.90
36	5	882	A	C6-N1-C2	-5.58	115.25	118.60
44	l7	229	PHE	CB-CG-CD2	-5.58	116.89	120.80
36	1	817	A	C8-N9-C4	5.58	108.03	105.80
36	1	2387	A	C8-N9-C4	5.58	108.03	105.80
36	1	2905	U	N3-C2-O2	5.58	126.10	122.20
1	2	1600	A	C2-N3-C4	-5.57	107.81	110.60
36	1	1300	G	C4-C5-N7	5.57	113.03	110.80
36	5	1391	C	C6-N1-C2	5.57	122.53	120.30
36	1	1495	U	C6-N1-C1'	5.57	129.00	121.20
36	1	3190	C	C6-N1-C2	5.57	122.53	120.30
36	5	874	U	O5'-P-OP1	-5.57	100.69	105.70
36	5	2823	G	N1-C6-O6	5.57	123.24	119.90
36	1	3143	C	N1-C2-O2	-5.56	115.56	118.90
1	6	687	G	N3-C2-N2	-5.56	116.00	119.90
1	2	720	G	OP1-P-O3'	5.56	117.44	105.20
36	1	2966	G	N9-C4-C5	-5.56	103.17	105.40
1	6	453	U	C6-N1-C2	-5.56	117.66	121.00
1	6	1058	U	P-O3'-C3'	5.56	126.38	119.70
36	1	14	U	O5'-P-OP2	-5.56	100.69	105.70
36	1	1380	G	O5'-P-OP1	5.56	117.37	110.70
36	5	1192	C	N3-C2-O2	-5.56	118.01	121.90
36	1	1929	G	C8-N9-C4	5.56	108.62	106.40
38	4	53	A	C2-N3-C4	5.56	113.38	110.60
36	5	867	G	O5'-P-OP2	5.56	117.37	110.70
36	1	1875	G	N7-C8-N9	-5.56	110.32	113.10
36	1	3268	A	N1-C6-N6	5.56	121.93	118.60
36	5	2156	C	C6-N1-C2	5.56	122.52	120.30
36	1	2403	G	C6-C5-N7	-5.55	127.07	130.40
36	1	2726	C	N1-C2-N3	5.55	123.09	119.20
1	6	308	C	N3-C4-N4	-5.55	114.11	118.00
36	5	3140	G	N9-C4-C5	-5.55	103.18	105.40
36	1	2376	G	N7-C8-N9	5.55	115.88	113.10
36	5	406	G	C8-N9-C1'	5.55	134.22	127.00
36	1	2208	A	C6-N1-C2	-5.55	115.27	118.60
1	6	1022	C	O5'-P-OP1	-5.55	100.70	105.70
36	1	2861	U	O5'-P-OP1	-5.54	100.71	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3362	A	C2-N3-C4	-5.54	107.83	110.60
1	6	581	U	C2-N1-C1'	-5.54	111.05	117.70
36	5	2132	C	C6-N1-C2	-5.54	118.08	120.30
36	5	2621	G	C5-C6-O6	-5.54	125.28	128.60
36	5	2901	G	O5'-P-OP2	-5.54	100.71	105.70
1	2	158	U	P-O3'-C3'	5.54	126.35	119.70
36	5	2404	A	C6-C5-N7	5.54	136.18	132.30
36	5	2979	U	C2-N3-C4	5.54	130.32	127.00
36	1	2983	C	O4'-C1'-N1	5.54	112.63	108.20
12	C0	76	LEU	CA-CB-CG	5.54	128.03	115.30
36	1	3001	C	C6-N1-C2	5.54	122.51	120.30
1	6	1279	C	C6-N1-C2	-5.53	118.09	120.30
36	5	566	G	N7-C8-N9	5.53	115.87	113.10
36	1	1815	U	P-O3'-C3'	5.53	126.33	119.70
36	5	2772	C	P-O3'-C3'	5.53	126.34	119.70
36	5	2804	A	O5'-P-OP1	-5.53	100.72	105.70
36	1	2279	A	N1-C6-N6	5.53	121.92	118.60
36	1	1345	G	OP2-P-O3'	5.52	117.35	105.20
36	5	964	G	OP2-P-O3'	5.52	117.35	105.20
1	2	1573	A	P-O3'-C3'	5.52	126.33	119.70
38	8	77	A	C8-N9-C4	5.52	108.01	105.80
36	1	1207	G	C5-C6-O6	-5.52	125.29	128.60
36	1	953	G	N3-C4-C5	5.52	131.36	128.60
36	1	1368	U	O5'-P-OP1	-5.52	100.73	105.70
36	1	1484	U	P-O3'-C3'	5.52	126.32	119.70
36	1	2393	G	N3-C4-N9	5.52	129.31	126.00
36	5	2572	C	C6-N1-C1'	-5.52	114.18	120.80
36	1	2870	C	C2-N1-C1'	-5.51	112.73	118.80
36	5	1424	C	O5'-P-OP2	-5.51	100.74	105.70
36	5	645	A	C8-N9-C4	-5.51	103.59	105.80
36	5	2971	A	N3-C4-N9	5.51	131.81	127.40
37	7	1	G	C6-C5-N7	-5.51	127.09	130.40
36	1	2996	U	N3-C2-O2	-5.51	118.34	122.20
36	5	826	G	N1-C6-O6	5.51	123.21	119.90
36	5	3152	U	C2-N1-C1'	5.51	124.31	117.70
1	2	737	A	O4'-C1'-N9	5.51	112.61	108.20
36	1	57	A	C8-N9-C4	5.51	108.00	105.80
36	1	752	C	C6-N1-C2	5.51	122.50	120.30
1	2	74	U	P-O3'-C3'	5.50	126.30	119.70
1	2	502	U	C5-C6-N1	5.50	125.45	122.70
1	2	853	G	C4-C5-N7	5.50	113.00	110.80
36	5	922	U	C2-N3-C4	-5.50	123.70	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2385	G	N3-C4-N9	-5.50	122.70	126.00
36	5	2524	A	C5-N7-C8	-5.50	101.15	103.90
36	1	2875	U	N1-C1'-C2'	-5.50	105.95	112.00
36	5	2639	G	C8-N9-C4	-5.50	104.20	106.40
36	5	3214	U	O4'-C1'-N1	5.50	112.60	108.20
36	1	2283	G	N1-C6-O6	5.49	123.20	119.90
1	6	1736	G	N1-C6-O6	5.49	123.20	119.90
36	5	189	G	N1-C6-O6	-5.49	116.61	119.90
1	6	1596	C	N3-C2-O2	-5.49	118.06	121.90
36	5	1300	G	C5-C6-O6	-5.49	125.31	128.60
36	5	1487	G	N1-C6-O6	-5.49	116.61	119.90
36	1	2149	A	C8-N9-C4	5.49	108.00	105.80
1	6	214	G	N1-C6-O6	5.49	123.19	119.90
36	5	3195	U	N1-C2-O2	5.49	126.64	122.80
36	1	1929	G	N9-C4-C5	-5.48	103.21	105.40
36	1	2419	A	O5'-P-OP2	-5.48	100.77	105.70
36	1	226	C	C6-N1-C2	-5.48	118.11	120.30
36	1	1300	G	N9-C4-C5	-5.48	103.21	105.40
36	1	2314	U	C6-N1-C1'	-5.48	113.52	121.20
36	5	873	C	P-O3'-C3'	5.48	126.28	119.70
36	5	1445	U	C6-N1-C2	5.48	124.29	121.00
36	1	545	U	C2-N1-C1'	5.48	124.28	117.70
36	5	2298	U	C2-N1-C1'	-5.48	111.12	117.70
36	1	895	A	N7-C8-N9	5.48	116.54	113.80
36	5	2345	A	N1-C6-N6	5.48	121.89	118.60
36	1	2369	G	N3-C4-C5	-5.48	125.86	128.60
38	4	137	C	C6-N1-C2	5.48	122.49	120.30
1	2	1489	U	N3-C2-O2	-5.47	118.37	122.20
36	5	657	A	C8-N9-C4	5.47	107.99	105.80
36	5	1536	G	N1-C6-O6	5.47	123.18	119.90
36	1	1307	G	P-O3'-C3'	5.47	126.27	119.70
48	m1	43	GLN	C-N-CA	-5.47	108.02	121.70
1	2	1458	G	C4-N9-C1'	5.47	133.61	126.50
36	1	1300	G	C5-C6-O6	-5.47	125.32	128.60
1	6	359	A	C4-C5-C6	-5.47	114.27	117.00
1	2	1761	U	N3-C2-O2	-5.46	118.38	122.20
36	1	1741	A	N1-C2-N3	5.46	132.03	129.30
1	6	321	C	C6-N1-C2	-5.46	118.11	120.30
36	1	776	U	C5-C6-N1	-5.46	119.97	122.70
36	1	1269	U	C2-N1-C1'	5.46	124.25	117.70
62	N6	6	LEU	CA-CB-CG	-5.46	102.74	115.30
1	6	1421	A	C8-N9-C4	5.46	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1314	C	C5-C4-N4	-5.46	116.38	120.20
38	4	97	A	N1-C6-N6	-5.46	115.33	118.60
1	6	400	A	N1-C6-N6	5.46	121.88	118.60
36	1	2403	G	C5-C6-N1	-5.46	108.77	111.50
1	6	1458	G	C8-N9-C1'	-5.46	119.91	127.00
36	5	1367	G	C5-C6-N1	-5.46	108.77	111.50
36	1	1849	C	O5'-P-OP1	-5.45	100.79	105.70
1	6	1657	U	N1-C2-O2	5.45	126.62	122.80
36	1	1331	U	O4'-C1'-N1	-5.45	103.84	108.20
36	1	2766	U	N3-C2-O2	-5.45	118.39	122.20
36	1	2966	G	C4-C5-N7	5.45	112.98	110.80
1	6	1361	U	C6-N1-C1'	-5.45	113.57	121.20
36	5	2145	A	C8-N9-C4	-5.45	103.62	105.80
1	2	453	U	C6-N1-C2	-5.45	117.73	121.00
36	5	1867	A	N1-C6-N6	5.45	121.87	118.60
36	1	672	A	N1-C6-N6	5.45	121.87	118.60
36	5	282	G	C2'-C3'-O3'	5.45	122.42	113.70
36	1	2343	C	N3-C4-C5	5.44	124.08	121.90
36	1	3278	C	C6-N1-C2	-5.44	118.12	120.30
36	5	1453	A	C8-N9-C4	5.44	107.98	105.80
36	1	2593	A	P-O3'-C3'	5.44	126.23	119.70
36	1	397	A	N1-C6-N6	-5.44	115.34	118.60
36	1	2679	A	C2-N3-C4	-5.44	107.88	110.60
1	2	1596	C	C6-N1-C2	-5.44	118.13	120.30
36	1	651	G	N3-C4-C5	-5.44	125.88	128.60
1	2	75	U	N3-C2-O2	-5.43	118.40	122.20
36	1	760	G	O4'-C1'-N9	5.43	112.55	108.20
1	6	427	C	C5-C6-N1	-5.43	118.28	121.00
36	5	2618	G	C5-C6-N1	5.43	114.22	111.50
1	6	555	A	C8-N9-C4	-5.43	103.63	105.80
36	1	1306	G	C5-C6-O6	-5.43	125.34	128.60
36	1	1108	U	C5-C6-N1	-5.43	119.99	122.70
36	5	767	U	O4'-C1'-N1	5.43	112.54	108.20
36	5	1017	C	N1-C2-O2	5.43	122.16	118.90
36	1	2818	U	P-O3'-C3'	5.43	126.21	119.70
1	6	194	U	N3-C2-O2	-5.43	118.40	122.20
36	5	1506	A	C8-N9-C4	-5.43	103.63	105.80
36	5	2837	A	C8-N9-C4	5.43	107.97	105.80
36	1	1495	U	N1-C2-N3	5.42	118.16	114.90
1	6	339	C	C6-N1-C2	-5.42	118.13	120.30
36	1	1497	C	C6-N1-C2	-5.42	118.13	120.30
36	1	651	G	N3-C4-N9	5.42	129.25	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S1	181	LEU	CA-CB-CG	5.42	127.77	115.30
36	1	2650	U	C6-N1-C2	-5.42	117.75	121.00
36	5	2823	G	C5-C6-O6	-5.42	125.35	128.60
36	1	2714	G	C4-N9-C1'	-5.42	119.46	126.50
38	4	113	U	C2-N1-C1'	-5.42	111.20	117.70
1	6	1033	C	C5-C6-N1	-5.42	118.29	121.00
36	1	3214	U	C2-N1-C1'	5.41	124.20	117.70
38	4	57	C	C6-N1-C2	5.41	122.47	120.30
1	6	1514	U	N3-C2-O2	-5.41	118.41	122.20
36	5	2353	G	N1-C6-O6	5.41	123.15	119.90
36	1	501	A	C8-N9-C4	5.41	107.96	105.80
36	1	645	A	C5-C6-N1	5.41	120.41	117.70
1	2	1568	C	P-O3'-C3'	5.41	126.19	119.70
36	5	1794	G	N1-C2-N2	-5.41	111.33	116.20
36	1	30	G	N1-C6-O6	-5.41	116.66	119.90
36	1	1366	A	N1-C6-N6	5.41	121.84	118.60
36	1	1589	A	O4'-C1'-N9	-5.40	103.88	108.20
36	1	200	C	N3-C2-O2	-5.40	118.12	121.90
36	1	2808	A	N1-C6-N6	5.40	121.84	118.60
36	1	2873	U	N1-C2-N3	5.40	118.14	114.90
1	6	1657	U	N3-C2-O2	-5.40	118.42	122.20
36	5	2707	C	N3-C4-C5	5.40	124.06	121.90
1	2	1473	U	N3-C2-O2	-5.39	118.42	122.20
36	1	1377	G	C4-C5-N7	5.39	112.96	110.80
38	4	79	A	C8-N9-C4	-5.39	103.64	105.80
36	5	2950	G	O4'-C1'-N9	5.39	112.51	108.20
1	2	499	U	P-O3'-C3'	5.39	126.17	119.70
1	6	1340	U	N1-C2-O2	5.39	126.57	122.80
36	5	2519	A	O5'-P-OP1	-5.39	100.85	105.70
36	5	2802	A	OP2-P-O3'	5.38	117.04	105.20
36	1	2887	A	C5-C6-N6	-5.38	119.40	123.70
36	5	1000	C	C6-N1-C2	5.38	122.45	120.30
1	6	1745	G	C6-C5-N7	-5.38	127.17	130.40
36	1	3140	G	N1-C6-O6	5.38	123.12	119.90
36	5	283	G	C4-C5-N7	5.38	112.95	110.80
36	5	3323	A	N9-C4-C5	5.38	107.95	105.80
1	2	864	U	N3-C2-O2	-5.37	118.44	122.20
1	2	1361	U	N1-C2-O2	5.37	126.56	122.80
36	5	97	U	N3-C2-O2	5.37	125.96	122.20
36	5	2890	A	OP2-P-O3'	5.37	117.02	105.20
19	C7	84	TYR	C-N-CA	5.37	135.13	121.70
36	1	2745	G	C4-N9-C1'	-5.37	119.52	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	53	A	N1-C6-N6	-5.37	115.38	118.60
36	1	2366	C	O5'-P-OP2	-5.37	100.87	105.70
36	5	3073	A	C8-N9-C4	5.37	107.95	105.80
38	4	32	C	C6-N1-C2	5.37	122.45	120.30
1	2	830	U	C2-N1-C1'	5.36	124.14	117.70
36	1	645	A	C6-N1-C2	-5.36	115.38	118.60
36	1	1308	A	N1-C2-N3	5.36	131.98	129.30
36	5	2885	C	O5'-P-OP2	-5.36	100.87	105.70
36	1	274	G	C8-N9-C4	5.36	108.54	106.40
36	5	2402	A	C8-N9-C4	5.36	107.94	105.80
36	5	2280	A	N1-C6-N6	5.36	121.81	118.60
36	1	49	A	C5-C6-N1	-5.36	115.02	117.70
1	6	925	G	N1-C6-O6	5.36	123.11	119.90
36	5	1373	A	C5-C6-N6	-5.35	119.42	123.70
1	2	704	C	O4'-C1'-N1	5.35	112.48	108.20
1	6	934	C	C2-N1-C1'	5.35	124.69	118.80
36	5	639	G	C8-N9-C4	5.35	108.54	106.40
36	5	2211	U	C5-C4-O4	5.35	129.11	125.90
1	2	732	G	N9-C4-C5	-5.35	103.26	105.40
36	1	3308	C	N1-C2-O2	-5.35	115.69	118.90
38	4	124	G	P-O3'-C3'	-5.35	113.28	119.70
36	5	3195	U	P-O3'-C3'	5.35	126.12	119.70
36	1	1844	C	C6-N1-C2	5.35	122.44	120.30
38	4	20	U	C5-C6-N1	-5.34	120.03	122.70
36	1	2283	G	C5-C6-O6	-5.34	125.39	128.60
36	5	200	C	C6-N1-C2	-5.34	118.16	120.30
36	1	1733	G	N3-C4-C5	-5.34	125.93	128.60
36	1	1898	G	O5'-P-OP1	-5.34	100.89	105.70
36	1	1838	G	C5-C6-O6	-5.34	125.40	128.60
36	5	948	C	C5-C6-N1	-5.34	118.33	121.00
36	5	3104	U	N1-C2-O2	-5.34	119.06	122.80
36	5	3154	C	C6-N1-C1'	-5.34	114.40	120.80
1	6	1698	G	P-O3'-C3'	5.33	126.10	119.70
36	5	2385	G	O5'-P-OP1	-5.33	100.90	105.70
36	1	71	A	C8-N9-C4	-5.33	103.67	105.80
36	1	213	A	C8-N9-C4	5.33	107.93	105.80
1	6	214	G	C5-C6-O6	-5.33	125.40	128.60
36	1	3316	A	C2-N3-C4	-5.33	107.94	110.60
1	6	696	C	C2-N1-C1'	-5.33	112.94	118.80
36	5	2388	U	N3-C4-C5	-5.33	111.40	114.60
1	2	864	U	C5-C4-O4	5.33	129.10	125.90
36	1	2836	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2584	G	OP2-P-O3’	5.32	116.91	105.20
36	5	3088	G	O5’-P-OP2	5.32	117.09	110.70
36	1	859	G	N1-C2-N2	-5.32	111.41	116.20
36	1	2172	A	N1-C6-N6	5.32	121.79	118.60
1	6	194	U	C6-N1-C1’	-5.32	113.75	121.20
36	5	1462	A	C8-N9-C4	5.32	107.93	105.80
36	5	2514	U	O5’-P-OP1	-5.32	100.91	105.70
36	1	3362	A	N7-C8-N9	5.32	116.46	113.80
36	1	2946	A	C6-C5-N7	-5.32	128.58	132.30
36	5	1156	C	C6-N1-C2	-5.32	118.17	120.30
36	5	2385	G	C8-N9-C4	5.32	108.53	106.40
1	2	1051	G	P-O3’-C3’	5.32	126.08	119.70
36	1	1639	C	C6-N1-C2	-5.32	118.17	120.30
36	1	2700	G	C5-C6-O6	-5.32	125.41	128.60
1	6	25	C	N1-C2-O2	5.32	122.09	118.90
36	5	348	A	O5’-P-OP1	-5.32	100.92	105.70
36	5	2421	U	N1-C2-N3	5.32	118.09	114.90
1	2	1027	A	C4-C5-N7	5.31	113.36	110.70
36	1	27	C	O5’-P-OP1	-5.31	100.92	105.70
36	1	49	A	C2-N3-C4	-5.31	107.94	110.60
36	1	2846	U	N3-C2-O2	-5.31	118.48	122.20
1	2	386	G	N3-C4-C5	-5.31	125.95	128.60
36	1	2101	C	P-O3’-C3’	5.31	126.07	119.70
36	1	915	A	C8-N9-C4	-5.30	103.68	105.80
37	3	69	C	C6-N1-C2	-5.30	118.18	120.30
1	6	272	U	P-O3’-C3’	5.30	126.06	119.70
36	5	90	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1503	A	O4’-C1’-N9	5.30	112.44	108.20
36	1	199	A	O4’-C1’-N9	5.30	112.44	108.20
36	5	2383	C	N1-C2-O2	-5.30	115.72	118.90
1	6	305	C	N1-C2-O2	-5.30	115.72	118.90
36	5	718	G	O4’-C1’-N9	5.30	112.44	108.20
1	2	1280	C	N3-C4-C5	-5.30	119.78	121.90
36	1	670	C	C6-N1-C2	5.30	122.42	120.30
36	1	2572	C	C6-N1-C1’	-5.30	114.44	120.80
36	5	1665	C	N1-C2-O2	5.30	122.08	118.90
36	5	2836	C	O4’-C1’-N1	5.30	112.44	108.20
1	2	577	G	N1-C6-O6	5.29	123.08	119.90
36	1	1604	G	C8-N9-C1’	-5.29	120.12	127.00
1	6	321	C	N1-C2-O2	5.29	122.08	118.90
36	1	334	A	N1-C6-N6	5.29	121.78	118.60
1	6	308	C	C2-N1-C1’	-5.29	112.98	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	188	A	O5'-P-OP1	-5.29	100.94	105.70
36	1	811	U	C4-C5-C6	5.29	122.87	119.70
36	1	3083	G	N3-C4-C5	-5.29	125.96	128.60
36	5	374	A	P-O3'-C3'	5.29	126.05	119.70
36	5	1628	C	C6-N1-C2	-5.29	118.19	120.30
36	1	3276	G	N3-C4-C5	5.29	131.24	128.60
1	6	558	U	C2-N1-C1'	5.29	124.04	117.70
1	6	877	G	N1-C6-O6	-5.29	116.73	119.90
36	5	922	U	N3-C2-O2	-5.29	118.50	122.20
1	2	1596	C	C2-N1-C1'	5.28	124.61	118.80
36	1	406	G	C4-C5-N7	-5.28	108.69	110.80
36	5	1430	U	C6-N1-C2	5.28	124.17	121.00
36	5	2231	C	O4'-C1'-N1	5.28	112.43	108.20
48	m1	112	LEU	CA-CB-CG	5.28	127.45	115.30
36	5	1448	U	C5-C6-N1	-5.28	120.06	122.70
36	5	2890	A	C8-N9-C4	-5.28	103.69	105.80
64	n8	73	LEU	CA-CB-CG	5.28	127.44	115.30
1	6	1750	A	O5'-P-OP2	-5.27	100.95	105.70
36	1	1822	C	C6-N1-C2	-5.27	118.19	120.30
64	N8	115	LYS	C-N-CA	-5.27	111.23	122.30
1	2	36	C	C6-N1-C2	5.27	122.41	120.30
36	1	2207	A	O4'-C1'-N9	5.27	112.42	108.20
38	4	22	U	C5-C6-N1	-5.27	120.06	122.70
36	1	547	G	P-O3'-C3'	5.27	126.02	119.70
1	6	609	U	N3-C4-O4	-5.27	115.71	119.40
1	6	965	U	N3-C2-O2	-5.27	118.51	122.20
36	1	304	G	N9-C4-C5	5.26	107.51	105.40
1	6	1523	G	N3-C4-N9	5.26	129.16	126.00
36	5	224	C	N1-C2-O2	5.26	122.06	118.90
36	5	1196	C	N1-C2-N3	-5.26	115.52	119.20
1	2	553	G	N1-C6-O6	5.26	123.06	119.90
18	c6	97	VAL	CA-CB-CG2	5.26	118.79	110.90
1	6	1361	U	N1-C2-O2	5.25	126.48	122.80
1	6	813	U	N1-C2-O2	5.25	126.48	122.80
36	5	3090	U	N3-C4-O4	-5.25	115.72	119.40
1	6	984	G	C8-N9-C4	5.25	108.50	106.40
36	5	2964	G	N9-C4-C5	5.25	107.50	105.40
1	2	610	G	C4-N9-C1'	5.25	133.32	126.50
1	2	704	C	C6-N1-C1'	-5.25	114.50	120.80
36	5	216	G	O5'-P-OP1	-5.25	100.98	105.70
36	1	2298	U	N3-C4-O4	-5.24	115.73	119.40
36	1	1113	G	N3-C2-N2	-5.24	116.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2872	A	N3-C4-C5	5.24	130.47	126.80
36	1	2809	C	C6-N1-C2	-5.24	118.20	120.30
36	5	418	A	N1-C6-N6	5.24	121.74	118.60
36	5	2744	U	O5’-P-OP2	-5.24	100.98	105.70
36	1	799	G	O5’-P-OP1	-5.24	100.98	105.70
36	1	2662	G	C6-C5-N7	-5.24	127.26	130.40
36	5	109	A	N1-C6-N6	-5.24	115.46	118.60
36	5	1379	G	C8-N9-C1’	-5.24	120.19	127.00
1	2	1027	A	C5-N7-C8	-5.23	101.28	103.90
36	1	2995	A	C8-N9-C4	5.23	107.89	105.80
24	D2	104	LEU	CA-CB-CG	5.23	127.33	115.30
36	1	715	A	P-O3’-C3’	5.23	125.98	119.70
36	5	2278	C	N1-C2-O2	5.23	122.04	118.90
36	5	3092	C	O4’-C1’-N1	5.23	112.39	108.20
36	5	2204	C	OP1-P-O3’	5.23	116.70	105.20
1	2	499	U	C6-N1-C1’	-5.23	113.88	121.20
36	1	2875	U	C4-C5-C6	5.23	122.84	119.70
36	5	1582	C	C5-C6-N1	5.23	123.61	121.00
36	5	1216	C	C6-N1-C2	-5.22	118.21	120.30
36	5	2663	G	C5-C6-O6	-5.22	125.47	128.60
36	1	658	G	C4-N9-C1’	5.22	133.29	126.50
36	1	676	G	N3-C4-C5	-5.22	125.99	128.60
36	1	1716	U	P-O3’-C3’	5.22	125.97	119.70
38	4	103	G	C8-N9-C4	-5.22	104.31	106.40
1	2	192	U	C2-N1-C1’	5.22	123.96	117.70
36	1	1433	A	N1-C6-N6	-5.22	115.47	118.60
36	1	2996	U	C6-N1-C1’	-5.22	113.89	121.20
1	6	1781	A	C8-N9-C4	-5.22	103.71	105.80
36	5	1117	G	C4-C5-N7	5.22	112.89	110.80
36	1	2852	C	C6-N1-C2	5.22	122.39	120.30
56	N0	24	LEU	CA-CB-CG	5.22	127.30	115.30
1	2	1658	G	C4-C5-N7	5.21	112.89	110.80
36	5	2372	A	C4-C5-C6	5.21	119.61	117.00
36	5	406	G	C5-C6-O6	5.21	131.73	128.60
36	5	2283	G	C8-N9-C4	5.21	108.48	106.40
36	1	2403	G	C5-C6-O6	-5.21	125.47	128.60
36	5	2388	U	N3-C4-O4	5.21	123.05	119.40
36	1	2620	G	C8-N9-C4	5.21	108.48	106.40
1	6	1696	G	C3’-C2’-C1’	5.21	105.66	101.50
36	5	3157	U	N1-C2-O2	5.20	126.44	122.80
3	S1	184	LEU	CA-CB-CG	5.20	127.26	115.30
1	2	1202	A	N1-C6-N6	-5.20	115.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	430	U	O5'-P-OP1	-5.20	101.02	105.70
36	5	660	A	OP1-P-OP2	5.20	127.40	119.60
36	5	2172	A	C8-N9-C4	5.20	107.88	105.80
36	1	76	G	N3-C4-C5	-5.20	126.00	128.60
36	1	883	A	N1-C2-N3	5.20	131.90	129.30
36	5	1879	A	N9-C4-C5	-5.20	103.72	105.80
36	5	2405	C	N3-C2-O2	-5.20	118.26	121.90
36	1	339	C	N3-C4-N4	-5.20	114.36	118.00
1	6	1185	U	N1-C2-O2	5.20	126.44	122.80
36	5	200	C	N3-C4-C5	-5.20	119.82	121.90
1	6	1535	U	N3-C2-O2	-5.19	118.56	122.20
36	1	968	G	C5-C6-O6	-5.19	125.48	128.60
36	1	2137	U	O4'-C1'-N1	5.19	112.35	108.20
36	1	2745	G	C8-N9-C4	5.19	108.48	106.40
33	e1	86	THR	C-N-CA	5.19	134.68	121.70
36	1	54	C	C6-N1-C2	5.19	122.38	120.30
36	5	2635	A	O5'-P-OP2	-5.19	101.03	105.70
36	5	2800	G	N1-C6-O6	5.19	123.01	119.90
36	1	783	A	N9-C4-C5	-5.19	103.73	105.80
36	5	2512	C	C5-C6-N1	5.19	123.59	121.00
1	2	1100	G	N1-C6-O6	5.18	123.01	119.90
36	1	1851	G	C5-C6-O6	-5.18	125.49	128.60
36	5	2662	G	N3-C4-C5	-5.18	126.01	128.60
36	5	3278	C	C6-N1-C2	5.18	122.37	120.30
36	5	1848	G	C4-C5-N7	5.18	112.87	110.80
36	5	1856	C	O5'-P-OP1	-5.18	101.04	105.70
1	6	1773	C	N1-C2-O2	-5.18	115.79	118.90
36	5	1885	U	N3-C2-O2	5.18	125.83	122.20
24	D2	65	LEU	CA-CB-CG	5.18	127.21	115.30
1	6	214	G	C4-C5-N7	5.18	112.87	110.80
1	6	295	A	C8-N9-C4	5.17	107.87	105.80
36	5	437	G	N7-C8-N9	5.17	115.69	113.10
1	2	321	C	O4'-C1'-N1	5.17	112.34	108.20
36	1	1604	G	N3-C4-C5	-5.17	126.01	128.60
36	1	2541	U	P-O3'-C3'	5.17	125.91	119.70
1	6	965	U	N1-C2-O2	5.17	126.42	122.80
37	7	81	U	C6-N1-C2	5.17	124.10	121.00
36	1	939	U	N3-C2-O2	5.17	125.82	122.20
36	1	1129	A	N1-C6-N6	5.17	121.70	118.60
36	1	2537	U	P-O3'-C3'	5.17	125.90	119.70
36	5	226	C	N1-C2-O2	5.17	122.00	118.90
36	5	2211	U	N3-C4-C5	-5.17	111.50	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	L7	207	LEU	CB-CG-CD1	-5.17	102.22	111.00
36	5	421	G	C4-N9-C1’	5.16	133.21	126.50
1	2	278	U	P-O3’-C3’	5.16	125.89	119.70
1	6	937	C	C6-N1-C2	-5.16	118.23	120.30
36	1	1838	G	N9-C4-C5	-5.16	103.34	105.40
37	3	115	G	N9-C4-C5	-5.16	103.34	105.40
1	2	187	G	P-O3’-C3’	5.16	125.89	119.70
36	1	2147	A	C8-N9-C4	5.16	107.86	105.80
36	5	2887	A	O4’-C1’-N9	-5.16	104.07	108.20
36	1	1111	U	C5-C6-N1	-5.16	120.12	122.70
37	7	1	G	C4-N9-C1’	5.16	133.20	126.50
36	1	1419	A	O5’-P-OP1	5.15	116.89	110.70
36	1	1902	G	N9-C4-C5	-5.15	103.34	105.40
36	5	1134	G	C8-N9-C4	5.15	108.46	106.40
36	1	2316	G	N9-C4-C5	-5.15	103.34	105.40
36	1	3046	A	C8-N9-C4	-5.15	103.74	105.80
1	6	987	G	N3-C4-N9	5.15	129.09	126.00
36	5	2234	G	N9-C4-C5	-5.15	103.34	105.40
36	5	3373	U	C5-C6-N1	-5.15	120.13	122.70
1	2	1363	U	N3-C2-O2	-5.14	118.60	122.20
36	1	1497	C	N3-C4-C5	-5.14	119.84	121.90
36	1	2983	C	C5-C4-N4	5.14	123.80	120.20
36	1	3276	G	O4’-C1’-N9	-5.14	104.08	108.20
36	5	2996	U	O5’-P-OP2	-5.14	101.07	105.70
1	2	240	U	OP2-P-O3’	5.14	116.51	105.20
36	1	817	A	N1-C6-N6	5.14	121.69	118.60
1	6	453	U	C5-C6-N1	5.14	125.27	122.70
1	6	1058	U	OP1-P-O3’	5.14	116.51	105.20
36	5	635	G	C4-C5-N7	5.14	112.86	110.80
36	5	1238	C	P-O3’-C3’	5.14	125.87	119.70
36	5	3228	C	C6-N1-C1’	-5.14	114.63	120.80
36	5	1389	G	C4-C5-N7	5.14	112.86	110.80
1	2	251	A	O5’-P-OP1	-5.14	101.08	105.70
1	6	813	U	N3-C2-O2	-5.14	118.61	122.20
1	2	136	C	C6-N1-C2	-5.13	118.25	120.30
1	2	1100	G	C5-C6-O6	-5.13	125.52	128.60
36	5	3362	A	C2-N3-C4	-5.13	108.03	110.60
1	6	1744	A	C8-N9-C4	5.13	107.85	105.80
36	5	939	U	O5’-P-OP1	5.13	116.86	110.70
1	2	321	C	C5-C6-N1	5.13	123.56	121.00
1	2	794	U	P-O3’-C3’	5.13	125.85	119.70
36	1	2816	G	N9-C4-C5	-5.13	103.35	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2828	G	N3-C2-N2	5.13	123.49	119.90
38	4	46	G	C4-N9-C1’	5.13	133.17	126.50
37	7	121	U	C2-N1-C1’	5.13	123.85	117.70
38	8	126	A	OP1-P-O3’	5.13	116.48	105.20
36	1	2809	C	N3-C2-O2	-5.13	118.31	121.90
37	7	100	C	C5-C6-N1	-5.13	118.44	121.00
36	5	2818	U	P-O3’-C3’	5.12	125.85	119.70
38	4	2	A	C8-N9-C4	-5.12	103.75	105.80
36	5	1429	G	C4-C5-N7	5.12	112.85	110.80
36	5	3309	G	C4-N9-C1’	5.12	133.16	126.50
36	5	3327	G	N3-C2-N2	-5.12	116.31	119.90
36	5	1457	U	O5’-P-OP2	5.12	116.84	110.70
36	5	2411	U	N3-C4-O4	-5.12	115.81	119.40
36	5	2621	G	N3-C2-N2	-5.12	116.32	119.90
1	2	1767	G	O4’-C1’-N9	5.12	112.29	108.20
36	1	57	A	N1-C6-N6	5.12	121.67	118.60
1	2	144	U	N3-C2-O2	-5.12	118.62	122.20
1	2	251	A	O5’-P-OP2	5.12	116.84	110.70
36	5	962	A	N1-C6-N6	5.12	121.67	118.60
1	2	782	U	OP2-P-O3’	5.12	116.45	105.20
1	6	1697	G	N3-C4-C5	-5.12	126.04	128.60
36	5	30	G	C4-C5-N7	5.12	112.85	110.80
36	5	2634	U	C2-N3-C4	-5.12	123.93	127.00
1	2	1773	C	N3-C4-C5	-5.11	119.86	121.90
36	1	355	A	N7-C8-N9	-5.11	111.25	113.80
36	1	2364	G	C4-N9-C1’	-5.11	119.86	126.50
36	5	2118	C	N1-C2-O2	5.11	121.97	118.90
38	8	27	U	C5-C6-N1	5.11	125.25	122.70
1	6	337	G	C6-C5-N7	-5.11	127.33	130.40
36	5	1065	A	C8-N9-C4	5.11	107.84	105.80
36	1	2966	G	C6-C5-N7	-5.11	127.34	130.40
36	5	77	A	OP2-P-O3’	5.11	116.43	105.20
36	5	2816	G	C6-C5-N7	-5.11	127.34	130.40
1	6	151	G	N3-C2-N2	-5.10	116.33	119.90
38	8	96	A	C8-N9-C4	5.10	107.84	105.80
1	2	1595	U	O4’-C1’-N1	5.10	112.28	108.20
1	2	1745	G	N9-C4-C5	-5.10	103.36	105.40
36	1	2337	C	C6-N1-C2	-5.10	118.26	120.30
36	5	1314	C	C6-N1-C1’	-5.10	114.68	120.80
36	1	399	A	OP1-P-OP2	-5.10	111.95	119.60
36	1	2399	A	OP1-P-O3’	5.10	116.42	105.20
36	1	3275	U	C2-N1-C1’	5.10	123.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	644	G	C5-C6-O6	5.10	131.66	128.60
1	6	359	A	C8-N9-C1'	5.10	136.88	127.70
38	4	145	U	N3-C2-O2	-5.10	118.63	122.20
36	1	689	U	O5'-P-OP2	-5.09	101.11	105.70
36	5	1043	C	O5'-P-OP1	5.09	116.81	110.70
1	6	421	A	N1-C6-N6	5.09	121.66	118.60
36	5	291	C	C6-N1-C2	5.09	122.34	120.30
37	7	1	G	C8-N9-C1'	-5.09	120.38	127.00
36	5	824	C	O5'-P-OP2	-5.09	101.12	105.70
36	5	2885	C	C6-N1-C2	5.09	122.34	120.30
36	1	2964	G	C2-N3-C4	-5.09	109.36	111.90
18	C6	28	LEU	CA-CB-CG	5.09	127.00	115.30
36	1	3306	U	N1-C2-O2	5.09	126.36	122.80
36	5	2257	C	C6-N1-C2	-5.09	118.27	120.30
36	5	2293	C	N1-C2-O2	5.09	121.95	118.90
36	1	503	C	C6-N1-C2	5.08	122.33	120.30
36	1	2918	G	C4-N9-C1'	5.08	133.11	126.50
1	6	402	C	O5'-P-OP1	5.08	116.80	110.70
1	2	736	C	C6-N1-C1'	-5.08	114.70	120.80
36	1	2874	G	N1-C6-O6	-5.08	116.85	119.90
36	1	922	U	N3-C2-O2	-5.08	118.64	122.20
42	l5	179	ARG	C-N-CA	5.08	134.40	121.70
1	2	639	U	C2-N1-C1'	5.08	123.80	117.70
36	5	1143	A	C2-N3-C4	-5.08	108.06	110.60
36	5	2818	U	C5'-C4'-O4'	-5.08	103.00	109.10
36	5	3309	G	N3-C4-C5	-5.08	126.06	128.60
36	1	350	C	C6-N1-C2	-5.08	118.27	120.30
1	6	548	G	C5-C6-O6	-5.08	125.56	128.60
36	5	1764	U	C5-C6-N1	5.08	125.24	122.70
36	5	1872	C	N1-C2-O2	5.08	121.94	118.90
1	2	1082	C	N1-C2-O2	5.07	121.94	118.90
1	6	418	G	O5'-P-OP1	-5.07	101.13	105.70
1	6	1523	G	N3-C4-C5	-5.07	126.06	128.60
1	2	1027	A	N1-C6-N6	5.07	121.64	118.60
36	1	3005	A	C8-N9-C4	-5.07	103.77	105.80
1	6	1730	A	C5-C6-N6	-5.07	119.64	123.70
36	1	1858	A	N3-C4-N9	5.07	131.46	127.40
1	6	417	A	P-O3'-C3'	5.07	125.78	119.70
36	5	838	G	C5-C6-O6	5.07	131.64	128.60
36	1	282	G	P-O3'-C3'	5.07	125.78	119.70
36	5	704	U	C6-N1-C2	-5.07	117.96	121.00
36	1	2283	G	C4-C5-N7	5.07	112.83	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	66	A	O5'-P-OP1	-5.07	101.14	105.70
36	5	1297	C	C6-N1-C2	-5.07	118.27	120.30
21	C9	28	LEU	CA-CB-CG	5.06	126.94	115.30
1	6	1196	A	P-O3'-C3'	5.06	125.78	119.70
36	1	859	G	N3-C2-N2	5.06	123.44	119.90
1	6	670	U	C2-N1-C1'	5.06	123.77	117.70
36	5	3343	G	N3-C4-N9	5.06	129.04	126.00
1	2	1489	U	C6-N1-C2	-5.06	117.96	121.00
36	1	2401	A	C4-C5-C6	-5.06	114.47	117.00
36	1	3181	C	C6-N1-C2	-5.06	118.28	120.30
36	5	1239	C	C6-N1-C2	-5.06	118.28	120.30
36	5	3004	C	N3-C2-O2	5.06	125.44	121.90
1	2	2	A	O4'-C1'-N9	-5.06	104.15	108.20
47	m0	48	LEU	CA-CB-CG	5.06	126.93	115.30
1	2	577	G	C5-N7-C8	-5.06	101.77	104.30
36	1	770	G	O4'-C1'-N9	5.05	112.24	108.20
1	6	306	U	C6-N1-C2	5.05	124.03	121.00
1	6	1700	C	C6-N1-C1'	-5.05	114.73	120.80
36	5	880	G	C6-C5-N7	5.05	133.43	130.40
38	4	46	G	C8-N9-C1'	-5.05	120.43	127.00
36	1	1849	C	N3-C2-O2	5.05	125.44	121.90
36	1	2966	G	N1-C6-O6	5.05	122.93	119.90
36	1	3057	U	C5-C4-O4	5.05	128.93	125.90
36	5	2512	C	C6-N1-C2	-5.05	118.28	120.30
1	2	992	A	O4'-C1'-N9	5.05	112.24	108.20
36	1	274	G	N1-C6-O6	5.05	122.93	119.90
6	s4	3	ARG	NE-CZ-NH1	-5.05	117.78	120.30
36	1	2903	A	C8-N9-C4	5.04	107.82	105.80
81	c2	58	LEU	CA-CB-CG	5.04	126.90	115.30
1	6	1573	A	P-O3'-C3'	5.04	125.75	119.70
36	5	2376	G	C8-N9-C1'	-5.04	120.44	127.00
36	1	1149	G	N7-C8-N9	-5.04	110.58	113.10
36	5	1300	G	N1-C6-O6	5.04	122.92	119.90
1	2	1486	G	C5-N7-C8	-5.04	101.78	104.30
38	4	99	C	C6-N1-C2	5.04	122.32	120.30
36	5	2611	U	C5-C6-N1	-5.04	120.18	122.70
36	5	3134	A	C5-C6-N6	-5.04	119.67	123.70
1	2	610	G	C8-N9-C1'	-5.04	120.45	127.00
36	1	3362	A	C5-N7-C8	-5.04	101.38	103.90
36	5	1604	G	C4-C5-C6	5.04	121.82	118.80
36	1	1595	U	C6-N1-C2	5.04	124.02	121.00
36	1	1875	G	C5-N7-C8	5.03	106.82	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	136	C	C2-N1-C1'	5.03	124.33	118.80
36	1	659	G	C2-N3-C4	5.03	114.42	111.90
36	1	1512	U	C6-N1-C2	-5.03	117.98	121.00
36	1	1590	G	N1-C6-O6	-5.03	116.88	119.90
39	l2	238	ILE	CG1-CB-CG2	-5.03	100.34	111.40
36	1	2554	A	P-O3'-C3'	5.03	125.73	119.70
45	L8	65	LEU	CA-CB-CG	5.03	126.86	115.30
36	1	676	G	C8-N9-C4	-5.03	104.39	106.40
36	1	2939	G	OP2-P-O3'	5.03	116.26	105.20
36	5	1604	G	N1-C2-N3	5.03	126.92	123.90
36	5	2872	A	C8-N9-C1'	5.03	136.75	127.70
36	5	3289	G	N7-C8-N9	5.03	115.61	113.10
36	1	334	A	N9-C4-C5	-5.02	103.79	105.80
36	1	1433	A	N9-C4-C5	5.02	107.81	105.80
1	2	1196	A	P-O3'-C3'	5.02	125.73	119.70
36	1	851	C	C2-N1-C1'	5.02	124.33	118.80
36	5	1292	C	C6-N1-C2	5.02	122.31	120.30
38	8	53	A	C2-N3-C4	5.02	113.11	110.60
1	2	1745	G	N3-C2-N2	5.02	123.42	119.90
36	5	2659	G	N1-C6-O6	5.02	122.91	119.90
36	5	3382	U	N3-C2-O2	-5.02	118.69	122.20
36	1	2376	G	C8-N9-C4	-5.02	104.39	106.40
36	1	3276	G	C5-C6-O6	-5.02	125.59	128.60
36	1	3302	U	C6-N1-C2	5.02	124.01	121.00
1	6	1389	C	N3-C2-O2	-5.02	118.39	121.90
36	5	1155	C	N3-C4-C5	5.02	123.91	121.90
38	8	96	A	O5'-P-OP2	-5.02	101.18	105.70
36	1	80	G	C8-N9-C4	5.02	108.41	106.40
36	1	2808	A	O4'-C1'-N9	-5.02	104.19	108.20
1	6	1082	C	C6-N1-C2	-5.02	118.29	120.30
36	1	80	G	OP2-P-O3'	5.02	116.24	105.20
1	6	608	U	N3-C2-O2	-5.01	118.69	122.20
36	5	2118	C	C2-N1-C1'	5.01	124.31	118.80
90	a	75	C	N3-C2-O2	-5.01	118.39	121.90
36	5	3388	C	C5-C6-N1	-5.01	118.49	121.00
36	1	2426	U	C5-C4-O4	5.01	128.91	125.90
36	5	2978	U	N3-C4-O4	-5.01	115.89	119.40
36	1	545	U	N1-C2-O2	5.01	126.31	122.80
36	1	3143	C	C6-N1-C2	5.01	122.30	120.30
36	1	3303	G	O4'-C1'-N9	5.01	112.21	108.20
36	5	2440	G	N7-C8-N9	5.01	115.60	113.10
36	5	2849	C	N3-C2-O2	5.01	125.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3137	C	C6-N1-C2	5.01	122.30	120.30
36	5	1561	G	O4'-C1'-N9	5.01	112.21	108.20
36	1	1176	C	O5'-P-OP2	5.01	116.71	110.70
36	5	2918	G	N1-C6-O6	5.01	122.90	119.90
1	2	1101	G	N1-C6-O6	-5.00	116.90	119.90
36	1	2811	A	C8-N9-C4	-5.00	103.80	105.80
36	5	1445	U	C5-C6-N1	-5.00	120.20	122.70
36	5	3368	U	N1-C2-O2	-5.00	119.30	122.80
36	1	1165	A	C8-N9-C4	5.00	107.80	105.80
36	5	546	C	C2-N1-C1'	5.00	124.30	118.80
1	2	542	A	O4'-C1'-N9	5.00	112.20	108.20
36	1	2603	G	N1-C6-O6	5.00	122.90	119.90
36	5	2832	C	C5-C6-N1	-5.00	118.50	121.00
36	5	2870	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
24	D2	54	ASP	Peptide
25	D3	44	GLY	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	84	VAL	Peptide
28	D6	85	ARG	Peptide
33	E1	105	TYR	Peptide
39	L2	19	HIS	Peptide
40	L3	172	ALA	Peptide
43	L6	129	GLU	Peptide
43	L6	89	THR	Peptide
45	L8	74	THR	Peptide
49	M3	137	GLN	Peptide
52	M6	110	PRO	Peptide
53	M7	120	ASN	Peptide
56	N0	133	ALA	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide
61	N5	137	ASN	Peptide
65	N9	19	ASN	Peptide
65	N9	20	GLY	Peptide

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Mol	Chain	Res	Type	Group
70	O4	71	THR	Peptide
3	S1	131	ASP	Peptide
6	S4	193	GLY	Peptide
9	S7	131	PHE	Peptide
13	c1	119	VAL	Peptide
82	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
27	d5	85	LYS	Peptide
33	e1	106	TYR	Peptide
39	l2	143	GLU	Peptide
39	l2	171	GLY	Peptide
39	l2	211	HIS	Peptide
40	l3	185	GLY	Peptide
42	l5	270	LYS	Peptide
42	l5	271	LYS	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
50	m4	20	VAL	Peptide
52	m6	110	PRO	Peptide
53	m7	119	VAL	Peptide
56	n0	133	ALA	Peptide
87	n4	75	THR	Peptide
63	n7	5	LEU	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
65	n9	24	PRO	Peptide
68	o2	39	ASP	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
10	s8	60	ILE	Peptide
11	s9	100	LYS	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	
2	S0	204/206 (99%)	155 (76%)	34 (17%)	15 (7%)	1	7
2	s0	204/206 (99%)	163 (80%)	22 (11%)	19 (9%)	0	4
3	S1	212/216 (98%)	151 (71%)	35 (16%)	26 (12%)	0	2
3	s1	214/216 (99%)	173 (81%)	26 (12%)	15 (7%)	1	7
4	S2	215/217 (99%)	189 (88%)	19 (9%)	7 (3%)	4	22
4	s2	215/217 (99%)	179 (83%)	25 (12%)	11 (5%)	2	13
5	S3	221/223 (99%)	186 (84%)	25 (11%)	10 (4%)	2	15
5	s3	221/223 (99%)	177 (80%)	28 (13%)	16 (7%)	1	7
6	S4	258/260 (99%)	218 (84%)	30 (12%)	10 (4%)	3	18
6	s4	258/260 (99%)	218 (84%)	26 (10%)	14 (5%)	2	12
7	S5	204/206 (99%)	166 (81%)	22 (11%)	16 (8%)	1	6
7	s5	204/206 (99%)	160 (78%)	30 (15%)	14 (7%)	1	8
8	S6	224/226 (99%)	198 (88%)	16 (7%)	10 (4%)	2	15
8	s6	216/226 (96%)	190 (88%)	12 (6%)	14 (6%)	1	9
9	S7	182/186 (98%)	144 (79%)	19 (10%)	19 (10%)	0	3
9	s7	184/186 (99%)	150 (82%)	22 (12%)	12 (6%)	1	9
10	S8	184/199 (92%)	163 (89%)	10 (5%)	11 (6%)	1	10
10	s8	184/199 (92%)	159 (86%)	17 (9%)	8 (4%)	2	16
11	S9	183/185 (99%)	158 (86%)	17 (9%)	8 (4%)	2	15
11	s9	183/185 (99%)	157 (86%)	18 (10%)	8 (4%)	2	15
12	C0	82/96 (85%)	69 (84%)	9 (11%)	4 (5%)	2	14
13	C1	145/155 (94%)	119 (82%)	19 (13%)	7 (5%)	2	14
13	c1	144/155 (93%)	120 (83%)	18 (12%)	6 (4%)	3	16
14	C2	122/124 (98%)	74 (61%)	26 (21%)	22 (18%)	0	1
15	C3	148/150 (99%)	127 (86%)	15 (10%)	6 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	c3	148/150 (99%)	121 (82%)	19 (13%)	8 (5%)	2	12
16	C4	125/128 (98%)	97 (78%)	17 (14%)	11 (9%)	1	5
16	c4	126/128 (98%)	103 (82%)	17 (14%)	6 (5%)	2	14
17	C5	122/131 (93%)	96 (79%)	16 (13%)	10 (8%)	1	6
18	C6	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	1	10
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	2	16
19	C7	116/125 (93%)	94 (81%)	14 (12%)	8 (7%)	1	8
19	c7	113/125 (90%)	92 (81%)	12 (11%)	9 (8%)	1	6
20	C8	143/145 (99%)	113 (79%)	22 (15%)	8 (6%)	2	11
20	c8	143/145 (99%)	121 (85%)	16 (11%)	6 (4%)	3	16
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	25
21	c9	141/143 (99%)	124 (88%)	14 (10%)	3 (2%)	7	32
22	D0	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	3	19
22	d0	108/110 (98%)	86 (80%)	12 (11%)	10 (9%)	0	4
23	D1	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	2
23	d1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	10
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	6	28
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	52
25	D3	142/144 (99%)	118 (83%)	14 (10%)	10 (7%)	1	7
25	d3	142/144 (99%)	128 (90%)	11 (8%)	3 (2%)	7	32
26	D4	132/134 (98%)	111 (84%)	13 (10%)	8 (6%)	1	10
26	d4	132/134 (98%)	106 (80%)	17 (13%)	9 (7%)	1	8
27	D5	68/70 (97%)	47 (69%)	12 (18%)	9 (13%)	0	1
27	d5	67/70 (96%)	53 (79%)	10 (15%)	4 (6%)	1	10
28	D6	95/97 (98%)	60 (63%)	22 (23%)	13 (14%)	0	1
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	5
29	D7	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	3	19
29	d7	79/81 (98%)	61 (77%)	11 (14%)	7 (9%)	1	4
30	D8	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	14
30	d8	61/63 (97%)	46 (75%)	12 (20%)	3 (5%)	2	14
31	D9	51/53 (96%)	40 (78%)	8 (16%)	3 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	d9	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	10
32	E0	58/62 (94%)	46 (79%)	9 (16%)	3 (5%)	2	12
32	e0	60/62 (97%)	47 (78%)	7 (12%)	6 (10%)	0	3
33	E1	69/76 (91%)	38 (55%)	18 (26%)	13 (19%)	0	1
33	e1	74/76 (97%)	33 (45%)	23 (31%)	18 (24%)	0	0
34	SR	316/318 (99%)	275 (87%)	32 (10%)	9 (3%)	5	25
35	SM	131/159 (82%)	100 (76%)	17 (13%)	14 (11%)	0	3
39	L2	250/252 (99%)	229 (92%)	13 (5%)	8 (3%)	4	23
39	l2	250/252 (99%)	215 (86%)	26 (10%)	9 (4%)	3	20
40	L3	384/386 (100%)	334 (87%)	35 (9%)	15 (4%)	3	18
40	l3	384/386 (100%)	349 (91%)	25 (6%)	10 (3%)	5	27
41	L4	359/361 (99%)	301 (84%)	37 (10%)	21 (6%)	1	10
41	l4	359/361 (99%)	300 (84%)	41 (11%)	18 (5%)	2	13
42	L5	294/296 (99%)	239 (81%)	37 (13%)	18 (6%)	1	10
42	l5	292/296 (99%)	257 (88%)	28 (10%)	7 (2%)	6	28
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	7	33
43	l6	153/175 (87%)	135 (88%)	14 (9%)	4 (3%)	5	27
44	L7	220/223 (99%)	199 (90%)	15 (7%)	6 (3%)	5	26
44	l7	221/223 (99%)	201 (91%)	14 (6%)	6 (3%)	5	26
45	L8	231/233 (99%)	194 (84%)	26 (11%)	11 (5%)	2	14
46	L9	189/191 (99%)	167 (88%)	17 (9%)	5 (3%)	5	27
46	l9	189/191 (99%)	175 (93%)	8 (4%)	6 (3%)	4	23
47	M0	207/220 (94%)	180 (87%)	18 (9%)	9 (4%)	2	16
47	m0	209/220 (95%)	168 (80%)	31 (15%)	10 (5%)	2	14
48	M1	167/169 (99%)	127 (76%)	26 (16%)	14 (8%)	1	5
48	m1	167/169 (99%)	140 (84%)	17 (10%)	10 (6%)	1	10
49	M3	191/194 (98%)	159 (83%)	21 (11%)	11 (6%)	1	10
49	m3	192/194 (99%)	156 (81%)	24 (12%)	12 (6%)	1	9
50	M4	134/137 (98%)	118 (88%)	10 (8%)	6 (4%)	2	15
50	m4	135/137 (98%)	123 (91%)	9 (7%)	3 (2%)	6	31
51	M5	201/203 (99%)	182 (90%)	12 (6%)	7 (4%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	24
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	15	47
52	m6	195/197 (99%)	181 (93%)	12 (6%)	2 (1%)	15	47
53	M7	181/183 (99%)	152 (84%)	20 (11%)	9 (5%)	2	13
53	m7	153/183 (84%)	136 (89%)	12 (8%)	5 (3%)	4	22
54	M8	183/185 (99%)	161 (88%)	18 (10%)	4 (2%)	6	31
54	m8	183/185 (99%)	156 (85%)	21 (12%)	6 (3%)	4	22
55	M9	186/188 (99%)	173 (93%)	11 (6%)	2 (1%)	14	46
55	m9	186/188 (99%)	180 (97%)	4 (2%)	2 (1%)	14	46
56	N0	170/172 (99%)	153 (90%)	13 (8%)	4 (2%)	6	28
56	n0	170/172 (99%)	159 (94%)	8 (5%)	3 (2%)	8	35
57	N1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	8	34
57	n1	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	12	41
58	N2	98/100 (98%)	80 (82%)	16 (16%)	2 (2%)	7	33
58	n2	96/100 (96%)	85 (88%)	10 (10%)	1 (1%)	15	47
59	N3	134/136 (98%)	122 (91%)	8 (6%)	4 (3%)	4	24
59	n3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	39
60	N4	96/98 (98%)	76 (79%)	14 (15%)	6 (6%)	1	9
61	N5	119/121 (98%)	105 (88%)	12 (10%)	2 (2%)	9	36
61	n5	118/121 (98%)	99 (84%)	10 (8%)	9 (8%)	1	6
62	N6	124/126 (98%)	111 (90%)	10 (8%)	3 (2%)	6	28
62	n6	124/126 (98%)	112 (90%)	7 (6%)	5 (4%)	3	17
63	N7	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	2	12
63	n7	133/135 (98%)	106 (80%)	15 (11%)	12 (9%)	1	4
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	2	11
64	n8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	3	22
65	N9	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	12
65	n9	56/58 (97%)	40 (71%)	10 (18%)	6 (11%)	0	3
66	O0	95/100 (95%)	89 (94%)	5 (5%)	1 (1%)	14	46
66	o0	98/100 (98%)	88 (90%)	6 (6%)	4 (4%)	3	17
67	O1	107/109 (98%)	98 (92%)	5 (5%)	4 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	o1	107/109 (98%)	94 (88%)	9 (8%)	4 (4%)	3	19
68	O2	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	6	28
68	o2	125/127 (98%)	108 (86%)	12 (10%)	5 (4%)	3	17
69	O3	104/106 (98%)	94 (90%)	8 (8%)	2 (2%)	8	34
69	o3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4	25
70	O4	110/112 (98%)	97 (88%)	11 (10%)	2 (2%)	8	35
70	o4	110/112 (98%)	96 (87%)	11 (10%)	3 (3%)	5	26
71	O5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	5	27
71	o5	117/119 (98%)	102 (87%)	11 (9%)	4 (3%)	3	22
72	O6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1	7
72	o6	97/99 (98%)	83 (86%)	7 (7%)	7 (7%)	1	7
73	O7	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
73	o7	85/87 (98%)	76 (89%)	5 (6%)	4 (5%)	2	14
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	3	17
74	o8	75/77 (97%)	62 (83%)	12 (16%)	1 (1%)	12	41
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	32
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	32
76	Q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	17
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7	33
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	85 (82%)	12 (12%)	6 (6%)	1	10
78	q2	103/105 (98%)	94 (91%)	5 (5%)	4 (4%)	3	18
79	Q3	89/91 (98%)	79 (89%)	7 (8%)	3 (3%)	3	22
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	14	46
80	c0	78/96 (81%)	61 (78%)	10 (13%)	7 (9%)	1	4
81	c2	108/124 (87%)	67 (62%)	26 (24%)	15 (14%)	0	1
82	c5	133/142 (94%)	96 (72%)	19 (14%)	18 (14%)	0	1
83	sR	316/318 (99%)	268 (85%)	39 (12%)	9 (3%)	5	25
84	sM	61/104 (59%)	43 (70%)	10 (16%)	8 (13%)	0	1
85	l8	224/231 (97%)	184 (82%)	25 (11%)	15 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	n4	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	7
88	p0	117/219 (53%)	101 (86%)	12 (10%)	4 (3%)	3	22
All	All	22197/22912 (97%)	18787 (85%)	2314 (10%)	1096 (5%)	2	14

All (1096) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	5	ALA
2	S0	95	ALA
2	S0	158	VAL
2	S0	191	ARG
2	S0	203	PHE
3	S1	49	ASN
3	S1	113	MET
3	S1	148	ASN
3	S1	177	GLN
3	S1	179	SER
3	S1	206	PRO
4	S2	107	SER
4	S2	148	LEU
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	195	SER
5	S3	211	PRO
5	S3	220	PRO
6	S4	104	ASP
7	S5	26	ALA
7	S5	51	VAL
7	S5	101	GLY
7	S5	153	GLY
8	S6	25	ARG
8	S6	122	GLU
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG

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Mol	Chain	Res	Type
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
10	S8	147	ALA
10	S8	149	SER
11	S9	93	LEU
11	S9	134	ILE
12	C0	60	SER
12	C0	81	ASN
14	C2	89	ILE
14	C2	93	ASP
14	C2	127	GLY
15	C3	28	LEU
15	C3	138	ASN
16	C4	39	ILE
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	40	GLU
18	C6	41	PRO
18	C6	114	ARG
18	C6	138	PHE
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	25	ASN
20	C8	28	ILE
20	C8	60	GLU
20	C8	91	ASP
20	C8	92	ILE
21	C9	31	PRO
21	C9	53	TRP
23	D1	7	GLN
25	D3	114	LYS
25	D3	138	GLU
26	D4	36	SER
27	D5	39	ALA

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Mol	Chain	Res	Type
27	D5	44	GLN
27	D5	54	VAL
27	D5	71	ILE
27	D5	97	LYS
28	D6	36	ILE
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
29	D7	62	ILE
32	E0	47	VAL
33	E1	84	VAL
33	E1	102	VAL
33	E1	106	TYR
34	SR	318	ALA
35	SM	47	ALA
35	SM	52	PRO
35	SM	140	ASP
39	L2	47	GLN
40	L3	4	ARG
40	L3	5	LYS
40	L3	140	ASP
40	L3	142	ALA
40	L3	187	SER
40	L3	347	SER
40	L3	385	LYS
41	L4	130	ALA
41	L4	293	SER
41	L4	311	HIS
41	L4	317	PRO
42	L5	20	PHE
42	L5	234	ASP
42	L5	295	GLY
43	L6	6	ALA
43	L6	98	VAL
44	L7	26	VAL
44	L7	160	ARG
44	L7	164	SER
45	L8	25	PRO
45	L8	31	PRO
46	L9	50	ASN
47	M0	218	ALA

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Mol	Chain	Res	Type
48	M1	8	PRO
48	M1	11	ASP
48	M1	94	ARG
48	M1	115	LYS
48	M1	140	ARG
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
49	M3	131	LYS
49	M3	136	GLU
50	M4	8	LYS
50	M4	9	ALA
50	M4	29	ALA
50	M4	36	VAL
51	M5	74	PRO
51	M5	144	ARG
52	M6	111	PRO
53	M7	67	ILE
53	M7	75	GLU
53	M7	157	VAL
60	N4	81	PRO
60	N4	86	SER
61	N5	44	PRO
63	N7	17	ARG
63	N7	30	ASP
63	N7	125	GLY
64	N8	57	GLY
64	N8	66	ALA
67	O1	6	ASP
67	O1	83	GLU
67	O1	84	ASP
71	O5	119	LYS
72	O6	13	LYS
72	O6	33	ALA
78	Q2	17	CYS
78	Q2	30	ALA
79	Q3	58	SER
2	s0	4	PRO
2	s0	95	ALA
2	s0	158	VAL
2	s0	164	ASN
2	s0	189	VAL

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Mol	Chain	Res	Type
2	s0	206	ASP
3	s1	106	THR
3	s1	154	SER
3	s1	206	PRO
3	s1	223	PHE
4	s2	92	ALA
4	s2	162	CYS
5	s3	61	GLU
5	s3	115	ILE
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	219	ALA
5	s3	220	PRO
6	s4	95	THR
6	s4	163	ASP
6	s4	164	LEU
6	s4	196	VAL
7	s5	28	PRO
7	s5	39	GLU
7	s5	184	PHE
7	s5	204	GLY
8	s6	70	PRO
8	s6	154	ARG
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	67	LEU
9	s7	74	GLN
9	s7	131	PHE
11	s9	150	LEU
80	c0	32	HIS
13	c1	133	LYS
81	c2	89	ILE
16	c4	126	THR
82	c5	11	VAL
82	c5	17	TYR
82	c5	52	LYS
82	c5	68	PRO
82	c5	125	PRO
82	c5	126	VAL

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Mol	Chain	Res	Type
82	c5	127	ARG
18	c6	42	GLU
18	c6	116	LEU
19	c7	63	LYS
19	c7	88	VAL
19	c7	99	VAL
19	c7	104	ASN
20	c8	91	ASP
20	c8	92	ILE
21	c9	29	GLU
21	c9	33	TYR
21	c9	34	VAL
22	d0	17	GLN
22	d0	49	ASN
22	d0	97	VAL
26	d4	30	PRO
26	d4	33	ALA
26	d4	52	LYS
27	d5	85	LYS
27	d5	104	ALA
28	d6	47	ALA
29	d7	60	SER
30	d8	61	ARG
31	d9	6	VAL
32	e0	60	PRO
33	e1	79	LYS
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	106	TYR
83	sR	160	GLU
83	sR	163	ASP
83	sR	165	ASP
83	sR	318	ALA
84	sM	42	ALA
84	sM	50	ASN
39	l2	238	ILE
40	l3	22	ALA
40	l3	129	ALA
41	l4	301	PRO
41	l4	329	PRO

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Mol	Chain	Res	Type
42	l5	178	ASN
44	l7	159	GLN
85	l8	25	PRO
85	l8	34	PHE
85	l8	121	SER
85	l8	122	LYS
47	m0	82	ARG
47	m0	220	GLN
48	m1	8	PRO
48	m1	10	ARG
48	m1	94	ARG
48	m1	108	GLU
49	m3	47	ALA
49	m3	150	PRO
51	m5	76	PRO
52	m6	110	PRO
54	m8	99	THR
57	n1	136	ARG
87	n4	26	SER
87	n4	63	ILE
87	n4	71	ARG
87	n4	76	VAL
61	n5	24	LEU
61	n5	44	PRO
61	n5	45	LYS
61	n5	55	ASN
62	n6	83	ASP
62	n6	84	LYS
62	n6	125	LYS
62	n6	126	LEU
63	n7	7	ALA
63	n7	125	GLY
63	n7	129	TRP
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	45	GLY
68	o2	6	HIS
69	o3	88	ASN
72	o6	33	ALA
72	o6	64	SER

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Mol	Chain	Res	Type
72	o6	98	ARG
78	q2	17	CYS
88	p0	93	LEU
2	S0	4	PRO
2	S0	39	ASN
2	S0	49	ASN
2	S0	94	GLY
3	S1	21	VAL
3	S1	26	ARG
3	S1	35	PRO
3	S1	58	SER
3	S1	60	ALA
3	S1	62	LYS
3	S1	63	GLY
3	S1	158	SER
3	S1	182	ALA
3	S1	221	PRO
4	S2	106	ASP
5	S3	59	LEU
5	S3	216	PRO
6	S4	12	LEU
6	S4	195	ILE
7	S5	43	PHE
7	S5	63	GLN
7	S5	127	GLN
7	S5	150	GLY
8	S6	152	ASP
9	S7	29	ASN
9	S7	155	ASP
9	S7	186	PRO
10	S8	40	ALA
10	S8	104	ILE
10	S8	199	LYS
11	S9	98	ALA
11	S9	121	SER
11	S9	167	ALA
13	C1	30	ARG
13	C1	55	ASP
14	C2	25	GLU
14	C2	91	VAL
15	C3	22	ALA
15	C3	68	GLY

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Mol	Chain	Res	Type
16	C4	50	ALA
16	C4	51	ASP
16	C4	114	ARG
17	C5	11	VAL
17	C5	48	GLY
17	C5	101	ALA
18	C6	59	LYS
19	C7	23	LYS
19	C7	87	GLU
19	C7	115	LEU
20	C8	61	LEU
20	C8	142	GLY
21	C9	28	LEU
22	D0	17	GLN
23	D1	2	GLU
23	D1	4	ASP
23	D1	15	ARG
25	D3	70	LYS
25	D3	112	LYS
26	D4	5	VAL
27	D5	43	ASP
28	D6	11	ASN
28	D6	65	PRO
28	D6	86	VAL
29	D7	63	LEU
30	D8	36	THR
31	D9	20	GLN
32	E0	51	ASN
33	E1	83	LYS
33	E1	86	THR
33	E1	98	VAL
33	E1	144	CYS
33	E1	145	HIS
34	SR	161	ALA
35	SM	86	ASN
35	SM	87	THR
35	SM	111	GLY
39	L2	13	GLY
40	L3	3	HIS
40	L3	289	ASP
40	L3	351	LEU
41	L4	318	LEU

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Mol	Chain	Res	Type
41	L4	338	LYS
42	L5	6	ASP
42	L5	125	VAL
42	L5	137	ASP
42	L5	153	THR
42	L5	233	ALA
42	L5	253	PHE
42	L5	258	LYS
42	L5	276	LYS
44	L7	25	GLN
45	L8	36	ILE
45	L8	39	ALA
45	L8	75	ILE
47	M0	117	GLY
47	M0	145	LYS
47	M0	194	GLY
47	M0	220	GLN
48	M1	12	LEU
48	M1	74	PRO
48	M1	114	ILE
48	M1	152	HIS
49	M3	13	HIS
49	M3	141	ALA
49	M3	193	ALA
50	M4	10	SER
54	M8	98	LYS
55	M9	3	ASN
55	M9	53	LYS
56	N0	166	LYS
57	N1	123	GLY
57	N1	124	VAL
58	N2	51	GLY
59	N3	82	ALA
59	N3	134	GLY
60	N4	64	THR
61	N5	45	LYS
62	N6	84	LYS
62	N6	92	GLY
63	N7	35	SER
63	N7	102	GLU
64	N8	76	ASP
64	N8	96	LYS

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Mol	Chain	Res	Type
68	O2	27	ARG
71	O5	97	ALA
74	O8	18	ALA
74	O8	33	LYS
76	Q0	78	ILE
78	Q2	60	LYS
78	Q2	94	GLY
78	Q2	100	LYS
2	s0	8	ASP
2	s0	44	GLY
2	s0	66	ALA
2	s0	68	PRO
2	s0	186	GLY
3	s1	81	PHE
3	s1	82	ARG
3	s1	93	GLY
3	s1	218	LEU
5	s3	179	GLN
6	s4	12	LEU
6	s4	104	ASP
6	s4	195	ILE
6	s4	214	LEU
7	s5	36	ALA
7	s5	101	GLY
8	s6	138	ALA
8	s6	175	ILE
9	s7	66	SER
9	s7	133	THR
9	s7	155	ASP
10	s8	36	THR
10	s8	122	GLY
10	s8	199	LYS
11	s9	118	LEU
80	c0	23	ALA
80	c0	35	ILE
13	c1	7	VAL
81	c2	58	LEU
81	c2	66	VAL
81	c2	87	PRO
81	c2	101	ALA
81	c2	119	SER
81	c2	131	ASP

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Mol	Chain	Res	Type
15	c3	19	SER
15	c3	66	ILE
15	c3	139	TRP
16	c4	51	ASP
82	c5	51	SER
82	c5	131	ALA
82	c5	132	GLY
18	c6	39	VAL
18	c6	115	THR
19	c7	116	LYS
20	c8	60	GLU
22	d0	15	GLN
22	d0	52	LYS
22	d0	96	PRO
22	d0	118	VAL
26	d4	35	VAL
27	d5	44	GLN
28	d6	28	LYS
29	d7	53	ALA
32	e0	47	VAL
32	e0	51	ASN
32	e0	61	SER
33	e1	100	LEU
33	e1	102	VAL
33	e1	112	GLY
33	e1	136	LYS
84	sM	65	THR
84	sM	83	LYS
39	l2	24	GLN
39	l2	96	LEU
39	l2	127	ALA
39	l2	212	GLY
40	l3	140	ASP
41	l4	14	GLU
41	l4	15	ALA
41	l4	90	PHE
41	l4	146	PRO
41	l4	311	HIS
41	l4	345	GLU
42	l5	26	GLY
42	l5	123	GLU
42	l5	258	LYS

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Mol	Chain	Res	Type
42	l5	260	PHE
43	l6	98	VAL
44	l7	158	LYS
85	l8	26	LEU
85	l8	203	VAL
46	l9	144	ILE
46	l9	189	GLU
47	m0	83	ASP
47	m0	193	ASP
48	m1	95	ASN
48	m1	115	LYS
48	m1	167	TYR
49	m3	50	PRO
49	m3	93	ILE
49	m3	101	ARG
49	m3	134	GLU
49	m3	135	ALA
49	m3	141	ALA
50	m4	136	ALA
51	m5	183	THR
51	m5	184	LYS
51	m5	187	ARG
52	m6	16	VAL
53	m7	66	SER
53	m7	77	GLY
54	m8	84	VAL
54	m8	167	SER
56	n0	142	GLN
59	n3	42	SER
87	n4	25	ASP
87	n4	83	THR
87	n4	133	THR
61	n5	25	LYS
61	n5	40	LEU
63	n7	29	HIS
63	n7	70	PRO
63	n7	130	PHE
64	n8	47	LYS
65	n9	24	PRO
65	n9	25	LYS
66	o0	10	ILE
67	o1	83	GLU

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Mol	Chain	Res	Type
68	o2	124	GLY
70	o4	79	SER
71	o5	119	LYS
73	o7	67	LEU
73	o7	87	SER
74	o8	18	ALA
75	o9	3	ALA
78	q2	31	GLY
78	q2	32	LYS
88	p0	33	VAL
2	S0	192	THR
2	S0	195	TRP
3	S1	54	LEU
3	S1	156	ALA
6	S4	3	ARG
6	S4	245	LYS
7	S5	31	GLU
7	S5	39	GLU
7	S5	45	LYS
8	S6	69	LEU
9	S7	30	SER
9	S7	36	ALA
9	S7	74	GLN
9	S7	98	ILE
10	S8	22	ARG
11	S9	150	LEU
12	C0	64	TYR
13	C1	7	VAL
13	C1	146	ALA
14	C2	21	GLU
14	C2	87	PRO
14	C2	106	ILE
14	C2	107	ASP
14	C2	119	SER
15	C3	27	LYS
16	C4	40	ALA
16	C4	42	VAL
17	C5	52	LYS
17	C5	69	GLU
18	C6	111	SER
21	C9	69	LYS
22	D0	55	PRO

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Mol	Chain	Res	Type
24	D2	78	ARG
25	D3	131	SER
27	D5	41	ILE
28	D6	18	VAL
28	D6	35	ALA
29	D7	51	GLN
30	D8	61	ARG
31	D9	8	PHE
32	E0	50	VAL
33	E1	103	LEU
33	E1	111	GLU
33	E1	118	ARG
34	SR	98	GLU
34	SR	163	ASP
35	SM	82	THR
39	L2	144	ASN
39	L2	251	LYS
40	L3	174	LYS
40	L3	221	THR
41	L4	15	ALA
41	L4	90	PHE
41	L4	146	PRO
41	L4	182	LEU
41	L4	232	SER
41	L4	268	ALA
42	L5	7	ALA
42	L5	215	ASP
42	L5	260	PHE
43	L6	5	LYS
45	L8	76	ALA
46	L9	190	ASP
47	M0	187	ALA
47	M0	207	GLU
48	M1	95	ASN
48	M1	108	GLU
48	M1	145	LYS
49	M3	50	PRO
49	M3	76	THR
49	M3	130	GLY
49	M3	166	ALA
51	M5	81	TYR
53	M7	162	GLU

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Mol	Chain	Res	Type
53	M7	164	LYS
57	N1	159	PHE
58	N2	11	ILE
59	N3	46	LEU
59	N3	47	ASN
60	N4	97	LYS
62	N6	91	ASN
63	N7	36	HIS
64	N8	97	GLU
64	N8	117	ARG
68	O2	12	LYS
68	O2	68	PRO
72	O6	64	SER
79	Q3	7	LYS
79	Q3	84	ARG
2	s0	10	THR
2	s0	30	GLN
2	s0	185	ARG
2	s0	194	PRO
2	s0	203	PHE
3	s1	21	VAL
3	s1	39	GLU
3	s1	147	ALA
4	s2	106	ASP
4	s2	107	SER
4	s2	238	SER
5	s3	44	THR
5	s3	161	GLY
6	s4	245	LYS
7	s5	43	PHE
7	s5	151	GLY
8	s6	65	GLN
8	s6	68	LEU
8	s6	126	ASP
8	s6	152	ASP
8	s6	165	GLY
11	s9	169	PRO
13	c1	40	LEU
13	c1	121	ASP
81	c2	93	ASP
15	c3	87	ASP
15	c3	140	LYS

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Mol	Chain	Res	Type
16	c4	50	ALA
82	c5	7	ALA
82	c5	9	LYS
18	c6	113	ASP
20	c8	61	LEU
24	d2	56	HIS
26	d4	50	ALA
26	d4	78	SER
28	d6	13	LYS
29	d7	62	ILE
30	d8	62	GLU
31	d9	7	TRP
33	e1	81	LYS
33	e1	86	THR
33	e1	129	GLY
33	e1	131	PHE
33	e1	148	TYR
83	sR	4	ASN
84	sM	47	ALA
39	l2	56	ALA
39	l2	216	HIS
40	l3	155	ALA
40	l3	235	THR
41	l4	142	VAL
41	l4	190	GLY
41	l4	220	ARG
41	l4	233	LEU
41	l4	302	ALA
42	l5	270	LYS
44	l7	191	VAL
44	l7	228	SER
85	l8	39	ALA
85	l8	133	LYS
85	l8	239	GLY
85	l8	240	ASN
46	l9	2	LYS
47	m0	170	LYS
47	m0	174	THR
47	m0	176	LEU
47	m0	204	GLY
51	m5	181	ASN
54	m8	112	ALA

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Mol	Chain	Res	Type
56	n0	154	HIS
58	n2	91	ASP
87	n4	58	HIS
63	n7	56	LYS
63	n7	128	GLN
66	o0	100	ILE
66	o0	103	THR
67	o1	5	LYS
67	o1	84	ASP
71	o5	81	ARG
72	o6	34	SER
76	q0	78	ILE
78	q2	60	LYS
79	q3	50	GLY
88	p0	102	SER
2	S0	103	THR
2	S0	205	ARG
3	S1	130	SER
3	S1	209	ASN
3	S1	213	ARG
4	S2	235	LEU
4	S2	248	SER
5	S3	217	ILE
6	S4	193	GLY
6	S4	200	ARG
6	S4	234	PRO
6	S4	260	GLY
7	S5	58	LEU
7	S5	64	VAL
9	S7	5	GLN
9	S7	156	SER
10	S8	10	LYS
10	S8	52	ASN
10	S8	120	THR
10	S8	152	ILE
11	S9	118	LEU
12	C0	34	GLU
13	C1	147	ALA
14	C2	22	VAL
14	C2	112	ALA
14	C2	125	ASN
15	C3	3	ARG

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Mol	Chain	Res	Type
18	C6	32	ASN
19	C7	84	TYR
23	D1	81	ASN
24	D2	30	SER
24	D2	83	ILE
25	D3	41	SER
26	D4	6	THR
26	D4	34	ASN
26	D4	51	GLU
28	D6	46	GLU
28	D6	64	LEU
30	D8	6	PRO
33	E1	87	THR
34	SR	15	GLY
34	SR	231	MET
35	SM	12	VAL
39	L2	143	GLU
39	L2	246	LEU
42	L5	228	ALA
42	L5	259	LYS
45	L8	156	ASP
45	L8	157	VAL
45	L8	254	ASP
46	L9	2	LYS
46	L9	110	LYS
47	M0	217	PHE
51	M5	75	VAL
51	M5	184	LYS
53	M7	160	ALA
53	M7	161	ALA
53	M7	163	LYS
54	M8	99	THR
56	N0	24	LEU
60	N4	76	VAL
63	N7	103	GLN
65	N9	18	ARG
66	O0	96	GLY
71	O5	75	TYR
72	O6	34	SER
74	O8	35	GLY
78	Q2	34	SER
2	s0	103	THR

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Mol	Chain	Res	Type
3	s1	26	ARG
3	s1	179	SER
3	s1	224	ASP
4	s2	150	GLN
4	s2	235	LEU
5	s3	90	ARG
5	s3	93	ASP
5	s3	221	SER
6	s4	30	ARG
6	s4	90	ILE
6	s4	168	LYS
7	s5	29	ILE
7	s5	100	ASN
7	s5	153	GLY
8	s6	25	ARG
10	s8	94	ASN
11	s9	121	SER
11	s9	164	PHE
11	s9	167	ALA
80	c0	24	LYS
80	c0	30	ALA
13	c1	55	ASP
81	c2	39	ASP
81	c2	45	LEU
15	c3	60	VAL
15	c3	82	PRO
16	c4	48	VAL
16	c4	132	ARG
82	c5	14	THR
18	c6	97	VAL
19	c7	62	GLN
19	c7	113	LEU
22	d0	13	GLU
22	d0	51	VAL
23	d1	42	GLU
23	d1	44	ARG
26	d4	58	PHE
28	d6	15	ARG
28	d6	59	TYR
29	d7	20	LYS
29	d7	75	GLU
30	d8	33	LEU

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Mol	Chain	Res	Type
31	d9	11	PRO
33	e1	84	VAL
33	e1	103	LEU
83	sR	161	LYS
39	l2	80	GLU
40	l3	23	ALA
40	l3	187	SER
40	l3	386	ASP
41	l4	145	ILE
41	l4	193	LYS
41	l4	330	TYR
43	l6	10	TYR
43	l6	20	LYS
43	l6	172	HIS
85	l8	82	LEU
85	l8	163	VAL
85	l8	237	ILE
46	l9	110	LYS
48	m1	114	ILE
49	m3	60	ALA
49	m3	76	THR
49	m3	129	ASN
53	m7	67	ILE
53	m7	75	GLU
53	m7	78	VAL
54	m8	108	ALA
54	m8	155	MET
55	m9	3	ASN
56	n0	2	ALA
57	n1	135	PRO
59	n3	64	LYS
61	n5	38	LEU
61	n5	47	ALA
62	n6	77	LYS
63	n7	103	GLN
63	n7	127	ASN
63	n7	134	LEU
64	n8	110	GLY
68	o2	4	LEU
68	o2	5	PRO
68	o2	12	LYS
71	o5	82	ALA

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Mol	Chain	Res	Type
73	o7	85	LYS
73	o7	86	ALA
2	S0	66	ALA
3	S1	64	ARG
4	S2	150	GLN
5	S3	4	LEU
6	S4	77	ARG
7	S5	81	ARG
8	S6	146	GLY
9	S7	73	VAL
10	S8	59	ARG
13	C1	95	PRO
14	C2	39	ASP
14	C2	66	VAL
14	C2	68	GLU
14	C2	101	ALA
16	C4	18	ARG
16	C4	75	GLY
17	C5	9	LYS
22	D0	21	LYS
22	D0	49	ASN
23	D1	10	GLU
23	D1	42	GLU
23	D1	44	ARG
25	D3	3	LYS
25	D3	89	ASN
31	D9	11	PRO
33	E1	100	LEU
34	SR	160	GLU
34	SR	237	GLN
35	SM	46	LYS
35	SM	101	ASP
39	L2	127	ALA
40	L3	155	ALA
41	L4	5	GLN
41	L4	14	GLU
41	L4	233	LEU
41	L4	313	LEU
41	L4	339	LEU
41	L4	361	HIS
42	L5	19	PRO
42	L5	292	ALA

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Mol	Chain	Res	Type
46	L9	96	HIS
48	M1	117	ASP
51	M5	94	TYR
51	M5	145	ASP
54	M8	162	ALA
56	N0	2	ALA
60	N4	80	ARG
64	N8	47	LYS
65	N9	25	LYS
67	O1	7	VAL
69	O3	91	ALA
70	O4	46	ASP
72	O6	3	VAL
72	O6	21	THR
72	O6	77	LEU
75	O9	4	GLN
76	Q0	79	GLU
2	s0	127	ARG
4	s2	91	ARG
6	s4	94	ALA
6	s4	119	ALA
7	s5	35	GLN
7	s5	152	GLY
9	s7	8	ILE
9	s7	11	GLN
10	s8	78	ILE
11	s9	126	ARG
80	c0	3	MET
80	c0	31	LYS
81	c2	59	LEU
81	c2	82	PRO
81	c2	118	ALA
15	c3	22	ALA
19	c7	86	PRO
20	c8	14	ILE
20	c8	135	GLY
22	d0	72	ASN
23	d1	4	ASP
23	d1	77	GLY
25	d3	101	GLU
26	d4	51	GLU
26	d4	53	ASP

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Mol	Chain	Res	Type
28	d6	35	ALA
29	d7	3	LEU
29	d7	58	SER
33	e1	146	SER
83	sR	146	GLY
84	sM	43	ASP
84	sM	46	LYS
39	l2	143	GLU
41	l4	328	ASN
46	l9	96	HIS
46	l9	167	VAL
47	m0	43	VAL
48	m1	153	LYS
50	m4	135	LEU
63	n7	16	GLY
64	n8	24	LYS
66	o0	101	LEU
69	o3	33	GLU
69	o3	59	VAL
3	S1	210	ILE
7	S5	100	ASN
8	S6	123	GLY
8	S6	153	VAL
11	S9	162	SER
13	C1	96	LYS
14	C2	63	VAL
14	C2	85	LYS
14	C2	128	ALA
14	C2	131	ASP
18	C6	33	GLY
25	D3	96	VAL
28	D6	63	ALA
35	SM	17	VAL
35	SM	53	ARG
35	SM	89	ARG
35	SM	139	GLU
39	L2	180	LEU
40	L3	175	LYS
40	L3	317	ILE
41	L4	4	PRO
41	L4	140	HIS
44	L7	178	ILE

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Mol	Chain	Res	Type
45	L8	190	VAL
50	M4	6	ILE
52	M6	110	PRO
64	N8	27	LYS
2	s0	191	ARG
4	s2	163	GLY
4	s2	236	PRO
5	s3	43	PRO
5	s3	160	SER
5	s3	180	GLY
9	s7	115	SER
9	s7	185	ILE
10	s8	52	ASN
11	s9	162	SER
13	c1	76	VAL
16	c4	124	ASP
82	c5	71	GLU
82	c5	128	HIS
82	c5	130	ARG
23	d1	10	GLU
25	d3	70	LYS
27	d5	103	ARG
28	d6	58	VAL
32	e0	45	VAL
32	e0	54	ARG
40	l3	3	HIS
44	l7	229	PHE
85	l8	69	LEU
85	l8	81	THR
47	m0	101	LYS
48	m1	12	LEU
49	m3	152	THR
50	m4	49	PRO
51	m5	68	ARG
55	m9	36	ASN
87	n4	72	SER
64	n8	129	PHE
70	o4	78	GLY
70	o4	82	ALA
72	o6	36	ARG
23	D1	82	VAL
25	D3	8	GLY

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Mol	Chain	Res	Type
26	D4	100	VAL
56	N0	167	ARG
65	N9	21	ILE
69	O3	59	VAL
70	O4	77	GLY
4	s2	83	ILE
10	s8	50	GLY
10	s8	101	ILE
81	c2	63	VAL
82	c5	129	GLY
28	d6	60	PRO
41	l4	272	VAL
42	l5	125	VAL
72	o6	3	VAL
3	S1	48	VAL
3	S1	176	VAL
4	S2	182	PRO
14	C2	81	ASP
23	D1	6	GLY
26	D4	47	VAL
41	L4	131	VAL
54	M8	183	GLY
8	s6	69	LEU
82	c5	48	GLY
83	sR	97	GLY
83	sR	105	GLY
44	l7	178	ILE
71	o5	4	VAL
2	S0	189	VAL
17	C5	87	PRO
26	D4	95	GLY
27	D5	55	PRO
44	L7	191	VAL
45	L8	30	THR
47	M0	47	PRO
3	s1	22	ASP
81	c2	115	VAL
19	c7	117	LEU
25	d3	130	VAL
87	n4	132	GLY
3	S1	114	VAL
7	S5	21	THR

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Mol	Chain	Res	Type
9	S7	132	PRO
27	D5	88	ILE
34	SR	194	GLY
53	M7	36	ILE
8	s6	153	VAL
40	l3	141	GLY
61	n5	62	VAL
65	n9	37	PRO
72	o6	9	ILE
88	p0	196	VAL
7	s5	59	VAL
84	sM	51	ARG

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
2	S0	164/173 (95%)	132 (80%)	32 (20%)	1 5
2	s0	165/173 (95%)	136 (82%)	29 (18%)	2 8
3	S1	191/192 (100%)	155 (81%)	36 (19%)	1 6
3	s1	192/192 (100%)	162 (84%)	30 (16%)	2 11
4	S2	176/176 (100%)	141 (80%)	35 (20%)	1 5
4	s2	176/176 (100%)	137 (78%)	39 (22%)	1 3
5	S3	182/182 (100%)	150 (82%)	32 (18%)	2 8
5	s3	182/182 (100%)	157 (86%)	25 (14%)	3 16
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2 8
6	s4	221/221 (100%)	193 (87%)	28 (13%)	4 18
7	S5	173/173 (100%)	142 (82%)	31 (18%)	2 7
7	s5	173/173 (100%)	142 (82%)	31 (18%)	2 7
8	S6	188/193 (97%)	156 (83%)	32 (17%)	2 9
8	s6	187/193 (97%)	154 (82%)	33 (18%)	2 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/166 (99%)	139 (84%)	26 (16%)	2	11
9	s7	165/166 (99%)	138 (84%)	27 (16%)	2	10
10	S8	150/160 (94%)	128 (85%)	22 (15%)	3	13
10	s8	150/160 (94%)	132 (88%)	18 (12%)	5	20
11	S9	158/158 (100%)	127 (80%)	31 (20%)	1	5
11	s9	158/158 (100%)	136 (86%)	22 (14%)	3	15
12	C0	77/77 (100%)	64 (83%)	13 (17%)	2	9
13	C1	129/129 (100%)	113 (88%)	16 (12%)	4	19
13	c1	129/129 (100%)	102 (79%)	27 (21%)	1	4
14	C2	88/100 (88%)	69 (78%)	19 (22%)	1	4
15	C3	127/127 (100%)	108 (85%)	19 (15%)	3	12
15	c3	127/127 (100%)	106 (84%)	21 (16%)	2	10
16	C4	81/97 (84%)	63 (78%)	18 (22%)	1	3
16	c4	97/97 (100%)	74 (76%)	23 (24%)	1	2
17	C5	101/107 (94%)	87 (86%)	14 (14%)	3	15
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	7
18	c6	118/118 (100%)	101 (86%)	17 (14%)	3	14
19	C7	94/113 (83%)	72 (77%)	22 (23%)	1	3
19	c7	92/113 (81%)	78 (85%)	14 (15%)	3	12
20	C8	128/128 (100%)	93 (73%)	35 (27%)	0	1
20	c8	128/128 (100%)	105 (82%)	23 (18%)	1	7
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	5
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2	11
22	D0	100/103 (97%)	78 (78%)	22 (22%)	1	3
22	d0	103/103 (100%)	79 (77%)	24 (23%)	1	3
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3	12
23	d1	74/74 (100%)	61 (82%)	13 (18%)	2	8
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2	10
24	d2	110/110 (100%)	97 (88%)	13 (12%)	5	21
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	16
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	6
26	d4	112/112 (100%)	96 (86%)	16 (14%)	3	14
27	D5	61/61 (100%)	44 (72%)	17 (28%)	0	1
27	d5	61/61 (100%)	53 (87%)	8 (13%)	4	17
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	1
28	d6	83/83 (100%)	71 (86%)	12 (14%)	3	14
29	D7	70/70 (100%)	63 (90%)	7 (10%)	7	27
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/56 (100%)	45 (80%)	11 (20%)	1	5
30	d8	56/56 (100%)	44 (79%)	12 (21%)	1	4
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1	4
31	d9	47/47 (100%)	38 (81%)	9 (19%)	1	6
32	E0	51/53 (96%)	44 (86%)	7 (14%)	3	16
32	e0	53/53 (100%)	39 (74%)	14 (26%)	0	1
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	1
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
34	SR	259/260 (100%)	234 (90%)	25 (10%)	8	29
35	SM	97/107 (91%)	81 (84%)	16 (16%)	2	10
39	L2	193/194 (100%)	166 (86%)	27 (14%)	3	15
39	l2	192/194 (99%)	160 (83%)	32 (17%)	2	9
40	L3	321/322 (100%)	265 (83%)	56 (17%)	2	8
40	l3	321/322 (100%)	264 (82%)	57 (18%)	2	7
41	L4	288/288 (100%)	244 (85%)	44 (15%)	2	12
41	l4	288/288 (100%)	237 (82%)	51 (18%)	2	8
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	11
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2	10
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	16
43	l6	135/152 (89%)	117 (87%)	18 (13%)	4	16
44	L7	186/187 (100%)	168 (90%)	18 (10%)	8	29
44	l7	187/187 (100%)	162 (87%)	25 (13%)	4	16
45	L8	187/191 (98%)	154 (82%)	33 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L9	171/171 (100%)	138 (81%)	33 (19%)	1	5
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	4
47	M0	177/186 (95%)	147 (83%)	30 (17%)	2	9
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	9
48	M1	147/147 (100%)	122 (83%)	25 (17%)	2	9
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1	7
49	M3	154/154 (100%)	126 (82%)	28 (18%)	1	7
49	m3	154/154 (100%)	133 (86%)	21 (14%)	3	16
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	7
50	m4	108/108 (100%)	92 (85%)	16 (15%)	3	13
51	M5	175/175 (100%)	139 (79%)	36 (21%)	1	4
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3	14
52	M6	160/160 (100%)	144 (90%)	16 (10%)	7	27
52	m6	160/160 (100%)	140 (88%)	20 (12%)	4	19
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1	6
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	8
54	M8	150/150 (100%)	130 (87%)	20 (13%)	4	16
54	m8	150/150 (100%)	126 (84%)	24 (16%)	2	10
55	M9	153/153 (100%)	127 (83%)	26 (17%)	2	9
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	7
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	7
56	n0	156/156 (100%)	130 (83%)	26 (17%)	2	9
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/87 (100%)	75 (86%)	12 (14%)	3	16
58	n2	85/87 (98%)	70 (82%)	15 (18%)	2	8
59	N3	104/104 (100%)	88 (85%)	16 (15%)	2	12
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	25
60	N4	57/86 (66%)	50 (88%)	7 (12%)	4	20
61	N5	104/105 (99%)	83 (80%)	21 (20%)	1	5
61	n5	104/105 (99%)	85 (82%)	19 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	N6	109/109 (100%)	82 (75%)	27 (25%)	0	2
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	2
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	7
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	5
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	7
64	n8	118/118 (100%)	103 (87%)	15 (13%)	4	18
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	8
65	n9	46/46 (100%)	35 (76%)	11 (24%)	0	2
66	O0	81/84 (96%)	68 (84%)	13 (16%)	2	10
66	o0	84/84 (100%)	72 (86%)	12 (14%)	3	14
67	O1	92/96 (96%)	77 (84%)	15 (16%)	2	10
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	6
68	O2	109/109 (100%)	98 (90%)	11 (10%)	7	27
68	o2	109/109 (100%)	94 (86%)	15 (14%)	3	16
69	O3	90/90 (100%)	79 (88%)	11 (12%)	5	20
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	14
70	O4	95/95 (100%)	79 (83%)	16 (17%)	2	9
70	o4	95/95 (100%)	83 (87%)	12 (13%)	4	18
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1	6
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	4
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	3
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	59 (84%)	11 (16%)	2	11
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0	2
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	7
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	11
75	o9	45/45 (100%)	39 (87%)	6 (13%)	4	16
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	9
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	6
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	70 (78%)	20 (22%)	1	3
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	5
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	15
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	4
80	c0	73/73 (100%)	60 (82%)	13 (18%)	2	7
81	c2	88/88 (100%)	68 (77%)	20 (23%)	1	3
82	c5	103/118 (87%)	85 (82%)	18 (18%)	2	8
83	sR	260/261 (100%)	241 (93%)	19 (7%)	14	40
84	sM	54/54 (100%)	41 (76%)	13 (24%)	0	2
85	l8	177/185 (96%)	154 (87%)	23 (13%)	4	17
87	n4	100/114 (88%)	91 (91%)	9 (9%)	9	32
88	p0	105/165 (64%)	85 (81%)	20 (19%)	1	6
All	All	18729/19106 (98%)	15556 (83%)	3173 (17%)	2	9

All (3173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	7	PHE
2	S0	8	ASP
2	S0	9	LEU
2	S0	37	VAL
2	S0	43	ASP
2	S0	49	ASN
2	S0	50	VAL
2	S0	52	LYS
2	S0	59	LEU
2	S0	76	ILE
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	103	THR
2	S0	111	ILE
2	S0	117	GLU

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Mol	Chain	Res	Type
2	S0	119	ARG
2	S0	135	GLU
2	S0	139	VAL
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	170	ILE
2	S0	172	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
2	S0	200	ASP
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	61	LEU
3	S1	66	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	89	ASP
3	S1	91	VAL
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	111	ARG
3	S1	112	SER
3	S1	117	TRP
3	S1	124	ASN
3	S1	131	ASP
3	S1	135	LEU
3	S1	149	GLN
3	S1	170	GLU
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	198	GLU

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Mol	Chain	Res	Type
3	S1	202	LYS
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	54	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	70	ASP
4	S2	72	LEU
4	S2	73	LEU
4	S2	77	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	117	THR
4	S2	134	LEU
4	S2	136	VAL
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	159	THR
4	S2	166	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	237	VAL
4	S2	245	ASP

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Mol	Chain	Res	Type
5	S3	4	LEU
5	S3	7	LYS
5	S3	23	GLU
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	91	VAL
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	103	GLU
5	S3	104	SER
5	S3	105	MET
5	S3	113	LEU
5	S3	117	ARG
5	S3	127	MET
5	S3	134	CYS
5	S3	141	LYS
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	157	LEU
5	S3	158	ILE
5	S3	176	LEU
5	S3	178	ARG
5	S3	187	LYS
5	S3	190	ARG
5	S3	209	ILE
5	S3	218	LEU
5	S3	222	VAL
6	S4	7	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	39	ARG
6	S4	42	LEU
6	S4	65	LEU
6	S4	68	ARG
6	S4	70	VAL

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Mol	Chain	Res	Type
6	S4	77	ARG
6	S4	92	LEU
6	S4	93	ASP
6	S4	116	ASP
6	S4	126	VAL
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	139	VAL
6	S4	140	VAL
6	S4	146	THR
6	S4	148	ARG
6	S4	155	LYS
6	S4	164	LEU
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	197	HIS
6	S4	211	LYS
6	S4	214	LEU
6	S4	215	ASP
6	S4	222	LEU
6	S4	226	PHE
6	S4	227	VAL
6	S4	231	GLN
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	259	GLN
7	S5	24	VAL
7	S5	25	LEU
7	S5	32	GLU
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	49	GLU
7	S5	51	VAL
7	S5	53	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	86	GLN

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Mol	Chain	Res	Type
7	S5	89	ILE
7	S5	93	LEU
7	S5	119	ASP
7	S5	126	ASP
7	S5	147	THR
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	170	GLN
7	S5	186	ASN
7	S5	190	ILE
7	S5	194	LEU
7	S5	203	LYS
7	S5	206	SER
7	S5	216	GLU
7	S5	219	ARG
7	S5	225	ARG
8	S6	7	TYR
8	S6	25	ARG
8	S6	30	LYS
8	S6	45	PHE
8	S6	58	LYS
8	S6	59	GLN
8	S6	65	GLN
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	97	VAL
8	S6	98	ARG
8	S6	120	GLU
8	S6	122	GLU
8	S6	124	LEU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS

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Mol	Chain	Res	Type
8	S6	151	ASP
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	216	LEU
8	S6	223	LYS
9	S7	9	LEU
9	S7	24	PHE
9	S7	37	GLU
9	S7	38	LEU
9	S7	50	ASP
9	S7	70	PHE
9	S7	77	LEU
9	S7	79	ARG
9	S7	80	GLU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	105	THR
9	S7	109	VAL
9	S7	114	ARG
9	S7	116	ARG
9	S7	126	LEU
9	S7	131	PHE
9	S7	143	LEU
9	S7	144	VAL
9	S7	154	LEU
9	S7	159	VAL
9	S7	167	GLU
9	S7	181	ILE
9	S7	184	GLU
9	S7	185	ILE
10	S8	8	ARG
10	S8	21	PHE
10	S8	29	LEU
10	S8	32	GLN
10	S8	36	THR
10	S8	49	ARG
10	S8	58	LEU
10	S8	62	THR

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Mol	Chain	Res	Type
10	S8	66	SER
10	S8	70	GLU
10	S8	74	LYS
10	S8	123	LYS
10	S8	138	ASN
10	S8	140	GLU
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	164	ARG
10	S8	184	LEU
10	S8	185	GLU
10	S8	196	LEU
10	S8	199	LYS
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	28	LEU
11	S9	39	LYS
11	S9	49	LEU
11	S9	54	ARG
11	S9	60	LEU
11	S9	82	ARG
11	S9	88	GLU
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	96	VAL
11	S9	97	LEU
11	S9	99	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	120	LYS
11	S9	134	ILE
11	S9	138	LYS
11	S9	145	SER
11	S9	149	ARG
11	S9	151	ASP
11	S9	161	THR

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Mol	Chain	Res	Type
11	S9	171	ARG
11	S9	174	ARG
11	S9	182	GLU
12	C0	8	ARG
12	C0	20	VAL
12	C0	22	VAL
12	C0	27	PHE
12	C0	28	ASN
12	C0	32	HIS
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	82	LEU
13	C1	21	ASN
13	C1	29	LYS
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	54	ILE
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	83	THR
13	C1	99	ARG
13	C1	109	VAL
13	C1	123	VAL
13	C1	125	VAL
13	C1	136	ARG
13	C1	141	LYS
14	C2	28	LEU
14	C2	33	ARG
14	C2	36	LEU
14	C2	43	ARG
14	C2	50	LYS
14	C2	58	LEU
14	C2	61	VAL
14	C2	62	LEU
14	C2	63	VAL
14	C2	66	VAL

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Mol	Chain	Res	Type
14	C2	71	ILE
14	C2	74	LEU
14	C2	89	ILE
14	C2	103	LEU
14	C2	119	SER
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
15	C3	3	ARG
15	C3	9	LYS
15	C3	16	ILE
15	C3	21	ASN
15	C3	27	LYS
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	56	ASP
15	C3	64	ARG
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	115	LEU
15	C3	125	LEU
15	C3	134	VAL
15	C3	145	THR
15	C3	150	VAL
16	C4	13	VAL
16	C4	14	PHE
16	C4	20	TYR
16	C4	29	HIS
16	C4	31	THR
16	C4	39	ILE
16	C4	43	THR
16	C4	51	ASP
16	C4	81	VAL
16	C4	92	LYS
16	C4	102	LEU
16	C4	103	ARG
16	C4	107	ARG
16	C4	108	SER

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Mol	Chain	Res	Type
16	C4	123	SER
16	C4	124	ASP
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	22	LEU
17	C5	26	LEU
17	C5	35	LYS
17	C5	36	LEU
17	C5	44	ARG
17	C5	47	ARG
17	C5	50	THR
17	C5	52	LYS
17	C5	69	GLU
17	C5	86	VAL
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
18	C6	4	VAL
18	C6	14	LYS
18	C6	26	LYS
18	C6	28	LEU
18	C6	43	ILE
18	C6	52	LEU
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	97	VAL
18	C6	98	ASP
18	C6	101	SER
18	C6	106	LYS
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	138	PHE
18	C6	141	SER
19	C7	3	ARG
19	C7	6	THR
19	C7	25	THR

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Mol	Chain	Res	Type
19	C7	29	GLN
19	C7	30	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	43	SER
19	C7	46	LEU
19	C7	49	LYS
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	85	VAL
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	4	VAL
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	17	LEU
20	C8	20	THR
20	C8	21	ASN
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	32	LEU
20	C8	34	THR
20	C8	38	VAL
20	C8	40	ARG
20	C8	52	VAL
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN

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Mol	Chain	Res	Type
20	C8	77	THR
20	C8	80	LYS
20	C8	92	ILE
20	C8	107	SER
20	C8	110	ARG
20	C8	116	LEU
20	C8	132	ARG
20	C8	133	VAL
20	C8	136	GLN
20	C8	138	THR
20	C8	141	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	25	GLN
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	57	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	94	ILE
21	C9	125	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	132	LEU
21	C9	133	ASP
21	C9	134	ARG
21	C9	144	GLU
22	D0	15	GLN
22	D0	17	GLN
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS
22	D0	31	VAL

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Mol	Chain	Res	Type
22	D0	33	GLN
22	D0	34	LEU
22	D0	35	GLU
22	D0	42	VAL
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	60	THR
22	D0	61	LYS
22	D0	74	GLU
22	D0	76	SER
22	D0	89	ARG
22	D0	103	ILE
22	D0	108	ILE
22	D0	121	ASN
23	D1	3	ASN
23	D1	5	LYS
23	D1	32	VAL
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	65	SER
23	D1	68	SER
23	D1	78	LEU
23	D1	80	LYS
24	D2	4	SER
24	D2	7	LEU
24	D2	24	GLN
24	D2	26	LEU
24	D2	27	ILE
24	D2	43	LYS
24	D2	53	ILE
24	D2	65	LEU
24	D2	76	SER
24	D2	87	GLU
24	D2	93	LEU
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR

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Mol	Chain	Res	Type
24	D2	117	ARG
24	D2	121	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	18	HIS
25	D3	40	SER
25	D3	60	GLU
25	D3	73	ARG
25	D3	78	LYS
25	D3	82	LYS
25	D3	84	THR
25	D3	96	VAL
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	131	SER
25	D3	133	LEU
25	D3	144	ARG
26	D4	17	LEU
26	D4	29	HIS
26	D4	32	ARG
26	D4	34	ASN
26	D4	35	VAL
26	D4	36	SER
26	D4	47	VAL
26	D4	49	LYS
26	D4	51	GLU
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	84	LYS
26	D4	88	THR
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	121	THR
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
27	D5	37	GLN
27	D5	38	HIS
27	D5	42	LEU

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Mol	Chain	Res	Type
27	D5	58	ARG
27	D5	59	TYR
27	D5	67	ASP
27	D5	68	ARG
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	90	LYS
27	D5	92	ILE
27	D5	93	SER
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
28	D6	10	ARG
28	D6	12	LYS
28	D6	18	VAL
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	50	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	68	TYR
28	D6	69	ASN
28	D6	70	LYS
28	D6	79	ILE
28	D6	82	ARG
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
28	D6	90	GLU
28	D6	91	ASP
29	D7	3	LEU
29	D7	4	VAL
29	D7	20	LYS
29	D7	33	LEU
29	D7	34	ASP

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Mol	Chain	Res	Type
29	D7	61	THR
29	D7	67	THR
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	32	PHE
30	D8	33	LEU
30	D8	34	GLU
30	D8	39	THR
30	D8	49	ARG
30	D8	52	ASP
30	D8	58	GLU
30	D8	64	ARG
31	D9	6	VAL
31	D9	7	TRP
31	D9	9	SER
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	25	SER
31	D9	30	LEU
31	D9	36	LEU
31	D9	39	CYS
32	E0	20	LYS
32	E0	28	LYS
32	E0	29	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	47	VAL
32	E0	50	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	98	VAL
33	E1	103	LEU
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	126	CYS
33	E1	130	VAL

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Mol	Chain	Res	Type
33	E1	137	ASP
33	E1	138	ARG
33	E1	139	LEU
33	E1	151	ASN
34	SR	6	VAL
34	SR	29	GLN
34	SR	52	GLN
34	SR	59	ARG
34	SR	65	SER
34	SR	66	HIS
34	SR	76	ASP
34	SR	81	LEU
34	SR	98	GLU
34	SR	116	ASP
34	SR	117	LYS
34	SR	134	TRP
34	SR	136	ILE
34	SR	137	LYS
34	SR	145	LEU
34	SR	153	GLN
34	SR	165	ASP
34	SR	188	ILE
34	SR	191	ASP
34	SR	202	LEU
34	SR	238	ASP
34	SR	248	ASN
34	SR	268	GLN
34	SR	300	THR
34	SR	317	THR
35	SM	27	LYS
35	SM	46	LYS
35	SM	51	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	78	ASP
35	SM	82	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	94	HIS
35	SM	96	ARG

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Mol	Chain	Res	Type
35	SM	100	THR
35	SM	105	LYS
35	SM	139	GLU
39	L2	14	SER
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	72	ARG
39	L2	74	GLU
39	L2	84	THR
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	107	VAL
39	L2	109	GLU
39	L2	113	VAL
39	L2	116	VAL
39	L2	143	GLU
39	L2	157	VAL
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	191	LEU
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	224	THR
39	L2	227	ARG
39	L2	230	VAL
39	L2	241	ARG
40	L3	2	SER
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	55	THR
40	L3	56	ILE
40	L3	67	PHE
40	L3	70	ARG

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Mol	Chain	Res	Type
40	L3	85	VAL
40	L3	103	THR
40	L3	104	THR
40	L3	114	VAL
40	L3	126	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	173	GLN
40	L3	183	LEU
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	200	GLU
40	L3	202	THR
40	L3	212	ASN
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	260	VAL
40	L3	284	ARG
40	L3	296	THR
40	L3	300	ARG
40	L3	305	ILE
40	L3	317	ILE
40	L3	319	ASN
40	L3	320	ASP
40	L3	324	VAL
40	L3	325	LYS
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	347	SER
40	L3	354	VAL
40	L3	355	SER
40	L3	375	GLU

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Mol	Chain	Res	Type
40	L3	380	MET
40	L3	387	LEU
41	L4	21	PRO
41	L4	22	LEU
41	L4	64	SER
41	L4	69	ARG
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	108	LYS
41	L4	120	TYR
41	L4	133	SER
41	L4	138	ARG
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	153	SER
41	L4	156	LEU
41	L4	161	LYS
41	L4	172	VAL
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	216	VAL
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	259	ASP
41	L4	261	VAL
41	L4	267	VAL
41	L4	278	SER
41	L4	289	ILE
41	L4	306	THR

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Mol	Chain	Res	Type
41	L4	307	GLN
41	L4	313	LEU
41	L4	350	LYS
41	L4	354	VAL
42	L5	5	LYS
42	L5	10	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	69	ILE
42	L5	89	THR
42	L5	92	LEU
42	L5	93	THR
42	L5	105	ILE
42	L5	115	LEU
42	L5	131	LEU
42	L5	132	THR
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	188	GLU
42	L5	189	GLU
42	L5	197	SER
42	L5	222	LEU
42	L5	231	ILE
42	L5	232	ASP
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	264	GLN
42	L5	273	ARG
42	L5	293	LEU

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Mol	Chain	Res	Type
43	L6	2	SER
43	L6	5	LYS
43	L6	15	VAL
43	L6	21	THR
43	L6	28	GLN
43	L6	35	VAL
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	78	ARG
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	93	VAL
43	L6	99	GLU
43	L6	129	GLU
43	L6	134	ARG
44	L7	24	GLU
44	L7	25	GLN
44	L7	82	LYS
44	L7	83	LEU
44	L7	84	VAL
44	L7	87	VAL
44	L7	93	ASN
44	L7	100	ARG
44	L7	108	LEU
44	L7	121	LYS
44	L7	158	LYS
44	L7	175	LYS
44	L7	179	LEU
44	L7	184	LEU
44	L7	189	ILE
44	L7	234	GLU
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	38	GLN
45	L8	41	GLN
45	L8	50	VAL
45	L8	63	LYS

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Mol	Chain	Res	Type
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	82	LEU
45	L8	84	ARG
45	L8	90	THR
45	L8	92	LYS
45	L8	101	THR
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	145	ASN
45	L8	150	LEU
45	L8	156	ASP
45	L8	163	VAL
45	L8	169	LEU
45	L8	180	VAL
45	L8	185	ARG
45	L8	203	VAL
45	L8	204	ARG
45	L8	206	GLU
45	L8	218	ILE
45	L8	238	LEU
45	L8	240	ASN
45	L8	246	MET
45	L8	248	LYS
45	L8	251	LYS
46	L9	1	MET
46	L9	5	GLN
46	L9	9	GLN
46	L9	16	VAL
46	L9	18	VAL
46	L9	20	ILE
46	L9	24	ILE
46	L9	33	THR
46	L9	41	ILE
46	L9	48	VAL
46	L9	49	ASN
46	L9	52	LEU
46	L9	65	VAL
46	L9	68	LEU
46	L9	69	ARG

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Mol	Chain	Res	Type
46	L9	70	THR
46	L9	90	MET
46	L9	92	TYR
46	L9	132	VAL
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	140	VAL
46	L9	147	SER
46	L9	149	ASN
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	172	ILE
46	L9	177	ASP
46	L9	189	GLU
46	L9	190	ASP
47	M0	3	ARG
47	M0	7	ARG
47	M0	21	ARG
47	M0	24	ARG
47	M0	30	LYS
47	M0	32	ARG
47	M0	33	ILE
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	54	SER
47	M0	63	GLU
47	M0	74	LYS
47	M0	87	LEU
47	M0	116	ARG
47	M0	125	LEU
47	M0	130	ASP
47	M0	133	GLN
47	M0	139	ARG
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS

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Mol	Chain	Res	Type
47	M0	177	ASP
47	M0	184	LYS
47	M0	192	ASP
47	M0	197	VAL
47	M0	203	LYS
47	M0	207	GLU
48	M1	6	GLN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	19	LEU
48	M1	23	VAL
48	M1	31	THR
48	M1	44	THR
48	M1	46	VAL
48	M1	65	ILE
48	M1	70	THR
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	115	LYS
48	M1	120	ILE
48	M1	137	ARG
48	M1	140	ARG
48	M1	148	VAL
48	M1	166	LYS
48	M1	168	ASP
49	M3	5	LYS
49	M3	23	LYS
49	M3	24	VAL
49	M3	33	VAL
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG

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Mol	Chain	Res	Type
49	M3	69	VAL
49	M3	85	LEU
49	M3	114	GLN
49	M3	115	ARG
49	M3	117	LYS
49	M3	121	SER
49	M3	122	LYS
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	134	GLU
49	M3	136	GLU
49	M3	139	LEU
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG
49	M3	190	LYS
50	M4	8	LYS
50	M4	10	SER
50	M4	11	ASN
50	M4	20	VAL
50	M4	21	VAL
50	M4	27	GLN
50	M4	50	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	74	ARG
50	M4	82	SER
50	M4	91	CYS
50	M4	93	LYS
50	M4	102	LYS
50	M4	105	GLN
50	M4	108	ARG
50	M4	113	THR
50	M4	135	LEU
51	M5	10	LEU
51	M5	15	GLN
51	M5	18	VAL
51	M5	20	ARG
51	M5	22	LEU
51	M5	27	VAL

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Mol	Chain	Res	Type
51	M5	38	ARG
51	M5	49	ARG
51	M5	50	ARG
51	M5	62	TYR
51	M5	68	ARG
51	M5	75	VAL
51	M5	76	PRO
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	92	LEU
51	M5	93	LYS
51	M5	96	ARG
51	M5	104	GLU
51	M5	106	VAL
51	M5	109	ARG
51	M5	117	ASN
51	M5	133	ILE
51	M5	138	GLN
51	M5	144	ARG
51	M5	151	ILE
51	M5	155	VAL
51	M5	159	ARG
51	M5	182	ASN
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
51	M5	198	SER
51	M5	201	ARG
51	M5	204	LYS
52	M6	22	VAL
52	M6	34	VAL
52	M6	41	LEU
52	M6	68	ARG
52	M6	78	ARG
52	M6	85	ARG
52	M6	89	SER
52	M6	106	GLU
52	M6	116	LYS
52	M6	117	ARG
52	M6	119	VAL
52	M6	124	LEU

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Mol	Chain	Res	Type
52	M6	143	THR
52	M6	160	ARG
52	M6	184	THR
52	M6	190	VAL
53	M7	7	THR
53	M7	8	SER
53	M7	9	THR
53	M7	24	VAL
53	M7	32	THR
53	M7	36	ILE
53	M7	52	LEU
53	M7	56	ARG
53	M7	69	ARG
53	M7	70	THR
53	M7	111	LYS
53	M7	112	LEU
53	M7	115	SER
53	M7	118	GLN
53	M7	121	GLN
53	M7	126	ARG
53	M7	127	ARG
53	M7	144	SER
53	M7	149	VAL
53	M7	155	GLU
53	M7	157	VAL
53	M7	165	VAL
53	M7	168	LEU
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	7	SER
54	M8	17	THR
54	M8	22	ASP
54	M8	26	LEU
54	M8	32	LEU
54	M8	41	ASP
54	M8	49	LEU
54	M8	69	ARG
54	M8	74	GLU
54	M8	81	VAL
54	M8	98	LYS
54	M8	100	THR

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Mol	Chain	Res	Type
54	M8	127	LEU
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	168	THR
54	M8	171	LYS
54	M8	174	ARG
54	M8	180	ARG
55	M9	10	LEU
55	M9	17	VAL
55	M9	20	ARG
55	M9	24	LEU
55	M9	25	ASP
55	M9	30	SER
55	M9	31	GLU
55	M9	43	LYS
55	M9	44	LEU
55	M9	55	VAL
55	M9	61	SER
55	M9	71	ARG
55	M9	74	ARG
55	M9	81	ARG
55	M9	86	GLU
55	M9	91	SER
55	M9	98	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	116	ASP
55	M9	134	HIS
55	M9	138	LEU
55	M9	175	GLN
55	M9	182	ASP
56	N0	8	GLN
56	N0	12	ARG
56	N0	13	ARG
56	N0	40	ARG
56	N0	45	LEU
56	N0	51	VAL
56	N0	57	GLU
56	N0	61	ILE

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Mol	Chain	Res	Type
56	N0	63	GLN
56	N0	71	LYS
56	N0	79	VAL
56	N0	87	THR
56	N0	103	VAL
56	N0	105	THR
56	N0	106	LEU
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	123	ILE
56	N0	130	GLU
56	N0	137	ARG
56	N0	138	GLN
56	N0	144	LEU
56	N0	160	THR
56	N0	162	THR
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR
57	N1	4	SER
57	N1	9	SER
57	N1	12	ARG
57	N1	14	MET
57	N1	18	ASP
57	N1	27	LEU
57	N1	64	VAL
57	N1	68	THR
57	N1	71	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	88	ARG
57	N1	89	LEU
57	N1	97	LYS
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	122	GLN
57	N1	124	VAL

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Mol	Chain	Res	Type
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	143	THR
57	N1	149	GLN
57	N1	154	VAL
57	N1	159	PHE
58	N2	10	LYS
58	N2	29	ASP
58	N2	38	ILE
58	N2	39	ASP
58	N2	49	ASN
58	N2	52	ASN
58	N2	61	THR
58	N2	66	VAL
58	N2	70	LYS
58	N2	74	LYS
58	N2	100	THR
58	N2	104	ARG
59	N3	32	ARG
59	N3	54	LEU
59	N3	57	MET
59	N3	63	LYS
59	N3	64	LYS
59	N3	72	LYS
59	N3	74	MET
59	N3	83	LYS
59	N3	91	VAL
59	N3	102	ILE
59	N3	108	GLU
59	N3	109	MET
59	N3	115	THR
59	N3	120	LYS
59	N3	125	LEU
59	N3	135	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	19	THR
60	N4	26	SER
60	N4	34	SER
60	N4	39	LEU

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Mol	Chain	Res	Type
60	N4	54	LEU
61	N5	26	VAL
61	N5	27	ARG
61	N5	34	LEU
61	N5	38	LEU
61	N5	40	LEU
61	N5	45	LYS
61	N5	49	LYS
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	86	VAL
61	N5	104	GLU
61	N5	108	LEU
61	N5	112	THR
61	N5	115	ARG
61	N5	120	LYS
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	5	SER
62	N6	8	VAL
62	N6	10	SER
62	N6	13	ARG
62	N6	17	LYS
62	N6	26	GLN
62	N6	37	LYS
62	N6	39	LEU
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	56	VAL
62	N6	57	LEU
62	N6	71	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	94	SER
62	N6	105	VAL

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Mol	Chain	Res	Type
62	N6	111	LEU
62	N6	113	LYS
62	N6	115	ARG
62	N6	122	LYS
62	N6	125	LYS
62	N6	126	LEU
62	N6	127	GLU
63	N7	3	LYS
63	N7	14	VAL
63	N7	17	ARG
63	N7	24	VAL
63	N7	34	LYS
63	N7	46	ILE
63	N7	53	VAL
63	N7	54	THR
63	N7	64	LYS
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	90	GLU
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	107	ARG
63	N7	109	GLU
63	N7	121	ARG
63	N7	134	LEU
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	12	ARG
64	N8	14	HIS
64	N8	16	SER
64	N8	26	ARG
64	N8	42	ARG
64	N8	46	ASP
64	N8	56	VAL
64	N8	60	TYR
64	N8	72	VAL
64	N8	76	ASP
64	N8	84	GLU

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Mol	Chain	Res	Type
64	N8	91	LEU
64	N8	98	THR
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	139	ARG
65	N9	14	ARG
65	N9	18	ARG
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	16	LEU
66	O0	32	LYS
66	O0	34	LEU
66	O0	36	GLN
66	O0	54	SER
66	O0	61	MET
66	O0	66	LYS
66	O0	76	GLU
66	O0	79	THR
66	O0	83	LYS
66	O0	87	VAL
66	O0	100	ILE
66	O0	104	LEU
67	O1	6	ASP
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	46	THR
67	O1	55	LEU
67	O1	64	VAL
67	O1	73	LEU
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	89	LEU
67	O1	105	GLN

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Mol	Chain	Res	Type
67	O1	106	THR
68	O2	24	ARG
68	O2	31	ASN
68	O2	33	ARG
68	O2	61	LYS
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	84	THR
68	O2	103	LYS
68	O2	106	VAL
68	O2	128	LEU
69	O3	4	SER
69	O3	15	SER
69	O3	20	LYS
69	O3	59	VAL
69	O3	70	LYS
69	O3	74	THR
69	O3	78	SER
69	O3	81	VAL
69	O3	86	ARG
69	O3	98	VAL
69	O3	106	ASN
70	O4	3	GLN
70	O4	5	VAL
70	O4	20	ILE
70	O4	21	LYS
70	O4	24	LYS
70	O4	29	ILE
70	O4	46	ASP
70	O4	49	SER
70	O4	55	SER
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	79	SER
70	O4	86	LYS
70	O4	87	GLU
70	O4	104	VAL
71	O5	15	GLU
71	O5	20	GLN
71	O5	21	LEU

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Mol	Chain	Res	Type
71	O5	27	GLU
71	O5	31	LEU
71	O5	41	LEU
71	O5	44	ILE
71	O5	45	LYS
71	O5	48	ARG
71	O5	49	LYS
71	O5	71	LYS
71	O5	74	LYS
71	O5	89	ARG
71	O5	90	ARG
71	O5	96	GLU
71	O5	100	VAL
71	O5	101	THR
71	O5	104	GLN
71	O5	107	LYS
71	O5	119	LYS
72	O6	5	THR
72	O6	11	LEU
72	O6	17	VAL
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	36	ARG
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	68	ARG
72	O6	70	ARG
72	O6	72	VAL
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	99	ARG
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	55	ARG

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Mol	Chain	Res	Type
73	O7	59	THR
73	O7	67	LEU
73	O7	80	THR
73	O7	87	SER
74	O8	3	ARG
74	O8	5	ILE
74	O8	6	THR
74	O8	8	ILE
74	O8	12	LEU
74	O8	24	THR
74	O8	41	THR
74	O8	46	ARG
74	O8	50	SER
74	O8	52	TYR
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	29	LEU
75	O9	32	ASN
75	O9	45	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	106	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	127	LEU
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	21	ARG
77	Q1	24	SER
77	Q1	25	LYS
78	Q2	8	ARG

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Mol	Chain	Res	Type
78	Q2	9	LYS
78	Q2	26	THR
78	Q2	29	LYS
78	Q2	34	SER
78	Q2	35	LEU
78	Q2	48	SER
78	Q2	55	LYS
78	Q2	76	LYS
78	Q2	78	LYS
78	Q2	79	THR
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	32	GLN
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	56	THR
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	91	GLU
2	s0	6	THR
2	s0	12	GLU
2	s0	22	THR
2	s0	30	GLN
2	s0	45	VAL
2	s0	57	LEU
2	s0	59	LEU
2	s0	62	ARG
2	s0	87	LEU
2	s0	88	LYS
2	s0	110	TYR
2	s0	111	ILE
2	s0	119	ARG

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Mol	Chain	Res	Type
2	s0	131	GLN
2	s0	135	GLU
2	s0	139	VAL
2	s0	144	ILE
2	s0	154	GLU
2	s0	157	ASP
2	s0	167	LYS
2	s0	172	LEU
2	s0	180	GLU
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	196	SER
2	s0	198	MET
2	s0	200	ASP
2	s0	202	TYR
3	s1	21	VAL
3	s1	22	ASP
3	s1	25	THR
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	62	LYS
3	s1	66	VAL
3	s1	70	LEU
3	s1	73	LEU
3	s1	74	GLN
3	s1	78	ASP
3	s1	81	PHE
3	s1	83	LYS
3	s1	110	LEU
3	s1	115	ARG
3	s1	125	VAL
3	s1	137	ILE
3	s1	150	VAL
3	s1	151	LYS
3	s1	177	GLN
3	s1	179	SER
3	s1	180	THR
3	s1	181	LEU
3	s1	202	LYS
3	s1	212	VAL

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Mol	Chain	Res	Type
3	s1	215	VAL
3	s1	219	LYS
3	s1	223	PHE
3	s1	234	GLU
4	s2	41	LEU
4	s2	53	ILE
4	s2	54	GLU
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	73	LEU
4	s2	76	LEU
4	s2	80	VAL
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	94	GLN
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	117	THR
4	s2	139	ILE
4	s2	141	ARG
4	s2	148	LEU
4	s2	150	GLN
4	s2	152	HIS
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	185	LYS
4	s2	194	GLU
4	s2	206	THR
4	s2	221	THR
4	s2	222	TYR
4	s2	225	LEU
4	s2	226	THR
4	s2	229	LEU
4	s2	233	GLN
4	s2	240	LEU
4	s2	248	SER

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Mol	Chain	Res	Type
4	s2	250	GLN
5	s3	4	LEU
5	s3	9	ARG
5	s3	10	LYS
5	s3	26	THR
5	s3	41	VAL
5	s3	44	THR
5	s3	53	THR
5	s3	55	THR
5	s3	59	LEU
5	s3	67	ASN
5	s3	69	LEU
5	s3	76	ARG
5	s3	84	ILE
5	s3	90	ARG
5	s3	91	VAL
5	s3	93	ASP
5	s3	115	ILE
5	s3	116	ARG
5	s3	127	MET
5	s3	128	GLU
5	s3	142	LEU
5	s3	158	ILE
5	s3	162	GLN
5	s3	202	LEU
5	s3	204	ASP
6	s4	11	ARG
6	s4	23	LEU
6	s4	24	SER
6	s4	26	CYS
6	s4	37	LYS
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	56	LEU
6	s4	67	GLN
6	s4	78	THR
6	s4	104	ASP
6	s4	116	ASP
6	s4	126	VAL
6	s4	131	LEU

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Mol	Chain	Res	Type
6	s4	147	ILE
6	s4	148	ARG
6	s4	163	ASP
6	s4	181	VAL
6	s4	182	TYR
6	s4	214	LEU
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	245	LYS
6	s4	246	LEU
7	s5	24	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	41	LYS
7	s5	51	VAL
7	s5	59	VAL
7	s5	63	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	83	ARG
7	s5	89	ILE
7	s5	93	LEU
7	s5	109	LYS
7	s5	112	ARG
7	s5	119	ASP
7	s5	125	THR
7	s5	148	ARG
7	s5	149	VAL
7	s5	156	ARG
7	s5	157	ARG
7	s5	166	ARG
7	s5	167	ARG
7	s5	170	GLN
7	s5	187	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	208	SER
7	s5	213	LYS
7	s5	216	GLU

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Mol	Chain	Res	Type
7	s5	219	ARG
8	s6	12	SER
8	s6	15	THR
8	s6	25	ARG
8	s6	30	LYS
8	s6	31	ARG
8	s6	69	LEU
8	s6	71	THR
8	s6	76	LEU
8	s6	78	THR
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	112	VAL
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	137	ARG
8	s6	143	LYS
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	169	TYR
8	s6	170	THR
8	s6	171	LYS
8	s6	177	ARG
8	s6	182	GLN
8	s6	212	LEU
8	s6	215	ARG
9	s7	11	GLN
9	s7	28	GLU
9	s7	33	GLU
9	s7	41	LEU
9	s7	49	ILE
9	s7	67	LEU
9	s7	77	LEU
9	s7	81	LEU

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Mol	Chain	Res	Type
9	s7	86	GLN
9	s7	87	ASP
9	s7	97	ARG
9	s7	103	SER
9	s7	105	THR
9	s7	108	GLN
9	s7	109	VAL
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	126	LEU
9	s7	141	ARG
9	s7	143	LEU
9	s7	144	VAL
9	s7	159	VAL
9	s7	160	GLN
9	s7	166	LEU
9	s7	185	ILE
9	s7	187	SER
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	58	LEU
10	s8	61	GLU
10	s8	74	LYS
10	s8	76	THR
10	s8	82	VAL
10	s8	111	GLN
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	168	CYS
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	21	SER
11	s9	28	LEU

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Mol	Chain	Res	Type
11	s9	78	ARG
11	s9	82	ARG
11	s9	90	LYS
11	s9	93	LEU
11	s9	101	VAL
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	120	LYS
11	s9	126	ARG
11	s9	130	THR
11	s9	134	ILE
11	s9	142	ASN
11	s9	150	LEU
11	s9	161	THR
11	s9	171	ARG
11	s9	180	LYS
80	c0	5	LYS
80	c0	15	LEU
80	c0	20	VAL
80	c0	21	VAL
80	c0	27	PHE
80	c0	33	GLU
80	c0	36	ASP
80	c0	40	LEU
80	c0	52	LYS
80	c0	55	VAL
80	c0	57	THR
80	c0	71	GLU
80	c0	77	ARG
13	c1	3	THR
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	27	THR
13	c1	30	ARG
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	56	LYS

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Mol	Chain	Res	Type
13	c1	60	PHE
13	c1	61	THR
13	c1	67	ARG
13	c1	74	THR
13	c1	77	SER
13	c1	78	THR
13	c1	80	MET
13	c1	83	THR
13	c1	86	ILE
13	c1	94	ILE
13	c1	99	ARG
13	c1	118	GLN
13	c1	125	VAL
13	c1	129	ARG
13	c1	140	VAL
81	c2	28	LEU
81	c2	36	LEU
81	c2	39	ASP
81	c2	43	ARG
81	c2	58	LEU
81	c2	61	VAL
81	c2	62	LEU
81	c2	66	VAL
81	c2	71	ILE
81	c2	74	LEU
81	c2	85	LYS
81	c2	89	ILE
81	c2	91	VAL
81	c2	103	LEU
81	c2	116	VAL
81	c2	121	VAL
81	c2	129	GLU
81	c2	132	GLU
81	c2	136	ILE
81	c2	140	PHE
15	c3	12	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	28	LEU
15	c3	35	GLU
15	c3	37	ILE

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Mol	Chain	Res	Type
15	c3	39	LYS
15	c3	60	VAL
15	c3	64	ARG
15	c3	66	ILE
15	c3	73	ARG
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	97	SER
15	c3	102	LEU
15	c3	115	LEU
15	c3	125	LEU
15	c3	138	ASN
15	c3	150	VAL
16	c4	20	TYR
16	c4	28	VAL
16	c4	31	THR
16	c4	33	LEU
16	c4	42	VAL
16	c4	43	THR
16	c4	51	ASP
16	c4	61	MET
16	c4	62	LEU
16	c4	66	ASP
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	103	ARG
16	c4	114	ARG
16	c4	118	VAL
16	c4	119	THR
16	c4	123	SER
16	c4	124	ASP
16	c4	125	SER
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
82	c5	12	PHE
82	c5	21	ASP
82	c5	24	LYS
82	c5	27	GLU
82	c5	36	LEU

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Mol	Chain	Res	Type
82	c5	40	ARG
82	c5	44	ARG
82	c5	52	LYS
82	c5	69	GLU
82	c5	71	GLU
82	c5	97	TYR
82	c5	107	ILE
82	c5	110	GLU
82	c5	120	SER
82	c5	121	ILE
82	c5	122	THR
82	c5	124	THR
82	c5	127	ARG
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	90	VAL
18	c6	97	VAL
18	c6	98	ASP
18	c6	110	THR
18	c6	114	ARG
18	c6	128	LYS
18	c6	137	ARG
19	c7	8	THR
19	c7	19	ARG
19	c7	29	GLN
19	c7	34	LEU
19	c7	38	ILE
19	c7	43	SER
19	c7	45	ARG
19	c7	46	LEU
19	c7	60	ARG
19	c7	69	ILE
19	c7	85	VAL
19	c7	88	VAL

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Mol	Chain	Res	Type
19	c7	89	SER
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN
20	c8	27	LYS
20	c8	28	ILE
20	c8	36	LYS
20	c8	40	ARG
20	c8	55	HIS
20	c8	63	GLN
20	c8	80	LYS
20	c8	85	PHE
20	c8	94	ASP
20	c8	104	ASN
20	c8	116	LEU
20	c8	134	ARG
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	27	LYS
21	c9	28	LEU
21	c9	34	VAL
21	c9	37	VAL
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	111	ILE
21	c9	116	ILE
21	c9	122	ARG
21	c9	123	ARG
21	c9	126	GLU
21	c9	140	LEU
21	c9	141	GLU

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Mol	Chain	Res	Type
21	c9	144	GLU
22	d0	23	ARG
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	47	GLN
22	d0	52	LYS
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU
22	d0	66	SER
22	d0	70	THR
22	d0	74	GLU
22	d0	80	GLU
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	32	VAL
23	d1	38	LYS
23	d1	50	TYR
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	78	LEU
23	d1	81	ASN
24	d2	4	SER
24	d2	7	LEU
24	d2	9	ASP
24	d2	23	ARG

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Mol	Chain	Res	Type
24	d2	37	PHE
24	d2	65	LEU
24	d2	74	VAL
24	d2	88	LYS
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	124	LYS
24	d2	126	LEU
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	23	ARG
25	d3	33	LEU
25	d3	40	SER
25	d3	56	LYS
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	96	VAL
25	d3	100	ASP
25	d3	107	PHE
25	d3	127	VAL
26	d4	10	ARG
26	d4	26	ASP
26	d4	34	ASN
26	d4	35	VAL
26	d4	42	GLU
26	d4	43	LYS
26	d4	44	LEU
26	d4	47	VAL
26	d4	49	LYS
26	d4	51	GLU
26	d4	62	THR
26	d4	88	THR
26	d4	105	ARG
26	d4	118	ILE
26	d4	128	LYS
26	d4	135	ASP
27	d5	43	ASP
27	d5	46	LYS

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Mol	Chain	Res	Type
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	81	ARG
27	d5	86	GLU
27	d5	105	THR
28	d6	10	ARG
28	d6	24	VAL
28	d6	28	LYS
28	d6	33	ASP
28	d6	44	ILE
28	d6	53	LEU
28	d6	58	VAL
28	d6	67	THR
28	d6	82	ARG
28	d6	84	VAL
28	d6	85	ARG
28	d6	90	GLU
29	d7	11	THR
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	61	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	7	VAL
30	d8	15	VAL
30	d8	19	THR
30	d8	22	ARG
30	d8	28	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	42	ARG
30	d8	49	ARG
30	d8	54	LEU
30	d8	64	ARG
31	d9	10	HIS
31	d9	16	LYS
31	d9	21	CYS

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Mol	Chain	Res	Type
31	d9	28	THR
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	54	LYS
32	e0	13	LYS
32	e0	22	GLU
32	e0	23	LYS
32	e0	26	LYS
32	e0	28	LYS
32	e0	29	LYS
32	e0	39	LEU
32	e0	44	PHE
32	e0	45	VAL
32	e0	47	VAL
32	e0	50	VAL
32	e0	54	ARG
32	e0	55	ARG
32	e0	56	MET
33	e1	80	ARG
33	e1	86	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	97	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	113	LYS
33	e1	115	THR
33	e1	120	GLU
33	e1	135	HIS
33	e1	140	TYR
33	e1	141	CYS
33	e1	146	SER
33	e1	147	VAL
33	e1	151	ASN
83	sR	22	SER
83	sR	29	GLN
83	sR	52	GLN
83	sR	58	VAL

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Mol	Chain	Res	Type
83	sR	59	ARG
83	sR	64	HIS
83	sR	65	SER
83	sR	76	ASP
83	sR	96	THR
83	sR	145	LEU
83	sR	168	THR
83	sR	176	LYS
83	sR	188	ILE
83	sR	228	LYS
83	sR	232	TYR
83	sR	274	LEU
83	sR	278	PHE
83	sR	297	ASP
83	sR	309	VAL
84	sM	24	GLU
84	sM	30	THR
84	sM	33	LYS
84	sM	41	SER
84	sM	43	ASP
84	sM	48	ARG
84	sM	50	ASN
84	sM	61	ILE
84	sM	68	ARG
84	sM	74	LYS
84	sM	75	ASP
84	sM	77	THR
84	sM	82	THR
39	l2	19	HIS
39	l2	23	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	71	LEU
39	l2	74	GLU
39	l2	84	THR
39	l2	96	LEU
39	l2	101	VAL
39	l2	104	LEU
39	l2	107	VAL
39	l2	109	GLU

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Mol	Chain	Res	Type
39	l2	113	VAL
39	l2	114	SER
39	l2	119	LYS
39	l2	128	ARG
39	l2	137	ILE
39	l2	147	ARG
39	l2	155	LYS
39	l2	158	ILE
39	l2	159	SER
39	l2	165	VAL
39	l2	180	LEU
39	l2	193	ARG
39	l2	202	VAL
39	l2	204	MET
39	l2	223	SER
39	l2	226	SER
39	l2	246	LEU
39	l2	249	SER
40	l3	3	HIS
40	l3	7	GLU
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	21	ARG
40	l3	24	SER
40	l3	25	ILE
40	l3	30	LYS
40	l3	37	ARG
40	l3	41	VAL
40	l3	47	LEU
40	l3	50	LYS
40	l3	56	ILE
40	l3	73	VAL
40	l3	84	VAL
40	l3	85	VAL
40	l3	95	THR
40	l3	103	THR
40	l3	114	VAL
40	l3	116	ARG
40	l3	125	SER
40	l3	139	GLN
40	l3	146	ARG

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Mol	Chain	Res	Type
40	l3	148	LEU
40	l3	150	ARG
40	l3	169	THR
40	l3	183	LEU
40	l3	187	SER
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	202	THR
40	l3	205	VAL
40	l3	211	GLN
40	l3	212	ASN
40	l3	213	GLU
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	246	LEU
40	l3	252	ILE
40	l3	260	VAL
40	l3	270	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	304	THR
40	l3	308	MET
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	346	THR
40	l3	347	SER
40	l3	380	MET
40	l3	382	THR
41	l4	2	SER
41	l4	25	VAL
41	l4	41	SER
41	l4	47	ARG
41	l4	69	ARG
41	l4	73	ARG
41	l4	85	SER
41	l4	93	MET
41	l4	120	TYR

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Mol	Chain	Res	Type
41	l4	122	THR
41	l4	138	ARG
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU
41	l4	154	THR
41	l4	156	LEU
41	l4	160	GLN
41	l4	170	LYS
41	l4	172	VAL
41	l4	176	SER
41	l4	177	ASP
41	l4	179	LEU
41	l4	182	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	191	LYS
41	l4	203	ARG
41	l4	206	LEU
41	l4	220	ARG
41	l4	222	VAL
41	l4	230	VAL
41	l4	246	ARG
41	l4	258	LEU
41	l4	266	THR
41	l4	267	VAL
41	l4	276	LEU
41	l4	287	THR
41	l4	300	ARG
41	l4	301	PRO
41	l4	306	THR
41	l4	307	GLN
41	l4	313	LEU
41	l4	316	ASN
41	l4	319	LYS
41	l4	323	VAL
41	l4	327	LEU
41	l4	342	LYS
41	l4	345	GLU
41	l4	347	THR
41	l4	356	THR
41	l4	359	LEU

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Mol	Chain	Res	Type
42	l5	4	GLN
42	l5	5	LYS
42	l5	13	SER
42	l5	34	LYS
42	l5	35	ARG
42	l5	51	LEU
42	l5	62	CYS
42	l5	65	ILE
42	l5	70	THR
42	l5	73	VAL
42	l5	74	VAL
42	l5	93	THR
42	l5	110	LEU
42	l5	112	LYS
42	l5	113	LEU
42	l5	115	LEU
42	l5	118	THR
42	l5	130	GLU
42	l5	133	GLU
42	l5	140	ARG
42	l5	144	VAL
42	l5	146	LEU
42	l5	148	ILE
42	l5	151	GLN
42	l5	152	ARG
42	l5	155	THR
42	l5	185	PHE
42	l5	186	GLU
42	l5	194	LEU
42	l5	211	LEU
42	l5	218	ARG
42	l5	220	SER
42	l5	227	LEU
42	l5	254	LYS
42	l5	258	LYS
42	l5	259	LYS
42	l5	268	GLU
42	l5	273	ARG
42	l5	282	ARG
42	l5	293	LEU
43	l6	8	LYS
43	l6	20	LYS

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Mol	Chain	Res	Type
43	l6	21	THR
43	l6	46	ARG
43	l6	50	LYS
43	l6	64	LEU
43	l6	65	ILE
43	l6	66	SER
43	l6	79	VAL
43	l6	89	THR
43	l6	93	VAL
43	l6	98	VAL
43	l6	109	GLU
43	l6	131	LYS
43	l6	143	LYS
43	l6	152	THR
43	l6	155	LEU
43	l6	162	SER
44	l7	22	THR
44	l7	26	VAL
44	l7	41	ARG
44	l7	53	LYS
44	l7	56	GLU
44	l7	60	ARG
44	l7	77	VAL
44	l7	80	GLN
44	l7	83	LEU
44	l7	84	VAL
44	l7	87	VAL
44	l7	88	ARG
44	l7	98	LYS
44	l7	110	ARG
44	l7	115	THR
44	l7	121	LYS
44	l7	156	ILE
44	l7	158	LYS
44	l7	173	LEU
44	l7	175	LYS
44	l7	179	LEU
44	l7	184	LEU
44	l7	196	LYS
44	l7	229	PHE
44	l7	239	LEU
85	l8	26	LEU

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Mol	Chain	Res	Type
85	l8	68	ARG
85	l8	74	THR
85	l8	79	GLN
85	l8	81	THR
85	l8	95	ASN
85	l8	136	LEU
85	l8	146	LYS
85	l8	149	LYS
85	l8	160	ILE
85	l8	163	VAL
85	l8	169	LEU
85	l8	172	LYS
85	l8	183	LYS
85	l8	208	GLU
85	l8	211	LEU
85	l8	214	LEU
85	l8	216	SER
85	l8	217	THR
85	l8	230	LYS
85	l8	238	LEU
85	l8	245	LYS
85	l8	248	LYS
46	l9	4	ILE
46	l9	6	THR
46	l9	18	VAL
46	l9	22	SER
46	l9	33	THR
46	l9	44	THR
46	l9	48	VAL
46	l9	55	VAL
46	l9	68	LEU
46	l9	69	ARG
46	l9	70	THR
46	l9	80	THR
46	l9	82	VAL
46	l9	90	MET
46	l9	92	TYR
46	l9	105	GLU
46	l9	120	ASP
46	l9	129	ARG
46	l9	130	ASP
46	l9	132	VAL

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Mol	Chain	Res	Type
46	l9	133	THR
46	l9	137	SER
46	l9	138	THR
46	l9	140	VAL
46	l9	144	ILE
46	l9	151	VAL
46	l9	152	GLU
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	166	ARG
46	l9	167	VAL
46	l9	170	LYS
46	l9	173	ARG
46	l9	179	ILE
46	l9	184	LYS
46	l9	191	LEU
47	m0	3	ARG
47	m0	21	ARG
47	m0	24	ARG
47	m0	26	VAL
47	m0	36	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	74	LYS
47	m0	76	MET
47	m0	83	ASP
47	m0	87	LEU
47	m0	99	ILE
47	m0	101	LYS
47	m0	139	ARG
47	m0	143	SER
47	m0	144	ASN
47	m0	154	ARG
47	m0	162	GLN
47	m0	163	GLN
47	m0	169	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	178	ARG
47	m0	197	VAL
47	m0	200	LEU

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Mol	Chain	Res	Type
47	m0	208	ASN
47	m0	211	ARG
47	m0	212	GLU
47	m0	215	GLU
47	m0	217	PHE
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	31	THR
48	m1	34	SER
48	m1	35	LYS
48	m1	40	LEU
48	m1	44	THR
48	m1	54	VAL
48	m1	55	ARG
48	m1	80	LEU
48	m1	101	ASN
48	m1	106	ILE
48	m1	107	ASP
48	m1	108	GLU
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	150	ASN
48	m1	152	HIS
48	m1	159	THR
48	m1	160	VAL
48	m1	171	VAL
49	m3	13	HIS
49	m3	54	LEU
49	m3	58	VAL
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	85	LEU
49	m3	100	ARG
49	m3	104	ARG

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Mol	Chain	Res	Type
49	m3	107	GLU
49	m3	123	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	164	GLU
49	m3	168	ARG
49	m3	171	ARG
49	m3	176	GLU
49	m3	184	GLU
49	m3	189	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	6	ILE
50	m4	16	GLU
50	m4	27	GLN
50	m4	28	SER
50	m4	43	LYS
50	m4	64	VAL
50	m4	66	THR
50	m4	69	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	98	SER
50	m4	106	ARG
50	m4	124	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	10	LEU
51	m5	15	GLN
51	m5	18	VAL
51	m5	22	LEU
51	m5	24	ARG
51	m5	41	ARG
51	m5	49	ARG
51	m5	75	VAL
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	97	SER
51	m5	105	ARG

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Mol	Chain	Res	Type
51	m5	106	VAL
51	m5	117	ASN
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL
51	m5	170	LYS
51	m5	174	ILE
51	m5	178	HIS
51	m5	183	THR
51	m5	190	THR
52	m6	34	VAL
52	m6	41	LEU
52	m6	58	LEU
52	m6	67	THR
52	m6	78	ARG
52	m6	85	ARG
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	119	VAL
52	m6	124	LEU
52	m6	126	VAL
52	m6	130	LYS
52	m6	160	ARG
52	m6	171	LYS
52	m6	175	THR
52	m6	180	SER
52	m6	182	ASN
52	m6	184	THR
53	m7	7	THR
53	m7	8	SER
53	m7	9	THR
53	m7	13	LYS
53	m7	24	VAL
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	65	SER
53	m7	76	PHE
53	m7	79	THR
53	m7	80	LYS

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Mol	Chain	Res	Type
53	m7	94	LEU
53	m7	103	GLU
53	m7	107	LEU
53	m7	112	LEU
53	m7	124	LYS
53	m7	126	ARG
53	m7	144	SER
53	m7	148	LEU
53	m7	150	VAL
53	m7	155	GLU
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
54	m8	21	SER
54	m8	24	VAL
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	49	LEU
54	m8	57	ILE
54	m8	80	THR
54	m8	81	VAL
54	m8	100	THR
54	m8	113	LYS
54	m8	129	VAL
54	m8	135	GLN
54	m8	138	LEU
54	m8	147	ARG
54	m8	161	LYS
54	m8	165	ILE
54	m8	170	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	36	ASN
55	m9	37	SER
55	m9	43	LYS

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Mol	Chain	Res	Type
55	m9	49	THR
55	m9	55	VAL
55	m9	56	THR
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	88	ARG
55	m9	99	LEU
55	m9	105	LEU
55	m9	106	LEU
55	m9	126	GLU
55	m9	127	SER
55	m9	133	LYS
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	164	LEU
55	m9	171	ASP
55	m9	173	ARG
55	m9	186	LYS
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	40	ARG
56	n0	45	LEU
56	n0	50	LYS
56	n0	51	VAL
56	n0	73	LYS
56	n0	80	ARG
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	107	TYR
56	n0	115	ARG
56	n0	117	ARG
56	n0	130	GLU
56	n0	132	THR
56	n0	136	LYS
56	n0	137	ARG
56	n0	148	LEU
56	n0	149	LYS

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Mol	Chain	Res	Type
56	n0	155	ARG
56	n0	162	THR
56	n0	166	LYS
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	35	LYS
57	n1	36	VAL
57	n1	64	VAL
57	n1	68	THR
57	n1	71	SER
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	118	GLU
57	n1	126	VAL
57	n1	129	LYS
57	n1	130	ARG
57	n1	131	GLN
57	n1	135	PRO
57	n1	139	ARG
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	154	VAL
57	n1	160	ILE
58	n2	14	THR
58	n2	21	SER
58	n2	27	VAL
58	n2	37	LEU
58	n2	39	ASP
58	n2	43	VAL
58	n2	50	LEU
58	n2	52	ASN
58	n2	54	VAL

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Mol	Chain	Res	Type
58	n2	57	THR
58	n2	58	GLU
58	n2	63	VAL
58	n2	68	THR
58	n2	90	ARG
58	n2	98	THR
59	n3	7	GLN
59	n3	13	ILE
59	n3	14	SER
59	n3	35	TYR
59	n3	46	LEU
59	n3	64	LYS
59	n3	74	MET
59	n3	88	ARG
59	n3	91	VAL
59	n3	110	LYS
59	n3	115	THR
87	n4	1	MET
87	n4	7	SER
87	n4	19	THR
87	n4	39	LEU
87	n4	63	ILE
87	n4	89	LEU
87	n4	95	SER
87	n4	126	GLU
87	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	39	LYS
61	n5	40	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	63	ILE
61	n5	71	THR
61	n5	73	MET
61	n5	86	VAL
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG

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Mol	Chain	Res	Type
61	n5	133	LEU
61	n5	135	ILE
61	n5	142	ILE
62	n6	4	GLN
62	n6	8	VAL
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	52	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	66	GLN
62	n6	71	SER
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	87	LYS
62	n6	90	VAL
62	n6	94	SER
62	n6	97	ILE
62	n6	102	SER
62	n6	115	ARG
62	n6	120	GLN
63	n7	3	LYS
63	n7	17	ARG
63	n7	24	VAL
63	n7	29	HIS
63	n7	33	SER
63	n7	34	LYS
63	n7	52	LYS
63	n7	72	ILE
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR

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Mol	Chain	Res	Type
63	n7	95	VAL
63	n7	99	GLU
63	n7	100	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	121	ARG
63	n7	126	LYS
63	n7	127	ASN
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	26	ARG
64	n8	42	ARG
64	n8	60	TYR
64	n8	72	VAL
64	n8	82	ILE
64	n8	85	ASP
64	n8	91	LEU
64	n8	97	GLU
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
65	n9	19	ASN
65	n9	21	ILE
65	n9	26	THR
65	n9	33	LYS
65	n9	38	LYS
65	n9	42	ASN
65	n9	47	LEU
65	n9	50	THR
65	n9	52	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	6	SER
66	o0	8	GLU
66	o0	9	SER
66	o0	18	ILE
66	o0	32	LYS

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Mol	Chain	Res	Type
66	o0	41	LEU
66	o0	50	VAL
66	o0	61	MET
66	o0	76	GLU
66	o0	86	ARG
66	o0	87	VAL
66	o0	97	ASP
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	50	ARG
67	o1	55	LEU
67	o1	68	GLU
67	o1	76	SER
67	o1	96	VAL
67	o1	100	SER
67	o1	102	LYS
67	o1	106	THR
67	o1	110	GLU
68	o2	4	LEU
68	o2	16	LYS
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	41	VAL
68	o2	51	SER
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	89	THR
68	o2	106	VAL
68	o2	123	LYS
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS

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Mol	Chain	Res	Type
69	o3	28	SER
69	o3	31	LYS
69	o3	48	ARG
69	o3	59	VAL
69	o3	70	LYS
69	o3	74	THR
69	o3	81	VAL
69	o3	97	SER
69	o3	98	VAL
69	o3	105	SER
69	o3	106	ASN
70	o4	5	VAL
70	o4	20	ILE
70	o4	23	VAL
70	o4	24	LYS
70	o4	29	ILE
70	o4	58	ARG
70	o4	65	VAL
70	o4	68	THR
70	o4	80	ARG
70	o4	85	VAL
70	o4	86	LYS
70	o4	98	GLN
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	40	SER
71	o5	45	LYS
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	68	GLN
71	o5	69	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	90	ARG
71	o5	100	VAL
71	o5	101	THR

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Mol	Chain	Res	Type
71	o5	107	LYS
71	o5	119	LYS
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	12	ASN
72	o6	21	THR
72	o6	26	ILE
72	o6	34	SER
72	o6	35	ASN
72	o6	36	ARG
72	o6	38	LYS
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	62	ARG
72	o6	64	SER
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	81	THR
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS
73	o7	17	THR
73	o7	25	ARG
73	o7	33	THR
73	o7	44	THR
73	o7	46	SER
73	o7	55	ARG
73	o7	58	THR
73	o7	59	THR
73	o7	64	MET
73	o7	65	ARG
73	o7	67	LEU
73	o7	68	LYS
73	o7	74	PHE
73	o7	80	THR
73	o7	82	SER

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Mol	Chain	Res	Type
73	o7	84	SER
74	o8	5	ILE
74	o8	12	LEU
74	o8	17	ARG
74	o8	19	ASP
74	o8	22	THR
74	o8	24	THR
74	o8	41	THR
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	67	GLN
75	o9	5	LYS
75	o9	12	LYS
75	o9	15	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	45	ARG
76	q0	78	ILE
76	q0	83	LYS
76	q0	85	LEU
76	q0	106	ARG
76	q0	110	CYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	18	ARG
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	2	VAL
78	q2	7	THR
78	q2	8	ARG
78	q2	35	LEU
78	q2	38	GLN
78	q2	45	ARG
78	q2	47	GLN

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Mol	Chain	Res	Type
78	q2	61	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	3	LYS
79	q3	4	ARG
79	q3	21	SER
79	q3	24	ARG
79	q3	33	GLN
79	q3	42	CYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	57	CYS
79	q3	58	SER
79	q3	59	CYS
79	q3	62	LYS
79	q3	81	SER
88	p0	4	ILE
88	p0	5	ARG
88	p0	6	GLU
88	p0	10	GLU
88	p0	48	ARG
88	p0	50	VAL
88	p0	51	VAL
88	p0	55	LYS
88	p0	67	LEU
88	p0	70	LEU
88	p0	74	GLU
88	p0	76	LEU
88	p0	80	VAL
88	p0	81	LYS
88	p0	84	VAL
88	p0	91	GLU

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Mol	Chain	Res	Type
88	p0	93	LEU
88	p0	97	LYS
88	p0	104	ARG
88	p0	185	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	95	ASN
3	S1	149	GLN
6	S4	188	ASN
8	S6	59	GLN
9	S7	74	GLN
11	S9	110	GLN
19	C7	105	GLN
20	C8	136	GLN
27	D5	95	HIS
34	SR	159	ASN
43	L6	28	GLN
44	L7	244	ASN
47	M0	59	GLN
63	N7	127	ASN
74	O8	67	GLN
78	Q2	3	ASN
2	s0	140	ASN
3	s1	149	GLN
3	s1	209	ASN
11	s9	110	GLN
11	s9	142	ASN
80	c0	32	HIS
20	c8	12	GLN
22	d0	72	ASN
24	d2	56	HIS
26	d4	22	GLN
32	e0	17	GLN
41	l4	296	GLN
42	l5	81	HIS
42	l5	264	GLN
44	l7	112	ASN
51	m5	138	GLN
51	m5	178	HIS
55	m9	7	GLN

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Mol	Chain	Res	Type
61	n5	137	ASN
64	n8	25	HIS
64	n8	44	ASN
70	o4	3	GLN
72	o6	63	ASN
73	o7	13	ASN
74	o8	40	GLN
75	o9	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	458 (25%)	67 (3%)
1	6	1792/1800 (99%)	445 (24%)	51 (2%)
36	1	3146/3394 (92%)	647 (20%)	70 (2%)
36	5	3145/3394 (92%)	646 (20%)	82 (2%)
37	3	120/121 (99%)	17 (14%)	1 (0%)
37	7	120/121 (99%)	16 (13%)	0
38	4	157/158 (99%)	36 (22%)	2 (1%)
38	8	157/158 (99%)	38 (24%)	2 (1%)
90	A	1/3 (33%)	1 (100%)	0
90	a	1/3 (33%)	1 (100%)	0
All	All	10416/10952 (95%)	2305 (22%)	275 (2%)

All (2305) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G

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Mol	Chain	Res	Type
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	101	U
1	2	104	A
1	2	114	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	178	U
1	2	185	U
1	2	186	C
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A

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Mol	Chain	Res	Type
1	2	227	U
1	2	228	G
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	249	U
1	2	250	C
1	2	261	U
1	2	262	U
1	2	265	A
1	2	269	G
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	308	C
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	341	A
1	2	344	A
1	2	352	A

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Mol	Chain	Res	Type
1	2	359	A
1	2	360	A
1	2	361	C
1	2	387	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	421	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	448	C
1	2	468	A
1	2	470	A
1	2	475	A
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A

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Mol	Chain	Res	Type
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	516	G
1	2	520	A
1	2	527	A
1	2	532	U
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	585	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	611	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	630	A
1	2	639	U
1	2	640	U

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Mol	Chain	Res	Type
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G

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Mol	Chain	Res	Type
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U
1	2	795	U
1	2	803	A
1	2	806	A
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	840	U

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Mol	Chain	Res	Type
1	2	846	G
1	2	848	C
1	2	856	A
1	2	862	A
1	2	863	A
1	2	864	U
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	961	U
1	2	966	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1071	U

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Mol	Chain	Res	Type
1	2	1074	G
1	2	1079	U
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1138	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1152	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1243	G
1	2	1244	A
1	2	1245	G

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Mol	Chain	Res	Type
1	2	1250	U
1	2	1251	U
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1286	U
1	2	1292	G
1	2	1301	U
1	2	1314	U
1	2	1321	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1446	A
1	2	1448	G
1	2	1457	C
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1482	C

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Mol	Chain	Res	Type
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1624	C
1	2	1626	U
1	2	1631	A
1	2	1635	A
1	2	1657	U
1	2	1658	G
1	2	1680	G
1	2	1681	A
1	2	1683	C
1	2	1684	U
1	2	1693	A
1	2	1696	G

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Mol	Chain	Res	Type
1	2	1697	G
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1716	C
1	2	1731	A
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	14	U
36	1	16	A
36	1	24	G
36	1	26	A
36	1	40	A
36	1	49	A
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	73	C
36	1	83	U
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A

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Mol	Chain	Res	Type
36	1	109	A
36	1	110	G
36	1	113	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	166	C
36	1	169	U
36	1	170	G
36	1	173	G
36	1	182	U
36	1	183	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	200	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	226	C
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	315	C

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Mol	Chain	Res	Type
36	1	323	A
36	1	329	U
36	1	339	C
36	1	349	A
36	1	350	C
36	1	351	A
36	1	370	U
36	1	376	G
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	404	G
36	1	421	G
36	1	422	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
36	1	517	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	543	C
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	552	G
36	1	557	A
36	1	558	U
36	1	559	A
36	1	560	G
36	1	569	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	594	U
36	1	604	G
36	1	607	A
36	1	609	G

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Mol	Chain	Res	Type
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	637	C
36	1	638	C
36	1	649	A
36	1	660	A
36	1	677	A
36	1	681	U
36	1	684	G
36	1	691	A
36	1	705	A
36	1	709	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	722	G
36	1	725	G
36	1	727	G
36	1	758	C
36	1	764	U
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	792	G
36	1	806	A
36	1	817	A
36	1	830	A
36	1	842	G
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	885	U
36	1	890	C

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Mol	Chain	Res	Type
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	944	C
36	1	959	C
36	1	960	U
36	1	963	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1035	G
36	1	1037	C
36	1	1045	C
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
36	1	1071	U

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Mol	Chain	Res	Type
36	1	1072	G
36	1	1079	A
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1131	G
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1178	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1185	C
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1197	A
36	1	1201	C
36	1	1209	G
36	1	1212	A
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1221	A
36	1	1222	G
36	1	1225	A
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1236	G

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Mol	Chain	Res	Type
36	1	1237	G
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1272	C
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1330	A
36	1	1331	U
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1386	A

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Mol	Chain	Res	Type
36	1	1392	G
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1417	G
36	1	1419	A
36	1	1429	G
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1436	U
36	1	1437	C
36	1	1443	G
36	1	1446	A
36	1	1450	G
36	1	1460	A
36	1	1468	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1502	C
36	1	1508	C
36	1	1527	C
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1572	U
36	1	1576	G
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A

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Mol	Chain	Res	Type
36	1	1596	C
36	1	1605	A
36	1	1607	U
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1683	A
36	1	1702	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1736	G
36	1	1750	A
36	1	1751	G
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1775	G
36	1	1780	G
36	1	1781	C
36	1	1797	A
36	1	1805	C
36	1	1810	A
36	1	1812	G
36	1	1813	A
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A

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Mol	Chain	Res	Type
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1864	A
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1895	A
36	1	1901	A
36	1	1906	G
36	1	1935	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2175	U
36	1	2187	G
36	1	2198	A
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2222	A
36	1	2223	A
36	1	2225	U

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Mol	Chain	Res	Type
36	1	2228	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2262	A
36	1	2272	G
36	1	2273	G
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2334	U
36	1	2335	G
36	1	2336	U
36	1	2341	A
36	1	2361	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2395	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2435	G
36	1	2437	G

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Mol	Chain	Res	Type
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2507	C
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2525	G
36	1	2526	C
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2576	G
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G

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Mol	Chain	Res	Type
36	1	2614	G
36	1	2626	A
36	1	2629	U
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2674	A
36	1	2677	G
36	1	2685	C
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2714	G
36	1	2728	G
36	1	2737	C
36	1	2752	U
36	1	2753	G
36	1	2754	G
36	1	2755	C
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2779	A
36	1	2788	C
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2803	A
36	1	2810	C
36	1	2814	G
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2829	U
36	1	2834	G
36	1	2836	C
36	1	2842	U

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Mol	Chain	Res	Type
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2859	U
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2876	C
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2914	G
36	1	2923	U
36	1	2927	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2947	G
36	1	2955	U
36	1	2971	A
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3028	G
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3113	A
36	1	3119	U

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Mol	Chain	Res	Type
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3139	A
36	1	3142	A
36	1	3143	C
36	1	3150	A
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3269	U
36	1	3270	U

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Mol	Chain	Res	Type
36	1	3272	C
36	1	3276	G
36	1	3279	A
36	1	3280	U
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3289	G
36	1	3294	A
36	1	3295	A
36	1	3303	G
36	1	3304	U
36	1	3307	A
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3348	G
36	1	3349	C
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3368	U
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3396	U
37	3	7	G

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Mol	Chain	Res	Type
37	3	13	A
37	3	22	A
37	3	29	C
37	3	41	G
37	3	51	A
37	3	53	U
37	3	54	U
37	3	65	G
37	3	73	C
37	3	74	C
37	3	76	A
37	3	91	G
37	3	95	A
37	3	102	A
37	3	112	G
37	3	121	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	42	G
38	4	48	A
38	4	51	G
38	4	52	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	66	A
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A

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Mol	Chain	Res	Type
38	4	113	U
38	4	122	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	151	C
38	4	152	G
38	4	155	A
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	23	G
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	57	G
1	6	60	U
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	87	C
1	6	104	A
1	6	114	C
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G

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Mol	Chain	Res	Type
1	6	158	U
1	6	159	U
1	6	166	C
1	6	178	U
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	G
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	229	U
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	238	U
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	266	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U

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Mol	Chain	Res	Type
1	6	278	U
1	6	280	U
1	6	281	G
1	6	287	G
1	6	299	A
1	6	309	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	333	A
1	6	337	G
1	6	338	C
1	6	341	A
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A
1	6	381	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	464	A
1	6	468	A
1	6	470	A
1	6	475	A
1	6	477	A
1	6	480	G
1	6	484	C

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Mol	Chain	Res	Type
1	6	485	A
1	6	486	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	495	C
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	519	C
1	6	527	A
1	6	532	U
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	551	G
1	6	554	C
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C

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Mol	Chain	Res	Type
1	6	568	G
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	609	U
1	6	610	G
1	6	611	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	648	G
1	6	652	G
1	6	653	C
1	6	654	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	695	U

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Mol	Chain	Res	Type
1	6	696	C
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	731	C
1	6	742	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	773	C
1	6	774	A
1	6	775	G
1	6	777	C
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U

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Mol	Chain	Res	Type
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	863	A
1	6	864	U
1	6	898	A
1	6	906	A
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	944	A
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	992	A
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1023	A
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U

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Mol	Chain	Res	Type
1	6	1061	A
1	6	1063	U
1	6	1072	C
1	6	1074	G
1	6	1082	C
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1109	G
1	6	1111	G
1	6	1138	A
1	6	1139	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1164	G
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1197	C
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1221	A
1	6	1225	U
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
1	6	1239	U
1	6	1240	U

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Mol	Chain	Res	Type
1	6	1241	G
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1261	G
1	6	1286	U
1	6	1288	G
1	6	1291	G
1	6	1314	U
1	6	1316	G
1	6	1321	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1355	C
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1371	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1412	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1445	G
1	6	1446	A
1	6	1448	G

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Mol	Chain	Res	Type
1	6	1458	G
1	6	1459	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1486	G
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1572	G
1	6	1573	A
1	6	1574	G
1	6	1582	U
1	6	1584	G
1	6	1600	A
1	6	1601	G
1	6	1616	G
1	6	1618	C
1	6	1621	U
1	6	1634	C
1	6	1637	C
1	6	1638	G

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Mol	Chain	Res	Type
1	6	1657	U
1	6	1658	G
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1705	C
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G
1	6	1731	A
1	6	1736	G
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	21	G
36	5	24	G
36	5	26	A
36	5	40	A
36	5	43	A

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Mol	Chain	Res	Type
36	5	49	A
36	5	57	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	68	C
36	5	73	C
36	5	76	G
36	5	92	G
36	5	93	C
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	150	A
36	5	152	U
36	5	156	G
36	5	157	A
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	173	G
36	5	174	C
36	5	178	U
36	5	182	U
36	5	183	G
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C

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Mol	Chain	Res	Type
36	5	201	A
36	5	210	U
36	5	213	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	236	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	269	G
36	5	283	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	316	U
36	5	323	A
36	5	329	U
36	5	334	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	370	U
36	5	376	G
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C

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Mol	Chain	Res	Type
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	503	C
36	5	512	U
36	5	521	A
36	5	523	A
36	5	535	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	555	U
36	5	557	A
36	5	559	A
36	5	566	G
36	5	569	A
36	5	578	A
36	5	579	G
36	5	581	U
36	5	592	A
36	5	594	U
36	5	595	G
36	5	600	G
36	5	604	G
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	653	A
36	5	660	A
36	5	662	U
36	5	675	C
36	5	677	A
36	5	681	U
36	5	691	A
36	5	705	A

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Mol	Chain	Res	Type
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	726	G
36	5	727	G
36	5	736	A
36	5	760	G
36	5	766	U
36	5	767	U
36	5	768	C
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	837	A
36	5	846	A
36	5	861	C
36	5	874	U
36	5	879	U
36	5	890	C
36	5	896	A
36	5	907	G
36	5	908	G
36	5	910	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G

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Mol	Chain	Res	Type
36	5	964	G
36	5	979	U
36	5	981	U
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1034	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1088	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G

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Mol	Chain	Res	Type
36	5	1117	G
36	5	1131	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1178	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G
36	5	1223	A
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1254	C
36	5	1259	A
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1285	G
36	5	1295	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1330	A
36	5	1349	G
36	5	1351	U
36	5	1352	A

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Mol	Chain	Res	Type
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1380	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1431	G
36	5	1432	C
36	5	1434	G
36	5	1437	C
36	5	1438	U
36	5	1446	A
36	5	1450	G
36	5	1460	A
36	5	1465	A
36	5	1480	G
36	5	1481	A
36	5	1482	A
36	5	1484	U
36	5	1490	A
36	5	1503	A
36	5	1508	C
36	5	1536	G
36	5	1539	A
36	5	1541	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1566	A
36	5	1567	U

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Mol	Chain	Res	Type
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1580	A
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1605	A
36	5	1607	U
36	5	1608	C
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1657	C
36	5	1683	A
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1760	A
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G

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Mol	Chain	Res	Type
36	5	1775	G
36	5	1778	G
36	5	1780	G
36	5	1781	C
36	5	1795	U
36	5	1797	A
36	5	1812	G
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1891	A
36	5	1893	A
36	5	1906	G
36	5	1918	C
36	5	1935	G
36	5	1952	G
36	5	1953	G
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2114	C
36	5	2121	G
36	5	2122	G
36	5	2128	C
36	5	2131	A
36	5	2144	A
36	5	2158	A

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Mol	Chain	Res	Type
36	5	2169	G
36	5	2176	U
36	5	2188	A
36	5	2198	A
36	5	2201	G
36	5	2205	U
36	5	2210	G
36	5	2213	A
36	5	2222	A
36	5	2223	A
36	5	2225	U
36	5	2228	A
36	5	2244	A
36	5	2250	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2264	U
36	5	2273	G
36	5	2276	G
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2318	U
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2337	C
36	5	2338	C
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G

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Mol	Chain	Res	Type
36	5	2397	A
36	5	2398	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
36	5	2437	G
36	5	2438	A
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2513	U
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G

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Mol	Chain	Res	Type
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2609	A
36	5	2610	G
36	5	2614	G
36	5	2615	G
36	5	2626	A
36	5	2637	A
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2667	A
36	5	2674	A
36	5	2677	G
36	5	2678	A
36	5	2681	U
36	5	2683	U
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2726	C
36	5	2728	G
36	5	2729	U

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Mol	Chain	Res	Type
36	5	2742	C
36	5	2752	U
36	5	2753	G
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2779	A
36	5	2796	G
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2829	U
36	5	2843	U
36	5	2845	A
36	5	2849	C
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2873	U
36	5	2875	U
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2904	U
36	5	2923	U
36	5	2928	C
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2971	A
36	5	2972	G

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Mol	Chain	Res	Type
36	5	2979	U
36	5	2983	C
36	5	2992	U
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3049	A
36	5	3050	U
36	5	3056	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3080	G
36	5	3086	A
36	5	3092	C
36	5	3102	G
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3145	C
36	5	3152	U
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3207	U

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Mol	Chain	Res	Type
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3270	U
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3280	U
36	5	3281	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3309	G
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G

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Mol	Chain	Res	Type
36	5	3358	U
36	5	3363	U
36	5	3369	G
36	5	3378	C
36	5	3382	U
36	5	3389	U
36	5	3390	G
36	5	3391	A
36	5	3396	U
37	7	22	A
37	7	23	A
37	7	27	A
37	7	33	U
37	7	41	G
37	7	54	U
37	7	60	G
37	7	64	A
37	7	65	G
37	7	73	C
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
38	8	20	U
38	8	21	C
38	8	34	U
38	8	35	C
38	8	42	G
38	8	48	A
38	8	51	G
38	8	52	A
38	8	53	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C

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Mol	Chain	Res	Type
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	102	U
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	116	G
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U
90	A	75	C
90	a	75	C

All (275) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	136	C
1	2	139	C
1	2	158	U
1	2	187	G

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Mol	Chain	Res	Type
1	2	217	A
1	2	218	A
1	2	232	U
1	2	240	U
1	2	278	U
1	2	280	U
1	2	321	C
1	2	417	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	622	A
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	781	U
1	2	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	913	G
1	2	1051	G
1	2	1058	U
1	2	1081	A
1	2	1157	A
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C

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Mol	Chain	Res	Type
1	2	1489	U
1	2	1490	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1696	G
1	2	1698	G
1	2	1711	C
1	2	1761	U
36	1	65	A
36	1	169	U
36	1	239	G
36	1	282	G
36	1	397	A
36	1	547	G
36	1	594	U
36	1	637	C
36	1	715	A
36	1	763	G
36	1	873	C
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1181	U
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1484	U
36	1	1562	C
36	1	1582	C
36	1	1716	U
36	1	1751	G
36	1	1815	U

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Mol	Chain	Res	Type
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1842	A
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2281	A
36	1	2372	A
36	1	2374	C
36	1	2418	G
36	1	2501	U
36	1	2513	U
36	1	2525	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2801	A
36	1	2818	U
36	1	2859	U
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3207	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3276	G
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	52	G
38	4	85	G
38	4	111	A
1	6	25	C

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Mol	Chain	Res	Type
1	6	66	U
1	6	75	U
1	6	76	A
1	6	103	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	417	A
1	6	512	A
1	6	542	A
1	6	555	A
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1196	A
1	6	1207	C
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1490	C
1	6	1491	U
1	6	1535	U
1	6	1568	C

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Mol	Chain	Res	Type
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1637	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	67	A
36	5	151	A
36	5	183	G
36	5	238	A
36	5	282	G
36	5	397	A
36	5	438	A
36	5	546	C
36	5	647	A
36	5	715	A
36	5	735	A
36	5	765	C
36	5	786	A
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1033	U
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1554	U

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Mol	Chain	Res	Type
36	5	1560	G
36	5	1580	A
36	5	1607	U
36	5	1716	U
36	5	1724	U
36	5	1816	A
36	5	1819	U
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2401	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C
36	5	2593	A
36	5	2682	C
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2872	A
36	5	2970	C
36	5	2971	A
36	5	2979	U
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3167	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3269	U

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Mol	Chain	Res	Type
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
38	8	111	A
38	8	126	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
90	PPU	A	76	36,90	32,40,41	1.07	2 (6%)	33,57,60	1.74	8 (24%)
90	PPU	a	76	36,90	32,40,41	1.04	2 (6%)	33,57,60	1.74	6 (18%)

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
90	PPU	A	76	36,90	-	3/21/43/44	0/4/4/4
90	PPU	a	76	36,90	-	4/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	a	76	PPU	C2'-C3'	-2.87	1.48	1.53
90	a	76	PPU	C5-C4	2.32	1.47	1.40
90	A	76	PPU	C2'-C3'	-2.23	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	A	76	PPU	C5-C4	2.19	1.46	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	a	76	PPU	C3'-N3'-C	-5.38	115.10	123.21
90	A	76	PPU	C3'-N3'-C	-4.92	115.79	123.21
90	a	76	PPU	CG-CB-CA	-4.45	104.87	114.13
90	A	76	PPU	CA-C-N3'	3.52	121.03	116.15
90	A	76	PPU	N3-C2-N1	-3.52	123.18	128.68
90	a	76	PPU	N3-C2-N1	-3.40	123.36	128.68
90	a	76	PPU	CA-C-N3'	2.83	120.08	116.15
90	A	76	PPU	O4'-C4'-C3'	2.77	108.04	104.06
90	a	76	PPU	O2'-C2'-C3'	-2.76	104.42	111.16
90	A	76	PPU	CG-CB-CA	-2.59	108.75	114.13
90	a	76	PPU	C4-C5-N7	-2.40	106.89	109.40
90	A	76	PPU	CD2-CG-CD1	2.40	121.94	118.17
90	A	76	PPU	N1-C6-N6	2.24	119.42	117.06
90	A	76	PPU	C4-C5-N7	-2.10	107.21	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	A	76	PPU	C3'-C4'-C5'-O5'
90	a	76	PPU	CE2-CZ-OC-CM
90	a	76	PPU	CE1-CZ-OC-CM
90	A	76	PPU	O4'-C4'-C5'-O5'
90	a	76	PPU	CA-CB-CG-CD1
90	a	76	PPU	CA-CB-CG-CD2
90	A	76	PPU	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3553 ligands modelled in this entry, 2208 are monoatomic - leaving 1345 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	$\#\|Z\| > 2$
92	OHX	1	4368	-	0,6,6	-	-	-		
92	OHX	1	4427	36	0,6,6	-	-	-		
92	OHX	7	237	-	0,6,6	-	-	-		
92	OHX	1	4497	-	0,6,6	-	-	-		
92	OHX	5	4335	-	0,6,6	-	-	-		
92	OHX	5	4225	-	0,6,6	-	-	-		
92	OHX	4	247	92	0,6,6	-	-	-		
92	OHX	5	4406	92	0,6,6	-	-	-		
92	OHX	6	2294	1,92	0,6,6	-	-	-		
92	OHX	5	4502	-	0,6,6	-	-	-		
92	OHX	5	4220	-	0,6,6	-	-	-		
92	OHX	1	4139	-	0,6,6	-	-	-		
92	OHX	1	4204	-	0,6,6	-	-	-		
92	OHX	2	2092	-	0,6,6	-	-	-		
92	OHX	1	4183	-	0,6,6	-	-	-		
92	OHX	6	2274	92	0,6,6	-	-	-		
92	OHX	L4	408	-	0,6,6	-	-	-		
92	OHX	6	2193	1	0,6,6	-	-	-		
92	OHX	1	4444	-	0,6,6	-	-	-		
92	OHX	6	2166	-	0,6,6	-	-	-		
92	OHX	6	2199	1	0,6,6	-	-	-		
92	OHX	1	4171	92	0,6,6	-	-	-		
92	OHX	5	4523	92	0,6,6	-	-	-		
92	OHX	5	4555	92	0,6,6	-	-	-		
92	OHX	m5	303	-	0,6,6	-	-	-		
92	OHX	6	2279	-	0,6,6	-	-	-		
92	OHX	l3	412	-	0,6,6	-	-	-		
92	OHX	2	2253	-	0,6,6	-	-	-		
92	OHX	1	4149	-	0,6,6	-	-	-		
92	OHX	8	223	-	0,6,6	-	-	-		
92	OHX	1	4346	-	0,6,6	-	-	-		
92	OHX	5	4316	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
92	OHX	2	2117	-	0,6,6	-	-	-		
92	OHX	5	4448	-	0,6,6	-	-	-		
92	OHX	5	4289	-	0,6,6	-	-	-		
92	OHX	2	2109	-	0,6,6	-	-	-		
92	OHX	5	4434	-	0,6,6	-	-	-		
92	OHX	6	2282	92	0,6,6	-	-	-		
92	OHX	5	4176	-	0,6,6	-	-	-		
92	OHX	1	4101	-	0,6,6	-	-	-		
92	OHX	2	2185	-	0,6,6	-	-	-		
92	OHX	1	4129	-	0,6,6	-	-	-		
92	OHX	2	2071	-	0,6,6	-	-	-		
92	OHX	6	2278	-	0,6,6	-	-	-		
92	OHX	5	4334	92	0,6,6	-	-	-		
92	OHX	1	4480	-	0,6,6	-	-	-		
92	OHX	6	2331	92	0,6,6	-	-	-		
92	OHX	5	4180	-	0,6,6	-	-	-		
92	OHX	5	4200	92	0,6,6	-	-	-		
92	OHX	1	4274	-	0,6,6	-	-	-		
92	OHX	5	4492	-	0,6,6	-	-	-		
92	OHX	6	2299	92	0,6,6	-	-	-		
92	OHX	5	4384	-	0,6,6	-	-	-		
92	OHX	5	4549	-	0,6,6	-	-	-		
92	OHX	6	2203	-	0,6,6	-	-	-		
92	OHX	1	4311	-	0,6,6	-	-	-		
92	OHX	1	4466	92	0,6,6	-	-	-		
92	OHX	5	4417	-	0,6,6	-	-	-		
92	OHX	7	201	92	0,6,6	-	-	-		
92	OHX	1	4460	-	0,6,6	-	-	-		
92	OHX	5	4429	-	0,6,6	-	-	-		
92	OHX	5	4508	-	0,6,6	-	-	-		
92	OHX	1	4181	92	0,6,6	-	-	-		
92	OHX	5	4328	-	0,6,6	-	-	-		
92	OHX	1	4240	-	0,6,6	-	-	-		
92	OHX	5	4421	-	0,6,6	-	-	-		
92	OHX	1	4373	-	0,6,6	-	-	-		
92	OHX	1	4233	-	0,6,6	-	-	-		
92	OHX	1	4143	92	0,6,6	-	-	-		
92	OHX	1	4241	-	0,6,6	-	-	-		
92	OHX	5	4329	-	0,6,6	-	-	-		
92	OHX	1	4348	-	0,6,6	-	-	-		
92	OHX	6	2258	92	0,6,6	-	-	-		
92	OHX	1	4374	-	0,6,6	-	-	-		
92	OHX	5	4495	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4303	-	0,6,6	-	-	-		
92	OHX	2	2229	-	0,6,6	-	-	-		
92	OHX	M7	209	-	0,6,6	-	-	-		
92	OHX	1	4243	-	0,6,6	-	-	-		
92	OHX	5	4322	-	0,6,6	-	-	-		
92	OHX	1	4431	92	0,6,6	-	-	-		
92	OHX	2	2231	-	0,6,6	-	-	-		
92	OHX	2	2250	-	0,6,6	-	-	-		
92	OHX	1	4292	92	0,6,6	-	-	-		
92	OHX	5	4461	-	0,6,6	-	-	-		
92	OHX	5	4216	92	0,6,6	-	-	-		
92	OHX	1	4342	36	0,6,6	-	-	-		
92	OHX	6	2288	-	0,6,6	-	-	-		
92	OHX	4	241	-	0,6,6	-	-	-		
92	OHX	1	4301	-	0,6,6	-	-	-		
92	OHX	2	2224	-	0,6,6	-	-	-		
92	OHX	5	4376	-	0,6,6	-	-	-		
92	OHX	5	4181	-	0,6,6	-	-	-		
92	OHX	1	4339	-	0,6,6	-	-	-		
92	OHX	1	4100	-	0,6,6	-	-	-		
92	OHX	6	2269	-	0,6,6	-	-	-		
92	OHX	2	2131	-	0,6,6	-	-	-		
92	OHX	2	2166	92	0,6,6	-	-	-		
92	OHX	2	2199	92	0,6,6	-	-	-		
92	OHX	5	4337	92	0,6,6	-	-	-		
92	OHX	1	4248	-	0,6,6	-	-	-		
92	OHX	sR	401	-	0,6,6	-	-	-		
92	OHX	1	4365	-	0,6,6	-	-	-		
92	OHX	1	4299	-	0,6,6	-	-	-		
92	OHX	S6	302	-	0,6,6	-	-	-		
92	OHX	1	4132	-	0,6,6	-	-	-		
92	OHX	6	2259	-	0,6,6	-	-	-		
92	OHX	1	4422	-	0,6,6	-	-	-		
92	OHX	1	4184	-	0,6,6	-	-	-		
92	OHX	5	4510	-	0,6,6	-	-	-		
92	OHX	5	4506	92	0,6,6	-	-	-		
92	OHX	5	4548	-	0,6,6	-	-	-		
92	OHX	1	4289	92	0,6,6	-	-	-		
92	OHX	6	2253	-	0,6,6	-	-	-		
92	OHX	5	4312	92	0,6,6	-	-	-		
92	OHX	5	4253	92	0,6,6	-	-	-		
92	OHX	5	4348	92	0,6,6	-	-	-		
92	OHX	5	4359	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	2	2103	-	0,6,6	-	-	-		
92	OHX	1	4160	-	0,6,6	-	-	-		
92	OHX	6	2264	-	0,6,6	-	-	-		
92	OHX	5	4515	92	0,6,6	-	-	-		
92	OHX	1	4401	92	0,6,6	-	-	-		
92	OHX	1	4440	36,92	0,6,6	-	-	-		
92	OHX	1	4118	-	0,6,6	-	-	-		
92	OHX	6	2201	92	0,6,6	-	-	-		
92	OHX	5	4182	-	0,6,6	-	-	-		
92	OHX	5	4443	-	0,6,6	-	-	-		
92	OHX	2	2177	-	0,6,6	-	-	-		
92	OHX	5	4231	92	0,6,6	-	-	-		
92	OHX	1	4473	92	0,6,6	-	-	-		
92	OHX	6	2231	-	0,6,6	-	-	-		
92	OHX	2	2203	92	0,6,6	-	-	-		
92	OHX	1	4145	-	0,6,6	-	-	-		
92	OHX	2	2074	92	0,6,6	-	-	-		
92	OHX	5	4342	-	0,6,6	-	-	-		
92	OHX	1	4508	92	0,6,6	-	-	-		
92	OHX	6	2304	-	0,6,6	-	-	-		
92	OHX	1	4384	-	0,6,6	-	-	-		
92	OHX	5	4420	-	0,6,6	-	-	-		
92	OHX	1	4400	-	0,6,6	-	-	-		
92	OHX	l4	404	-	0,6,6	-	-	-		
92	OHX	1	4302	92	0,6,6	-	-	-		
92	OHX	2	2180	-	0,6,6	-	-	-		
92	OHX	6	2156	-	0,6,6	-	-	-		
92	OHX	1	4429	-	0,6,6	-	-	-		
92	OHX	5	4405	-	0,6,6	-	-	-		
92	OHX	5	4202	-	0,6,6	-	-	-		
92	OHX	1	4179	-	0,6,6	-	-	-		
92	OHX	1	4137	-	0,6,6	-	-	-		
92	OHX	1	4296	92	0,6,6	-	-	-		
92	OHX	6	2183	-	0,6,6	-	-	-		
92	OHX	6	2204	1	0,6,6	-	-	-		
92	OHX	1	4115	-	0,6,6	-	-	-		
92	OHX	5	4341	92	0,6,6	-	-	-		
92	OHX	1	4165	-	0,6,6	-	-	-		
92	OHX	1	4490	92	0,6,6	-	-	-		
92	OHX	5	4227	-	0,6,6	-	-	-		
92	OHX	5	4372	-	0,6,6	-	-	-		
92	OHX	L2	305	92	0,6,6	-	-	-		
92	OHX	5	4514	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4474	92	0,6,6	-	-	-		
92	OHX	O7	108	-	0,6,6	-	-	-		
92	OHX	6	2214	92	0,6,6	-	-	-		
92	OHX	5	4242	36	0,6,6	-	-	-		
92	OHX	6	2307	-	0,6,6	-	-	-		
92	OHX	1	4195	-	0,6,6	-	-	-		
92	OHX	5	4323	36,92	0,6,6	-	-	-		
92	OHX	1	4448	-	0,6,6	-	-	-		
92	OHX	6	2221	1	0,6,6	-	-	-		
92	OHX	6	2327	-	0,6,6	-	-	-		
92	OHX	5	4463	-	0,6,6	-	-	-		
92	OHX	5	4505	36	0,6,6	-	-	-		
92	OHX	1	4434	-	0,6,6	-	-	-		
92	OHX	2	2135	-	0,6,6	-	-	-		
92	OHX	2	2086	92	0,6,6	-	-	-		
92	OHX	5	4567	92	0,6,6	-	-	-		
92	OHX	1	4467	92	0,6,6	-	-	-		
92	OHX	6	2229	-	0,6,6	-	-	-		
92	OHX	N8	208	-	0,6,6	-	-	-		
92	OHX	2	2080	-	0,6,6	-	-	-		
92	OHX	1	4347	92	0,6,6	-	-	-		
92	OHX	1	4216	-	0,6,6	-	-	-		
92	OHX	5	4469	-	0,6,6	-	-	-		
92	OHX	1	4214	-	0,6,6	-	-	-		
92	OHX	6	2143	-	0,6,6	-	-	-		
92	OHX	5	4464	92	0,6,6	-	-	-		
92	OHX	1	4402	-	0,6,6	-	-	-		
92	OHX	5	4320	92	0,6,6	-	-	-		
92	OHX	6	2301	-	0,6,6	-	-	-		
92	OHX	8	231	92	0,6,6	-	-	-		
92	OHX	1	4298	-	0,6,6	-	-	-		
92	OHX	5	4511	92	0,6,6	-	-	-		
92	OHX	4	242	-	0,6,6	-	-	-		
92	OHX	5	4291	92	0,6,6	-	-	-		
92	OHX	6	2338	92	0,6,6	-	-	-		
92	OHX	2	2137	1	0,6,6	-	-	-		
92	OHX	1	4385	92	0,6,6	-	-	-		
92	OHX	5	4390	-	0,6,6	-	-	-		
92	OHX	5	4194	-	0,6,6	-	-	-		
92	OHX	8	229	-	0,6,6	-	-	-		
92	OHX	1	4362	-	0,6,6	-	-	-		
92	OHX	1	4328	-	0,6,6	-	-	-		
92	OHX	1	4504	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4102	-	0,6,6	-	-	-		
92	OHX	1	4169	92	0,6,6	-	-	-		
92	OHX	5	4490	-	0,6,6	-	-	-		
92	OHX	5	4557	92	0,6,6	-	-	-		
92	OHX	2	2221	92	0,6,6	-	-	-		
92	OHX	1	4245	92	0,6,6	-	-	-		
92	OHX	5	4520	92	0,6,6	-	-	-		
92	OHX	1	4443	-	0,6,6	-	-	-		
92	OHX	2	2134	-	0,6,6	-	-	-		
92	OHX	1	4203	92	0,6,6	-	-	-		
92	OHX	4	235	-	0,6,6	-	-	-		
92	OHX	l2	306	92	0,6,6	-	-	-		
92	OHX	5	4280	-	0,6,6	-	-	-		
92	OHX	7	236	-	0,6,6	-	-	-		
92	OHX	1	4284	-	0,6,6	-	-	-		
92	OHX	5	4456	-	0,6,6	-	-	-		
92	OHX	6	2181	92	0,6,6	-	-	-		
92	OHX	1	4136	-	0,6,6	-	-	-		
92	OHX	1	4127	-	0,6,6	-	-	-		
92	OHX	1	4182	-	0,6,6	-	-	-		
92	OHX	1	4392	-	0,6,6	-	-	-		
92	OHX	5	4263	-	0,6,6	-	-	-		
92	OHX	1	4225	-	0,6,6	-	-	-		
92	OHX	2	2178	-	0,6,6	-	-	-		
92	OHX	5	4234	92	0,6,6	-	-	-		
92	OHX	1	4366	-	0,6,6	-	-	-		
92	OHX	l9	204	-	0,6,6	-	-	-		
92	OHX	5	4482	92	0,6,6	-	-	-		
92	OHX	8	237	38	0,6,6	-	-	-		
92	OHX	l5	308	-	0,6,6	-	-	-		
92	OHX	1	4453	92	0,6,6	-	-	-		
92	OHX	6	2292	-	0,6,6	-	-	-		
92	OHX	5	4237	92	0,6,6	-	-	-		
92	OHX	1	4491	92	0,6,6	-	-	-		
92	OHX	5	4444	-	0,6,6	-	-	-		
92	OHX	5	4553	36,92	0,6,6	-	-	-		
92	OHX	1	4227	-	0,6,6	-	-	-		
92	OHX	5	4554	92	0,6,6	-	-	-		
92	OHX	1	4355	36,92	0,6,6	-	-	-		
92	OHX	1	4109	-	0,6,6	-	-	-		
92	OHX	1	4277	-	0,6,6	-	-	-		
92	OHX	1	4155	-	0,6,6	-	-	-		
92	OHX	5	4306	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4177	-	0,6,6	-	-	-		
92	OHX	2	2072	-	0,6,6	-	-	-		
92	OHX	1	4499	92	0,6,6	-	-	-		
92	OHX	1	4505	36,92	0,6,6	-	-	-		
92	OHX	6	2206	-	0,6,6	-	-	-		
92	OHX	2	2113	92	0,6,6	-	-	-		
92	OHX	2	2133	92	0,6,6	-	-	-		
92	OHX	6	2319	-	0,6,6	-	-	-		
92	OHX	s1	302	-	0,6,6	-	-	-		
92	OHX	6	2236	-	0,6,6	-	-	-		
92	OHX	1	4323	-	0,6,6	-	-	-		
92	OHX	6	2235	-	0,6,6	-	-	-		
92	OHX	5	4211	92	0,6,6	-	-	-		
92	OHX	4	240	-	0,6,6	-	-	-		
92	OHX	5	4413	92	0,6,6	-	-	-		
92	OHX	o7	105	-	0,6,6	-	-	-		
92	OHX	5	4484	92	0,6,6	-	-	-		
92	OHX	5	4339	-	0,6,6	-	-	-		
92	OHX	1	4231	92	0,6,6	-	-	-		
92	OHX	5	4311	-	0,6,6	-	-	-		
92	OHX	1	4433	92	0,6,6	-	-	-		
92	OHX	1	4356	-	0,6,6	-	-	-		
92	OHX	5	4411	-	0,6,6	-	-	-		
92	OHX	2	2095	-	0,6,6	-	-	-		
92	OHX	1	4166	-	0,6,6	-	-	-		
92	OHX	2	2119	-	0,6,6	-	-	-		
92	OHX	2	2128	-	0,6,6	-	-	-		
92	OHX	5	4532	-	0,6,6	-	-	-		
92	OHX	5	4166	-	0,6,6	-	-	-		
92	OHX	6	2316	92	0,6,6	-	-	-		
92	OHX	2	2239	-	0,6,6	-	-	-		
92	OHX	1	4236	-	0,6,6	-	-	-		
92	OHX	1	4318	-	0,6,6	-	-	-		
92	OHX	5	4340	-	0,6,6	-	-	-		
92	OHX	2	2088	-	0,6,6	-	-	-		
92	OHX	1	4458	-	0,6,6	-	-	-		
92	OHX	2	2156	92	0,6,6	-	-	-		
92	OHX	1	4283	-	0,6,6	-	-	-		
92	OHX	5	4160	-	0,6,6	-	-	-		
92	OHX	1	4388	-	0,6,6	-	-	-		
92	OHX	5	4494	-	0,6,6	-	-	-		
92	OHX	5	4333	92	0,6,6	-	-	-		
92	OHX	1	4252	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4343	-	0,6,6	-	-	-		
92	OHX	5	4356	-	0,6,6	-	-	-		
92	OHX	2	2107	-	0,6,6	-	-	-		
92	OHX	1	4142	-	0,6,6	-	-	-		
92	OHX	6	2306	-	0,6,6	-	-	-		
92	OHX	1	4476	92	0,6,6	-	-	-		
92	OHX	2	2079	-	0,6,6	-	-	-		
92	OHX	1	4378	36	0,6,6	-	-	-		
92	OHX	2	2085	-	0,6,6	-	-	-		
92	OHX	1	4426	-	0,6,6	-	-	-		
92	OHX	5	4530	92	0,6,6	-	-	-		
92	OHX	5	4243	-	0,6,6	-	-	-		
92	OHX	2	2214	1	0,6,6	-	-	-		
92	OHX	2	2112	-	0,6,6	-	-	-		
92	OHX	6	2255	1,92	0,6,6	-	-	-		
92	OHX	6	2154	-	0,6,6	-	-	-		
92	OHX	5	4349	92	0,6,6	-	-	-		
92	OHX	2	2077	1,92	0,6,6	-	-	-		
92	OHX	2	2083	92	0,6,6	-	-	-		
92	OHX	1	4360	-	0,6,6	-	-	-		
92	OHX	5	4386	-	0,6,6	-	-	-		
92	OHX	1	4130	92	0,6,6	-	-	-		
92	OHX	8	222	92	0,6,6	-	-	-		
92	OHX	1	4456	-	0,6,6	-	-	-		
92	OHX	6	2280	-	0,6,6	-	-	-		
92	OHX	1	4496	92	0,6,6	-	-	-		
92	OHX	5	4472	-	0,6,6	-	-	-		
92	OHX	1	4221	-	0,6,6	-	-	-		
92	OHX	5	4304	-	0,6,6	-	-	-		
92	OHX	6	2315	-	0,6,6	-	-	-		
92	OHX	1	4185	92	0,6,6	-	-	-		
92	OHX	6	2273	-	0,6,6	-	-	-		
92	OHX	5	4441	-	0,6,6	-	-	-		
92	OHX	1	4157	92	0,6,6	-	-	-		
92	OHX	5	4259	92	0,6,6	-	-	-		
92	OHX	1	4482	92	0,6,6	-	-	-		
92	OHX	4	237	38	0,6,6	-	-	-		
92	OHX	5	4215	92	0,6,6	-	-	-		
92	OHX	7	240	-	0,6,6	-	-	-		
92	OHX	2	2220	1	0,6,6	-	-	-		
92	OHX	2	2122	92	0,6,6	-	-	-		
92	OHX	5	4487	-	0,6,6	-	-	-		
92	OHX	6	2260	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	2	2245	92	0,6,6	-	-	-		
92	OHX	5	4305	-	0,6,6	-	-	-		
92	OHX	6	2190	1,92	0,6,6	-	-	-		
92	OHX	5	4271	36	0,6,6	-	-	-		
92	OHX	5	4445	-	0,6,6	-	-	-		
92	OHX	2	2237	92	0,6,6	-	-	-		
92	OHX	5	4446	-	0,6,6	-	-	-		
92	OHX	1	4164	36	0,6,6	-	-	-		
92	OHX	1	4498	-	0,6,6	-	-	-		
92	OHX	5	4412	-	0,6,6	-	-	-		
92	OHX	2	2207	92	0,6,6	-	-	-		
92	OHX	5	4288	92	0,6,6	-	-	-		
92	OHX	l3	413	-	0,6,6	-	-	-		
92	OHX	6	2243	-	0,6,6	-	-	-		
92	OHX	6	2334	92	0,6,6	-	-	-		
92	OHX	S8	303	-	0,6,6	-	-	-		
92	OHX	1	4151	-	0,6,6	-	-	-		
92	OHX	5	4407	-	0,6,6	-	-	-		
92	OHX	4	233	-	0,6,6	-	-	-		
92	OHX	1	4123	-	0,6,6	-	-	-		
92	OHX	2	2142	-	0,6,6	-	-	-		
92	OHX	5	4476	92	0,6,6	-	-	-		
92	OHX	1	4484	92	0,6,6	-	-	-		
92	OHX	5	4547	92	0,6,6	-	-	-		
92	OHX	5	4287	-	0,6,6	-	-	-		
92	OHX	2	2093	1	0,6,6	-	-	-		
92	OHX	1	4502	92	0,6,6	-	-	-		
92	OHX	6	2202	-	0,6,6	-	-	-		
92	OHX	Q2	505	-	0,6,6	-	-	-		
92	OHX	2	2141	92	0,6,6	-	-	-		
92	OHX	5	4477	-	0,6,6	-	-	-		
92	OHX	5	4416	-	0,6,6	-	-	-		
92	OHX	1	4246	-	0,6,6	-	-	-		
92	OHX	5	4387	36	0,6,6	-	-	-		
92	OHX	6	2311	92	0,6,6	-	-	-		
92	OHX	1	4321	-	0,6,6	-	-	-		
92	OHX	4	244	-	0,6,6	-	-	-		
92	OHX	1	4315	92	0,6,6	-	-	-		
92	OHX	1	4116	92	0,6,6	-	-	-		
92	OHX	5	4244	-	0,6,6	-	-	-		
92	OHX	4	243	-	0,6,6	-	-	-		
92	OHX	2	2087	-	0,6,6	-	-	-		
92	OHX	5	4363	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4121	-	0,6,6	-	-	-		
92	OHX	5	4285	92	0,6,6	-	-	-		
92	OHX	5	4478	92	0,6,6	-	-	-		
92	OHX	5	4346	92	0,6,6	-	-	-		
92	OHX	1	4316	-	0,6,6	-	-	-		
92	OHX	5	4232	-	0,6,6	-	-	-		
92	OHX	6	2228	-	0,6,6	-	-	-		
92	OHX	5	4358	-	0,6,6	-	-	-		
92	OHX	6	2184	-	0,6,6	-	-	-		
92	OHX	6	2220	-	0,6,6	-	-	-		
92	OHX	5	4489	36	0,6,6	-	-	-		
92	OHX	1	4176	-	0,6,6	-	-	-		
92	OHX	l5	309	-	0,6,6	-	-	-		
92	OHX	2	2160	-	0,6,6	-	-	-		
92	OHX	5	4439	-	0,6,6	-	-	-		
92	OHX	1	4352	-	0,6,6	-	-	-		
92	OHX	1	4463	-	0,6,6	-	-	-		
92	OHX	7	232	-	0,6,6	-	-	-		
92	OHX	6	2219	-	0,6,6	-	-	-		
92	OHX	6	2254	-	0,6,6	-	-	-		
92	OHX	2	2194	92	0,6,6	-	-	-		
92	OHX	1	4503	92	0,6,6	-	-	-		
92	OHX	1	4436	-	0,6,6	-	-	-		
92	OHX	5	4264	92	0,6,6	-	-	-		
92	OHX	5	4392	-	0,6,6	-	-	-		
92	OHX	2	2247	92	0,6,6	-	-	-		
92	OHX	5	4360	-	0,6,6	-	-	-		
92	OHX	5	4451	-	0,6,6	-	-	-		
92	OHX	5	4466	-	0,6,6	-	-	-		
92	OHX	1	4417	36	0,6,6	-	-	-		
92	OHX	5	4393	-	0,6,6	-	-	-		
92	OHX	1	4190	-	0,6,6	-	-	-		
92	OHX	2	2252	92	0,6,6	-	-	-		
92	OHX	6	2163	-	0,6,6	-	-	-		
92	OHX	1	4419	-	0,6,6	-	-	-		
92	OHX	2	2127	-	0,6,6	-	-	-		
92	OHX	2	2205	-	0,6,6	-	-	-		
92	OHX	1	4441	-	0,6,6	-	-	-		
92	OHX	6	2196	92	0,6,6	-	-	-		
92	OHX	6	2250	92	0,6,6	-	-	-		
92	OHX	1	4370	-	0,6,6	-	-	-		
92	OHX	5	4418	-	0,6,6	-	-	-		
92	OHX	5	4266	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4485	92	0,6,6	-	-	-		
92	OHX	5	4465	92	0,6,6	-	-	-		
92	OHX	1	4325	-	0,6,6	-	-	-		
92	OHX	5	4161	-	0,6,6	-	-	-		
92	OHX	O3	204	-	0,6,6	-	-	-		
92	OHX	1	4309	36	0,6,6	-	-	-		
92	OHX	5	4238	-	0,6,6	-	-	-		
92	OHX	6	2275	-	0,6,6	-	-	-		
92	OHX	1	4279	92	0,6,6	-	-	-		
92	OHX	1	4131	92	0,6,6	-	-	-		
92	OHX	5	4197	-	0,6,6	-	-	-		
92	OHX	5	4419	-	0,6,6	-	-	-		
92	OHX	1	4280	-	0,6,6	-	-	-		
92	OHX	1	4215	-	0,6,6	-	-	-		
92	OHX	1	4305	92	0,6,6	-	-	-		
92	OHX	1	4495	92	0,6,6	-	-	-		
92	OHX	1	4353	92	0,6,6	-	-	-		
92	OHX	5	4425	-	0,6,6	-	-	-		
92	OHX	5	4383	92	0,6,6	-	-	-		
92	OHX	1	4334	-	0,6,6	-	-	-		
92	OHX	5	4228	-	0,6,6	-	-	-		
92	OHX	6	2302	92	0,6,6	-	-	-		
92	OHX	2	2115	-	0,6,6	-	-	-		
92	OHX	5	4438	-	0,6,6	-	-	-		
92	OHX	5	4498	-	0,6,6	-	-	-		
92	OHX	5	4299	36	0,6,6	-	-	-		
92	OHX	6	2252	-	0,6,6	-	-	-		
92	OHX	5	4468	-	0,6,6	-	-	-		
92	OHX	2	2251	92	0,6,6	-	-	-		
92	OHX	2	2070	-	0,6,6	-	-	-		
92	OHX	6	2248	-	0,6,6	-	-	-		
92	OHX	c5	202	-	0,6,6	-	-	-		
92	OHX	1	4477	-	0,6,6	-	-	-		
92	OHX	3	227	-	0,6,6	-	-	-		
92	OHX	1	4285	-	0,6,6	-	-	-		
92	OHX	1	4478	92	0,6,6	-	-	-		
92	OHX	1	4254	-	0,6,6	-	-	-		
92	OHX	2	2123	-	0,6,6	-	-	-		
92	OHX	6	2283	92	0,6,6	-	-	-		
92	OHX	5	4462	92	0,6,6	-	-	-		
92	OHX	5	4300	-	0,6,6	-	-	-		
92	OHX	1	4295	92	0,6,6	-	-	-		
92	OHX	1	4359	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4265	-	0,6,6	-	-	-		
92	OHX	5	4212	-	0,6,6	-	-	-		
92	OHX	M5	309	-	0,6,6	-	-	-		
92	OHX	6	2151	-	0,6,6	-	-	-		
92	OHX	5	4424	-	0,6,6	-	-	-		
92	OHX	5	4252	92	0,6,6	-	-	-		
92	OHX	5	4364	-	0,6,6	-	-	-		
92	OHX	1	4205	-	0,6,6	-	-	-		
92	OHX	5	4440	92	0,6,6	-	-	-		
92	OHX	1	4223	-	0,6,6	-	-	-		
92	OHX	1	4489	92	0,6,6	-	-	-		
92	OHX	5	4404	92	0,6,6	-	-	-		
92	OHX	1	4105	92	0,6,6	-	-	-		
92	OHX	2	2190	92	0,6,6	-	-	-		
92	OHX	1	4408	92	0,6,6	-	-	-		
92	OHX	2	2226	-	0,6,6	-	-	-		
92	OHX	5	4455	-	0,6,6	-	-	-		
92	OHX	N9	102	-	0,6,6	-	-	-		
92	OHX	5	4559	92	0,6,6	-	-	-		
92	OHX	5	4290	-	0,6,6	-	-	-		
92	OHX	a	101	92,90	0,6,6	-	-	-		
92	OHX	5	4550	-	0,6,6	-	-	-		
92	OHX	6	2177	-	0,6,6	-	-	-		
92	OHX	3	228	92	0,6,6	-	-	-		
92	OHX	5	4496	36	0,6,6	-	-	-		
92	OHX	2	2163	-	0,6,6	-	-	-		
92	OHX	5	4175	-	0,6,6	-	-	-		
92	OHX	4	248	-	0,6,6	-	-	-		
92	OHX	5	4170	-	0,6,6	-	-	-		
92	OHX	2	2197	1	0,6,6	-	-	-		
92	OHX	2	2196	1	0,6,6	-	-	-		
92	OHX	2	2146	-	0,6,6	-	-	-		
92	OHX	1	4140	-	0,6,6	-	-	-		
92	OHX	A	101	90	0,6,6	-	-	-		
92	OHX	1	4222	-	0,6,6	-	-	-		
92	OHX	5	4186	-	0,6,6	-	-	-		
92	OHX	1	4282	-	0,6,6	-	-	-		
92	OHX	1	4428	92	0,6,6	-	-	-		
92	OHX	1	4194	92	0,6,6	-	-	-		
92	OHX	1	4380	36	0,6,6	-	-	-		
92	OHX	2	2244	1,92	0,6,6	-	-	-		
92	OHX	1	4405	92	0,6,6	-	-	-		
92	OHX	1	4337	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4522	92	0,6,6	-	-	-		
92	OHX	5	4296	-	0,6,6	-	-	-		
92	OHX	1	4108	-	0,6,6	-	-	-		
92	OHX	5	4561	92	0,6,6	-	-	-		
92	OHX	6	2222	-	0,6,6	-	-	-		
92	OHX	q2	203	-	0,6,6	-	-	-		
92	OHX	6	2155	92	0,6,6	-	-	-		
92	OHX	1	4341	-	0,6,6	-	-	-		
92	OHX	5	4536	-	0,6,6	-	-	-		
92	OHX	1	4435	92	0,6,6	-	-	-		
92	OHX	6	2297	92	0,6,6	-	-	-		
92	OHX	1	4475	92	0,6,6	-	-	-		
92	OHX	5	4210	-	0,6,6	-	-	-		
92	OHX	5	4159	-	0,6,6	-	-	-		
92	OHX	2	2108	92	0,6,6	-	-	-		
92	OHX	2	2184	-	0,6,6	-	-	-		
92	OHX	2	2161	1	0,6,6	-	-	-		
92	OHX	5	4507	-	0,6,6	-	-	-		
92	OHX	5	4191	-	0,6,6	-	-	-		
92	OHX	1	4449	-	0,6,6	-	-	-		
92	OHX	5	4233	92	0,6,6	-	-	-		
92	OHX	5	4293	92	0,6,6	-	-	-		
92	OHX	2	2138	92	0,6,6	-	-	-		
92	OHX	1	4410	-	0,6,6	-	-	-		
92	OHX	5	4538	-	0,6,6	-	-	-		
92	OHX	5	4267	-	0,6,6	-	-	-		
92	OHX	5	4546	-	0,6,6	-	-	-		
92	OHX	5	4566	92	0,6,6	-	-	-		
92	OHX	5	4382	-	0,6,6	-	-	-		
92	OHX	5	4529	-	0,6,6	-	-	-		
92	OHX	5	4273	-	0,6,6	-	-	-		
92	OHX	5	4355	-	0,6,6	-	-	-		
92	OHX	6	2324	92	0,6,6	-	-	-		
92	OHX	5	4246	-	0,6,6	-	-	-		
92	OHX	5	4344	92	0,6,6	-	-	-		
92	OHX	5	4479	-	0,6,6	-	-	-		
92	OHX	1	4199	-	0,6,6	-	-	-		
92	OHX	2	2215	-	0,6,6	-	-	-		
92	OHX	5	4500	-	0,6,6	-	-	-		
92	OHX	2	2148	92	0,6,6	-	-	-		
92	OHX	2	2213	-	0,6,6	-	-	-		
92	OHX	2	2248	92	0,6,6	-	-	-		
92	OHX	6	2339	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	6	2158	-	0,6,6	-	-	-		
92	OHX	1	4196	92	0,6,6	-	-	-		
92	OHX	2	2183	1,92	0,6,6	-	-	-		
92	OHX	1	4201	-	0,6,6	-	-	-		
92	OHX	6	2333	92	0,6,6	-	-	-		
92	OHX	1	4117	-	0,6,6	-	-	-		
92	OHX	6	2240	-	0,6,6	-	-	-		
92	OHX	5	4295	92	0,6,6	-	-	-		
92	OHX	5	4179	-	0,6,6	-	-	-		
92	OHX	2	2195	92	0,6,6	-	-	-		
92	OHX	M9	204	-	0,6,6	-	-	-		
92	OHX	6	2180	92	0,6,6	-	-	-		
92	OHX	4	238	-	0,6,6	-	-	-		
92	OHX	3	223	92	0,6,6	-	-	-		
92	OHX	2	2167	-	0,6,6	-	-	-		
92	OHX	1	4391	-	0,6,6	-	-	-		
92	OHX	5	4423	36,92	0,6,6	-	-	-		
92	OHX	5	4539	92	0,6,6	-	-	-		
92	OHX	6	2223	92	0,6,6	-	-	-		
92	OHX	1	4253	92	0,6,6	-	-	-		
92	OHX	6	2157	-	0,6,6	-	-	-		
92	OHX	c5	201	-	0,6,6	-	-	-		
92	OHX	1	4492	92	0,6,6	-	-	-		
92	OHX	6	2153	-	0,6,6	-	-	-		
92	OHX	5	4245	-	0,6,6	-	-	-		
92	OHX	2	2078	-	0,6,6	-	-	-		
92	OHX	5	4279	92	0,6,6	-	-	-		
92	OHX	5	4436	-	0,6,6	-	-	-		
92	OHX	4	236	-	0,6,6	-	-	-		
92	OHX	5	4450	36	0,6,6	-	-	-		
92	OHX	5	4371	-	0,6,6	-	-	-		
92	OHX	5	4251	-	0,6,6	-	-	-		
92	OHX	1	4242	-	0,6,6	-	-	-		
92	OHX	6	2210	-	0,6,6	-	-	-		
92	OHX	2	2238	92	0,6,6	-	-	-		
92	OHX	2	2114	-	0,6,6	-	-	-		
92	OHX	2	2069	-	0,6,6	-	-	-		
92	OHX	5	4214	-	0,6,6	-	-	-		
92	OHX	6	2226	-	0,6,6	-	-	-		
92	OHX	2	2121	-	0,6,6	-	-	-		
92	OHX	5	4192	-	0,6,6	-	-	-		
92	OHX	5	4336	-	0,6,6	-	-	-		
92	OHX	6	2313	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4235	-	0,6,6	-	-	-		
92	OHX	2	2182	-	0,6,6	-	-	-		
92	OHX	6	2178	-	0,6,6	-	-	-		
92	OHX	6	2263	-	0,6,6	-	-	-		
92	OHX	3	222	-	0,6,6	-	-	-		
92	OHX	6	2197	1	0,6,6	-	-	-		
92	OHX	5	4524	36	0,6,6	-	-	-		
92	OHX	6	2212	-	0,6,6	-	-	-		
92	OHX	5	4229	92	0,6,6	-	-	-		
92	OHX	5	4401	92	0,6,6	-	-	-		
92	OHX	6	2246	-	0,6,6	-	-	-		
92	OHX	6	2312	92	0,6,6	-	-	-		
92	OHX	1	4363	-	0,6,6	-	-	-		
92	OHX	6	2267	-	0,6,6	-	-	-		
92	OHX	6	2167	-	0,6,6	-	-	-		
92	OHX	2	2198	92	0,6,6	-	-	-		
92	OHX	5	4480	92	0,6,6	-	-	-		
92	OHX	5	4552	92	0,6,6	-	-	-		
92	OHX	5	4353	-	0,6,6	-	-	-		
92	OHX	1	4224	-	0,6,6	-	-	-		
92	OHX	1	4317	-	0,6,6	-	-	-		
92	OHX	5	4317	-	0,6,6	-	-	-		
92	OHX	C8	202	92	0,6,6	-	-	-		
92	OHX	6	2290	1	0,6,6	-	-	-		
92	OHX	1	4267	-	0,6,6	-	-	-		
92	OHX	5	4408	92	0,6,6	-	-	-		
92	OHX	1	4112	-	0,6,6	-	-	-		
92	OHX	6	2293	-	0,6,6	-	-	-		
92	OHX	3	225	92	0,6,6	-	-	-		
92	OHX	6	2238	-	0,6,6	-	-	-		
92	OHX	1	4211	92	0,6,6	-	-	-		
92	OHX	1	4479	92	0,6,6	-	-	-		
92	OHX	1	4413	92	0,6,6	-	-	-		
92	OHX	C3	201	-	0,6,6	-	-	-		
92	OHX	5	4218	-	0,6,6	-	-	-		
92	OHX	6	2249	92	0,6,6	-	-	-		
92	OHX	6	2171	-	0,6,6	-	-	-		
92	OHX	6	2318	92	0,6,6	-	-	-		
92	OHX	5	4560	92	0,6,6	-	-	-		
92	OHX	m7	208	-	0,6,6	-	-	-		
92	OHX	6	2262	92	0,6,6	-	-	-		
92	OHX	1	4407	92	0,6,6	-	-	-		
92	OHX	1	4234	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4350	-	0,6,6	-	-	-		
92	OHX	1	4322	-	0,6,6	-	-	-		
92	OHX	m5	304	-	0,6,6	-	-	-		
92	OHX	5	4366	-	0,6,6	-	-	-		
92	OHX	8	227	-	0,6,6	-	-	-		
92	OHX	5	4240	36	0,6,6	-	-	-		
92	OHX	2	2158	92	0,6,6	-	-	-		
92	OHX	2	2151	-	0,6,6	-	-	-		
92	OHX	5	4347	36	0,6,6	-	-	-		
92	OHX	1	4375	-	0,6,6	-	-	-		
92	OHX	5	4370	-	0,6,6	-	-	-		
92	OHX	D9	104	92	0,6,6	-	-	-		
92	OHX	1	4220	-	0,6,6	-	-	-		
92	OHX	5	4428	-	0,6,6	-	-	-		
92	OHX	4	234	-	0,6,6	-	-	-		
92	OHX	5	4563	-	0,6,6	-	-	-		
92	OHX	6	2323	92	0,6,6	-	-	-		
92	OHX	M0	307	92	0,6,6	-	-	-		
92	OHX	6	2179	-	0,6,6	-	-	-		
92	OHX	2	2144	92	0,6,6	-	-	-		
92	OHX	5	4236	-	0,6,6	-	-	-		
92	OHX	5	4283	-	0,6,6	-	-	-		
92	OHX	1	4270	-	0,6,6	-	-	-		
92	OHX	1	4421	92	0,6,6	-	-	-		
92	OHX	2	2223	-	0,6,6	-	-	-		
92	OHX	2	2098	-	0,6,6	-	-	-		
92	OHX	6	2337	1,92	0,6,6	-	-	-		
92	OHX	2	2155	-	0,6,6	-	-	-		
92	OHX	6	2149	92	0,6,6	-	-	-		
92	OHX	1	4287	92	0,6,6	-	-	-		
92	OHX	2	2256	92	0,6,6	-	-	-		
92	OHX	5	4543	92	0,6,6	-	-	-		
92	OHX	1	4329	-	0,6,6	-	-	-		
92	OHX	5	4426	-	0,6,6	-	-	-		
92	OHX	1	4470	-	0,6,6	-	-	-		
92	OHX	2	2210	1	0,6,6	-	-	-		
92	OHX	3	229	-	0,6,6	-	-	-		
92	OHX	1	4119	-	0,6,6	-	-	-		
92	OHX	1	4250	-	0,6,6	-	-	-		
92	OHX	6	2276	-	0,6,6	-	-	-		
92	OHX	5	4432	36,92	0,6,6	-	-	-		
92	OHX	1	4472	-	0,6,6	-	-	-		
92	OHX	5	4327	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4178	-	0,6,6	-	-	-		
92	OHX	5	4221	-	0,6,6	-	-	-		
92	OHX	5	4156	-	0,6,6	-	-	-		
92	OHX	5	4314	-	0,6,6	-	-	-		
92	OHX	6	2174	-	0,6,6	-	-	-		
92	OHX	5	4345	-	0,6,6	-	-	-		
92	OHX	5	4379	-	0,6,6	-	-	-		
92	OHX	1	4229	-	0,6,6	-	-	-		
92	OHX	5	4527	-	0,6,6	-	-	-		
92	OHX	5	4375	-	0,6,6	-	-	-		
92	OHX	5	4276	92	0,6,6	-	-	-		
92	OHX	2	2099	-	0,6,6	-	-	-		
92	OHX	5	4471	92	0,6,6	-	-	-		
92	OHX	2	2116	92	0,6,6	-	-	-		
92	OHX	2	2208	-	0,6,6	-	-	-		
92	OHX	5	4399	36	0,6,6	-	-	-		
92	OHX	5	4395	-	0,6,6	-	-	-		
92	OHX	1	4412	92	0,6,6	-	-	-		
92	OHX	5	4388	36	0,6,6	-	-	-		
92	OHX	1	4265	-	0,6,6	-	-	-		
92	OHX	2	2139	-	0,6,6	-	-	-		
92	OHX	2	2202	-	0,6,6	-	-	-		
92	OHX	1	4494	-	0,6,6	-	-	-		
92	OHX	1	4333	-	0,6,6	-	-	-		
92	OHX	1	4273	36	0,6,6	-	-	-		
92	OHX	2	2187	-	0,6,6	-	-	-		
92	OHX	1	4174	-	0,6,6	-	-	-		
92	OHX	6	2309	92	0,6,6	-	-	-		
92	OHX	6	2245	92	0,6,6	-	-	-		
92	OHX	5	4361	-	0,6,6	-	-	-		
92	OHX	5	4207	92	0,6,6	-	-	-		
92	OHX	6	2237	-	0,6,6	-	-	-		
92	OHX	5	4534	36	0,6,6	-	-	-		
92	OHX	6	2335	92	0,6,6	-	-	-		
92	OHX	5	4204	-	0,6,6	-	-	-		
92	OHX	O7	107	-	0,6,6	-	-	-		
92	OHX	2	2249	92	0,6,6	-	-	-		
92	OHX	1	4416	-	0,6,6	-	-	-		
92	OHX	c1	201	92	0,6,6	-	-	-		
92	OHX	5	4199	92	0,6,6	-	-	-		
92	OHX	1	4387	-	0,6,6	-	-	-		
92	OHX	2	2094	-	0,6,6	-	-	-		
92	OHX	6	2233	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4278	-	0,6,6	-	-	-		
92	OHX	2	2097	-	0,6,6	-	-	-		
92	OHX	2	2200	-	0,6,6	-	-	-		
92	OHX	2	2228	-	0,6,6	-	-	-		
92	OHX	6	2266	1	0,6,6	-	-	-		
92	OHX	5	4294	-	0,6,6	-	-	-		
92	OHX	1	4244	-	0,6,6	-	-	-		
92	OHX	2	2179	-	0,6,6	-	-	-		
92	OHX	8	226	92	0,6,6	-	-	-		
92	OHX	5	4282	-	0,6,6	-	-	-		
92	OHX	1	4104	-	0,6,6	-	-	-		
92	OHX	5	4222	92	0,6,6	-	-	-		
92	OHX	5	4256	92	0,6,6	-	-	-		
92	OHX	5	4213	-	0,6,6	-	-	-		
92	OHX	6	2144	-	0,6,6	-	-	-		
92	OHX	2	2165	-	0,6,6	-	-	-		
92	OHX	6	2322	-	0,6,6	-	-	-		
92	OHX	5	4257	36,92	0,6,6	-	-	-		
92	OHX	1	4364	-	0,6,6	-	-	-		
92	OHX	1	4430	-	0,6,6	-	-	-		
92	OHX	5	4397	-	0,6,6	-	-	-		
92	OHX	6	2310	92	0,6,6	-	-	-		
92	OHX	1	4452	92	0,6,6	-	-	-		
92	OHX	1	4483	-	0,6,6	-	-	-		
92	OHX	8	240	-	0,6,6	-	-	-		
92	OHX	3	230	92	0,6,6	-	-	-		
92	OHX	5	4517	92	0,6,6	-	-	-		
92	OHX	6	2187	-	0,6,6	-	-	-		
92	OHX	1	4288	-	0,6,6	-	-	-		
92	OHX	5	4354	-	0,6,6	-	-	-		
92	OHX	2	2176	92	0,6,6	-	-	-		
92	OHX	1	4455	-	0,6,6	-	-	-		
92	OHX	5	4519	-	0,6,6	-	-	-		
92	OHX	2	2230	-	0,6,6	-	-	-		
92	OHX	1	4113	-	0,6,6	-	-	-		
92	OHX	1	4451	-	0,6,6	-	-	-		
92	OHX	6	2194	92	0,6,6	-	-	-		
92	OHX	5	4190	-	0,6,6	-	-	-		
92	OHX	5	4501	-	0,6,6	-	-	-		
92	OHX	2	2111	92	0,6,6	-	-	-		
92	OHX	1	4345	-	0,6,6	-	-	-		
92	OHX	5	4402	-	0,6,6	-	-	-		
92	OHX	2	2242	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4260	-	0,6,6	-	-	-		
92	OHX	1	4326	-	0,6,6	-	-	-		
92	OHX	5	4531	-	0,6,6	-	-	-		
92	OHX	1	4418	-	0,6,6	-	-	-		
92	OHX	5	4321	-	0,6,6	-	-	-		
92	OHX	1	4266	92	0,6,6	-	-	-		
92	OHX	1	4485	-	0,6,6	-	-	-		
92	OHX	2	2204	-	0,6,6	-	-	-		
92	OHX	6	2205	-	0,6,6	-	-	-		
92	OHX	5	4526	-	0,6,6	-	-	-		
92	OHX	4	239	-	0,6,6	-	-	-		
92	OHX	1	4493	-	0,6,6	-	-	-		
92	OHX	1	4172	92	0,6,6	-	-	-		
92	OHX	5	4157	-	0,6,6	-	-	-		
92	OHX	5	4281	-	0,6,6	-	-	-		
92	OHX	1	4238	92	0,6,6	-	-	-		
92	OHX	1	4335	-	0,6,6	-	-	-		
92	OHX	L5	301	-	0,6,6	-	-	-		
92	OHX	5	4331	-	0,6,6	-	-	-		
92	OHX	1	4313	-	0,6,6	-	-	-		
92	OHX	5	4255	-	0,6,6	-	-	-		
92	OHX	8	228	-	0,6,6	-	-	-		
92	OHX	5	4187	92	0,6,6	-	-	-		
92	OHX	1	4228	92	0,6,6	-	-	-		
92	OHX	1	4128	-	0,6,6	-	-	-		
92	OHX	L3	408	-	0,6,6	-	-	-		
92	OHX	n1	204	-	0,6,6	-	-	-		
92	OHX	5	4330	-	0,6,6	-	-	-		
92	OHX	1	4438	-	0,6,6	-	-	-		
92	OHX	1	4269	-	0,6,6	-	-	-		
92	OHX	5	4533	-	0,6,6	-	-	-		
92	OHX	5	4541	-	0,6,6	-	-	-		
92	OHX	1	4264	-	0,6,6	-	-	-		
92	OHX	1	4396	-	0,6,6	-	-	-		
92	OHX	5	4250	-	0,6,6	-	-	-		
92	OHX	5	4481	92	0,6,6	-	-	-		
92	OHX	5	4562	-	0,6,6	-	-	-		
92	OHX	2	2193	-	0,6,6	-	-	-		
92	OHX	1	4464	-	0,6,6	-	-	-		
92	OHX	5	4568	92	0,6,6	-	-	-		
92	OHX	2	2246	-	0,6,6	-	-	-		
92	OHX	5	4457	92	0,6,6	-	-	-		
92	OHX	5	4275	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4147	92	0,6,6	-	-	-		
92	OHX	7	233	-	0,6,6	-	-	-		
92	OHX	6	2330	-	0,6,6	-	-	-		
92	OHX	1	4462	-	0,6,6	-	-	-		
92	OHX	5	4537	-	0,6,6	-	-	-		
92	OHX	1	4300	-	0,6,6	-	-	-		
92	OHX	1	4209	-	0,6,6	-	-	-		
92	OHX	1	4159	-	0,6,6	-	-	-		
92	OHX	5	4437	92	0,6,6	-	-	-		
92	OHX	1	4256	-	0,6,6	-	-	-		
92	OHX	1	4114	-	0,6,6	-	-	-		
92	OHX	2	2162	-	0,6,6	-	-	-		
92	OHX	2	2172	-	0,6,6	-	-	-		
92	OHX	8	221	-	0,6,6	-	-	-		
92	OHX	1	4372	92	0,6,6	-	-	-		
92	OHX	6	2296	-	0,6,6	-	-	-		
92	OHX	5	4516	-	0,6,6	-	-	-		
92	OHX	6	2271	-	0,6,6	-	-	-		
92	OHX	1	4124	92	0,6,6	-	-	-		
92	OHX	1	4390	92	0,6,6	-	-	-		
92	OHX	1	4308	-	0,6,6	-	-	-		
92	OHX	1	4208	-	0,6,6	-	-	-		
92	OHX	2	2211	-	0,6,6	-	-	-		
92	OHX	1	4425	-	0,6,6	-	-	-		
92	OHX	8	233	-	0,6,6	-	-	-		
92	OHX	1	4383	-	0,6,6	-	-	-		
92	OHX	2	2076	-	0,6,6	-	-	-		
92	OHX	1	4135	-	0,6,6	-	-	-		
92	OHX	7	230	-	0,6,6	-	-	-		
92	OHX	C8	203	36,92	0,6,6	-	-	-		
92	OHX	6	2230	-	0,6,6	-	-	-		
92	OHX	5	4497	-	0,6,6	-	-	-		
92	OHX	5	4367	-	0,6,6	-	-	-		
92	OHX	1	4206	92	0,6,6	-	-	-		
92	OHX	1	4447	-	0,6,6	-	-	-		
92	OHX	6	2291	1	0,6,6	-	-	-		
92	OHX	1	4486	-	0,6,6	-	-	-		
92	OHX	1	4186	92	0,6,6	-	-	-		
92	OHX	6	2329	92	0,6,6	-	-	-		
92	OHX	1	4468	92	0,6,6	-	-	-		
92	OHX	1	4261	-	0,6,6	-	-	-		
92	OHX	m0	303	92	0,6,6	-	-	-		
92	OHX	1	4423	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	6	2268	-	0,6,6	-	-	-		
92	OHX	6	2242	92	0,6,6	-	-	-		
92	OHX	6	2289	-	0,6,6	-	-	-		
92	OHX	5	4239	-	0,6,6	-	-	-		
92	OHX	2	2082	-	0,6,6	-	-	-		
92	OHX	5	4459	92	0,6,6	-	-	-		
92	OHX	6	2198	-	0,6,6	-	-	-		
92	OHX	1	4331	-	0,6,6	-	-	-		
92	OHX	1	4210	92	0,6,6	-	-	-		
92	OHX	6	2216	92	0,6,6	-	-	-		
92	OHX	1	4212	-	0,6,6	-	-	-		
92	OHX	6	2162	92	0,6,6	-	-	-		
92	OHX	1	4191	-	0,6,6	-	-	-		
92	OHX	6	2173	92	0,6,6	-	-	-		
92	OHX	5	4394	92	0,6,6	-	-	-		
92	OHX	L3	407	-	0,6,6	-	-	-		
92	OHX	5	4410	92	0,6,6	-	-	-		
92	OHX	1	4404	-	0,6,6	-	-	-		
92	OHX	6	2265	-	0,6,6	-	-	-		
92	OHX	5	4512	-	0,6,6	-	-	-		
92	OHX	1	4193	-	0,6,6	-	-	-		
92	OHX	2	2096	-	0,6,6	-	-	-		
92	OHX	1	4382	-	0,6,6	-	-	-		
92	OHX	6	2175	-	0,6,6	-	-	-		
92	OHX	1	4103	36	0,6,6	-	-	-		
92	OHX	5	4447	-	0,6,6	-	-	-		
92	OHX	M0	308	92	0,6,6	-	-	-		
92	OHX	2	2073	-	0,6,6	-	-	-		
92	OHX	2	2136	-	0,6,6	-	-	-		
92	OHX	6	2225	-	0,6,6	-	-	-		
92	OHX	1	4290	-	0,6,6	-	-	-		
92	OHX	1	4357	-	0,6,6	-	-	-		
92	OHX	6	2277	-	0,6,6	-	-	-		
92	OHX	s4	302	-	0,6,6	-	-	-		
92	OHX	5	4188	-	0,6,6	-	-	-		
92	OHX	5	4544	-	0,6,6	-	-	-		
92	OHX	1	4170	92	0,6,6	-	-	-		
92	OHX	6	2325	92	0,6,6	-	-	-		
92	OHX	5	4415	-	0,6,6	-	-	-		
92	OHX	5	4184	-	0,6,6	-	-	-		
92	OHX	5	4247	-	0,6,6	-	-	-		
92	OHX	2	2153	-	0,6,6	-	-	-		
92	OHX	1	4275	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	6	2148	-	0,6,6	-	-	-		
92	OHX	5	4454	-	0,6,6	-	-	-		
92	OHX	1	4168	92	0,6,6	-	-	-		
92	OHX	2	2255	92	0,6,6	-	-	-		
92	OHX	6	2186	-	0,6,6	-	-	-		
92	OHX	6	2251	-	0,6,6	-	-	-		
92	OHX	5	4556	36,92	0,6,6	-	-	-		
92	OHX	6	2336	-	0,6,6	-	-	-		
92	OHX	5	4241	-	0,6,6	-	-	-		
92	OHX	5	4172	-	0,6,6	-	-	-		
92	OHX	5	4409	36	0,6,6	-	-	-		
92	OHX	6	2287	-	0,6,6	-	-	-		
92	OHX	1	4144	-	0,6,6	-	-	-		
92	OHX	8	225	-	0,6,6	-	-	-		
92	OHX	o9	102	-	0,6,6	-	-	-		
92	OHX	6	2332	92	0,6,6	-	-	-		
92	OHX	5	4452	-	0,6,6	-	-	-		
92	OHX	5	4475	-	0,6,6	-	-	-		
92	OHX	m0	304	92	0,6,6	-	-	-		
92	OHX	5	4217	-	0,6,6	-	-	-		
92	OHX	5	4297	-	0,6,6	-	-	-		
92	OHX	1	4450	-	0,6,6	-	-	-		
92	OHX	6	2207	92	0,6,6	-	-	-		
92	OHX	5	4398	-	0,6,6	-	-	-		
92	OHX	5	4351	-	0,6,6	-	-	-		
92	OHX	2	2147	92	0,6,6	-	-	-		
92	OHX	1	4110	-	0,6,6	-	-	-		
92	OHX	1	4146	-	0,6,6	-	-	-		
92	OHX	4	245	-	0,6,6	-	-	-		
92	OHX	5	4324	92	0,6,6	-	-	-		
92	OHX	2	2212	-	0,6,6	-	-	-		
92	OHX	5	4332	-	0,6,6	-	-	-		
92	OHX	1	4192	-	0,6,6	-	-	-		
92	OHX	2	2209	-	0,6,6	-	-	-		
92	OHX	6	2305	-	0,6,6	-	-	-		
92	OHX	6	2227	-	0,6,6	-	-	-		
92	OHX	6	2141	-	0,6,6	-	-	-		
92	OHX	5	4310	-	0,6,6	-	-	-		
92	OHX	5	4292	92	0,6,6	-	-	-		
92	OHX	1	4154	-	0,6,6	-	-	-		
92	OHX	8	224	-	0,6,6	-	-	-		
92	OHX	1	4239	92	0,6,6	-	-	-		
92	OHX	2	2130	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	2	2181	1	0,6,6	-	-	-		
92	OHX	5	4369	92	0,6,6	-	-	-		
92	OHX	1	4161	92	0,6,6	-	-	-		
92	OHX	5	4338	92	0,6,6	-	-	-		
92	OHX	5	4525	-	0,6,6	-	-	-		
92	OHX	1	4381	36,92	0,6,6	-	-	-		
92	OHX	1	4271	-	0,6,6	-	-	-		
92	OHX	5	4230	-	0,6,6	-	-	-		
92	OHX	6	2170	1	0,6,6	-	-	-		
92	OHX	2	2201	-	0,6,6	-	-	-		
92	OHX	6	2244	-	0,6,6	-	-	-		
92	OHX	1	4465	-	0,6,6	-	-	-		
92	OHX	2	2173	-	0,6,6	-	-	-		
92	OHX	5	4503	92	0,6,6	-	-	-		
92	OHX	5	4167	-	0,6,6	-	-	-		
92	OHX	5	4269	92	0,6,6	-	-	-		
92	OHX	5	4564	92	0,6,6	-	-	-		
92	OHX	1	4120	-	0,6,6	-	-	-		
92	OHX	1	4371	-	0,6,6	-	-	-		
92	OHX	1	4251	92	0,6,6	-	-	-		
92	OHX	6	2188	-	0,6,6	-	-	-		
92	OHX	6	2160	-	0,6,6	-	-	-		
92	OHX	5	4158	-	0,6,6	-	-	-		
92	OHX	6	2168	-	0,6,6	-	-	-		
92	OHX	2	2217	-	0,6,6	-	-	-		
92	OHX	1	4111	-	0,6,6	-	-	-		
92	OHX	1	4247	-	0,6,6	-	-	-		
92	OHX	2	2081	-	0,6,6	-	-	-		
92	OHX	5	4270	-	0,6,6	-	-	-		
92	OHX	5	4565	92	0,6,6	-	-	-		
92	OHX	1	4188	-	0,6,6	-	-	-		
92	OHX	1	4336	-	0,6,6	-	-	-		
92	OHX	5	4551	92	0,6,6	-	-	-		
92	OHX	5	4309	-	0,6,6	-	-	-		
92	OHX	m4	202	-	0,6,6	-	-	-		
92	OHX	5	4198	-	0,6,6	-	-	-		
92	OHX	6	2218	-	0,6,6	-	-	-		
92	OHX	5	4307	-	0,6,6	-	-	-		
92	OHX	1	4414	92	0,6,6	-	-	-		
92	OHX	5	4226	-	0,6,6	-	-	-		
92	OHX	6	2281	-	0,6,6	-	-	-		
92	OHX	6	2159	92	0,6,6	-	-	-		
92	OHX	6	2308	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	6	2169	-	0,6,6	-	-	-		
92	OHX	6	2328	-	0,6,6	-	-	-		
92	OHX	3	231	-	0,6,6	-	-	-		
92	OHX	1	4200	92	0,6,6	-	-	-		
92	OHX	1	4351	-	0,6,6	-	-	-		
92	OHX	1	4180	92	0,6,6	-	-	-		
92	OHX	5	4208	-	0,6,6	-	-	-		
92	OHX	5	4378	-	0,6,6	-	-	-		
92	OHX	5	4470	-	0,6,6	-	-	-		
92	OHX	1	4126	-	0,6,6	-	-	-		
92	OHX	2	2232	92	0,6,6	-	-	-		
92	OHX	5	4467	36	0,6,6	-	-	-		
92	OHX	6	2286	92	0,6,6	-	-	-		
92	OHX	1	4122	-	0,6,6	-	-	-		
92	OHX	7	238	92	0,6,6	-	-	-		
92	OHX	2	2227	92	0,6,6	-	-	-		
92	OHX	c3	201	-	0,6,6	-	-	-		
92	OHX	1	4153	92	0,6,6	-	-	-		
92	OHX	2	2175	-	0,6,6	-	-	-		
92	OHX	5	4178	-	0,6,6	-	-	-		
92	OHX	1	4156	92	0,6,6	-	-	-		
92	OHX	2	2191	-	0,6,6	-	-	-		
92	OHX	2	2171	1	0,6,6	-	-	-		
92	OHX	2	2240	92	0,6,6	-	-	-		
92	OHX	5	4254	36	0,6,6	-	-	-		
92	OHX	5	4183	-	0,6,6	-	-	-		
92	OHX	1	4406	92	0,6,6	-	-	-		
92	OHX	6	2200	-	0,6,6	-	-	-		
92	OHX	2	2084	-	0,6,6	-	-	-		
92	OHX	5	4377	-	0,6,6	-	-	-		
92	OHX	2	2174	-	0,6,6	-	-	-		
92	OHX	m0	305	92	0,6,6	-	-	-		
92	OHX	1	4379	92	0,6,6	-	-	-		
92	OHX	5	4262	-	0,6,6	-	-	-		
92	OHX	1	4332	-	0,6,6	-	-	-		
92	OHX	2	2120	1	0,6,6	-	-	-		
92	OHX	5	4223	-	0,6,6	-	-	-		
92	OHX	6	2303	-	0,6,6	-	-	-		
92	OHX	2	2170	-	0,6,6	-	-	-		
92	OHX	2	2236	92	0,6,6	-	-	-		
92	OHX	1	4399	92	0,6,6	-	-	-		
92	OHX	8	236	-	0,6,6	-	-	-		
92	OHX	1	4395	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4291	92	0,6,6	-	-	-		
92	OHX	1	4202	36	0,6,6	-	-	-		
92	OHX	1	4293	-	0,6,6	-	-	-		
92	OHX	6	2326	1	0,6,6	-	-	-		
92	OHX	2	2125	-	0,6,6	-	-	-		
92	OHX	5	4326	-	0,6,6	-	-	-		
92	OHX	7	239	-	0,6,6	-	-	-		
92	OHX	d4	201	-	0,6,6	-	-	-		
92	OHX	1	4361	92	0,6,6	-	-	-		
92	OHX	5	4203	92	0,6,6	-	-	-		
92	OHX	1	4207	-	0,6,6	-	-	-		
92	OHX	6	2232	-	0,6,6	-	-	-		
92	OHX	6	2164	-	0,6,6	-	-	-		
92	OHX	1	4197	92	0,6,6	-	-	-		
92	OHX	5	4286	-	0,6,6	-	-	-		
92	OHX	7	235	-	0,6,6	-	-	-		
92	OHX	SR	401	-	0,6,6	-	-	-		
92	OHX	O7	109	92	0,6,6	-	-	-		
92	OHX	1	4158	-	0,6,6	-	-	-		
92	OHX	6	2247	-	0,6,6	-	-	-		
92	OHX	6	2211	-	0,6,6	-	-	-		
92	OHX	6	2256	1	0,6,6	-	-	-		
92	OHX	6	2142	-	0,6,6	-	-	-		
92	OHX	5	4173	-	0,6,6	-	-	-		
92	OHX	m0	302	92	0,6,6	-	-	-		
92	OHX	1	4133	-	0,6,6	-	-	-		
92	OHX	N1	202	-	0,6,6	-	-	-		
92	OHX	2	2189	1	0,6,6	-	-	-		
92	OHX	6	2224	-	0,6,6	-	-	-		
92	OHX	5	4380	-	0,6,6	-	-	-		
92	OHX	5	4460	-	0,6,6	-	-	-		
92	OHX	1	4294	-	0,6,6	-	-	-		
92	OHX	5	3401	1	0,6,6	-	-	-		
92	OHX	6	2191	92	0,6,6	-	-	-		
92	OHX	5	4365	-	0,6,6	-	-	-		
92	OHX	1	4500	36,92	0,6,6	-	-	-		
92	OHX	2	2090	92	0,6,6	-	-	-		
92	OHX	1	4314	-	0,6,6	-	-	-		
92	OHX	5	4491	-	0,6,6	-	-	-		
92	OHX	6	2146	-	0,6,6	-	-	-		
92	OHX	1	4312	-	0,6,6	-	-	-		
92	OHX	1	4306	92	0,6,6	-	-	-		
92	OHX	5	4350	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
92	OHX	5	4168	-	0,6,6	-	-	-		
92	OHX	5	4164	-	0,6,6	-	-	-		
92	OHX	2	2152	92	0,6,6	-	-	-		
92	OHX	1	4213	-	0,6,6	-	-	-		
92	OHX	1	4276	-	0,6,6	-	-	-		
92	OHX	1	4474	-	0,6,6	-	-	-		
92	OHX	1	4471	36	0,6,6	-	-	-		
92	OHX	2	2124	-	0,6,6	-	-	-		
92	OHX	2	2159	1,92	0,6,6	-	-	-		
92	OHX	6	2217	-	0,6,6	-	-	-		
92	OHX	1	4319	92	0,6,6	-	-	-		
92	OHX	1	4397	-	0,6,6	-	-	-		
92	OHX	1	4369	92	0,6,6	-	-	-		
92	OHX	6	2208	-	0,6,6	-	-	-		
92	OHX	1	4338	92	0,6,6	-	-	-		
92	OHX	6	2165	-	0,6,6	-	-	-		
92	OHX	5	4518	-	0,6,6	-	-	-		
92	OHX	5	4473	-	0,6,6	-	-	-		
92	OHX	5	4374	-	0,6,6	-	-	-		
92	OHX	1	4324	-	0,6,6	-	-	-		
92	OHX	5	4303	-	0,6,6	-	-	-		
92	OHX	3	221	-	0,6,6	-	-	-		
92	OHX	2	2225	-	0,6,6	-	-	-		
92	OHX	1	4481	92	0,6,6	-	-	-		
92	OHX	1	4343	-	0,6,6	-	-	-		
92	OHX	5	4431	-	0,6,6	-	-	-		
92	OHX	1	4461	-	0,6,6	-	-	-		
92	OHX	2	2104	-	0,6,6	-	-	-		
92	OHX	5	4542	-	0,6,6	-	-	-		
92	OHX	1	4420	-	0,6,6	-	-	-		
92	OHX	3	219	-	0,6,6	-	-	-		
92	OHX	3	220	-	0,6,6	-	-	-		
92	OHX	1	4175	-	0,6,6	-	-	-		
92	OHX	2	2235	92	0,6,6	-	-	-		
92	OHX	6	2176	-	0,6,6	-	-	-		
92	OHX	6	2161	92	0,6,6	-	-	-		
92	OHX	5	4488	-	0,6,6	-	-	-		
92	OHX	5	4196	-	0,6,6	-	-	-		
92	OHX	O1	202	92	0,6,6	-	-	-		
92	OHX	1	4320	36	0,6,6	-	-	-		
92	OHX	1	4235	-	0,6,6	-	-	-		
92	OHX	5	4260	-	0,6,6	-	-	-		
92	OHX	1	4376	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	2	2101	92	0,6,6	-	-	-		
92	OHX	5	4325	-	0,6,6	-	-	-		
92	OHX	1	4278	36	0,6,6	-	-	-		
92	OHX	2	2186	92	0,6,6	-	-	-		
92	OHX	5	4248	-	0,6,6	-	-	-		
92	OHX	2	2168	-	0,6,6	-	-	-		
92	OHX	1	4099	-	0,6,6	-	-	-		
92	OHX	5	4352	92	0,6,6	-	-	-		
92	OHX	2	2100	-	0,6,6	-	-	-		
92	OHX	1	4262	92	0,6,6	-	-	-		
92	OHX	m1	203	-	0,6,6	-	-	-		
92	OHX	2	2091	1	0,6,6	-	-	-		
92	OHX	6	2152	-	0,6,6	-	-	-		
92	OHX	8	239	92	0,6,6	-	-	-		
92	OHX	5	4219	92	0,6,6	-	-	-		
92	OHX	n9	103	-	0,6,6	-	-	-		
92	OHX	6	2285	-	0,6,6	-	-	-		
92	OHX	d9	104	92	0,6,6	-	-	-		
92	OHX	2	2145	92	0,6,6	-	-	-		
92	OHX	1	4230	-	0,6,6	-	-	-		
92	OHX	M0	305	92	0,6,6	-	-	-		
92	OHX	1	4257	-	0,6,6	-	-	-		
92	OHX	6	2298	1,92	0,6,6	-	-	-		
92	OHX	5	4313	-	0,6,6	-	-	-		
92	OHX	8	235	-	0,6,6	-	-	-		
92	OHX	1	4255	-	0,6,6	-	-	-		
92	OHX	1	4187	92	0,6,6	-	-	-		
92	OHX	1	4218	-	0,6,6	-	-	-		
92	OHX	1	4263	-	0,6,6	-	-	-		
92	OHX	5	4430	-	0,6,6	-	-	-		
92	OHX	1	4286	92	0,6,6	-	-	-		
92	OHX	2	2164	-	0,6,6	-	-	-		
92	OHX	5	4261	92	0,6,6	-	-	-		
92	OHX	6	2195	-	0,6,6	-	-	-		
92	OHX	2	2089	92	0,6,6	-	-	-		
92	OHX	1	4173	-	0,6,6	-	-	-		
92	OHX	1	4354	-	0,6,6	-	-	-		
92	OHX	5	4396	-	0,6,6	-	-	-		
92	OHX	7	229	-	0,6,6	-	-	-		
92	OHX	7	231	92	0,6,6	-	-	-		
92	OHX	1	4249	-	0,6,6	-	-	-		
92	OHX	2	2234	-	0,6,6	-	-	-		
92	OHX	1	4501	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4162	-	0,6,6	-	-	-		
92	OHX	1	4457	92	0,6,6	-	-	-		
92	OHX	6	2189	-	0,6,6	-	-	-		
92	OHX	5	4400	92	0,6,6	-	-	-		
92	OHX	L3	409	-	0,6,6	-	-	-		
92	OHX	5	4298	-	0,6,6	-	-	-		
92	OHX	5	4302	-	0,6,6	-	-	-		
92	OHX	2	2126	-	0,6,6	-	-	-		
92	OHX	2	2219	-	0,6,6	-	-	-		
92	OHX	5	4209	92	0,6,6	-	-	-		
92	OHX	2	2254	92	0,6,6	-	-	-		
92	OHX	5	4385	92	0,6,6	-	-	-		
92	OHX	5	4171	-	0,6,6	-	-	-		
92	OHX	1	4437	92	0,6,6	-	-	-		
92	OHX	5	4362	-	0,6,6	-	-	-		
92	OHX	2	2102	-	0,6,6	-	-	-		
92	OHX	5	4504	-	0,6,6	-	-	-		
92	OHX	1	4141	-	0,6,6	-	-	-		
92	OHX	5	4224	-	0,6,6	-	-	-		
92	OHX	1	4281	92	0,6,6	-	-	-		
92	OHX	6	2241	-	0,6,6	-	-	-		
92	OHX	5	4165	-	0,6,6	-	-	-		
92	OHX	6	2320	-	0,6,6	-	-	-		
92	OHX	6	2192	-	0,6,6	-	-	-		
92	OHX	5	4521	36	0,6,6	-	-	-		
92	OHX	1	4358	-	0,6,6	-	-	-		
92	OHX	6	2295	-	0,6,6	-	-	-		
92	OHX	6	2321	-	0,6,6	-	-	-		
92	OHX	6	2172	-	0,6,6	-	-	-		
92	OHX	2	2143	92	0,6,6	-	-	-		
92	OHX	1	4272	92	0,6,6	-	-	-		
92	OHX	1	4330	92	0,6,6	-	-	-		
92	OHX	2	2106	-	0,6,6	-	-	-		
92	OHX	2	2110	-	0,6,6	-	-	-		
92	OHX	1	4258	-	0,6,6	-	-	-		
92	OHX	5	4493	-	0,6,6	-	-	-		
92	OHX	1	4367	-	0,6,6	-	-	-		
92	OHX	5	4206	92	0,6,6	-	-	-		
92	OHX	M5	310	-	0,6,6	-	-	-		
92	OHX	1	4469	92	0,6,6	-	-	-		
92	OHX	5	4422	92	0,6,6	-	-	-		
92	OHX	5	4528	-	0,6,6	-	-	-		
92	OHX	1	4432	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	5	4558	92	0,6,6	-	-	-		
92	OHX	1	4327	-	0,6,6	-	-	-		
92	OHX	1	4134	92	0,6,6	-	-	-		
92	OHX	5	4535	-	0,6,6	-	-	-		
92	OHX	6	2234	-	0,6,6	-	-	-		
92	OHX	5	4513	-	0,6,6	-	-	-		
92	OHX	2	2216	92	0,6,6	-	-	-		
92	OHX	2	2218	1	0,6,6	-	-	-		
92	OHX	5	4373	92	0,6,6	-	-	-		
92	OHX	5	4277	-	0,6,6	-	-	-		
92	OHX	S2	303	92	0,6,6	-	-	-		
92	OHX	2	2132	-	0,6,6	-	-	-		
92	OHX	5	4389	-	0,6,6	-	-	-		
92	OHX	5	4368	-	0,6,6	-	-	-		
92	OHX	5	4573	92	0,6,6	-	-	-		
92	OHX	1	4394	-	0,6,6	-	-	-		
92	OHX	1	4150	-	0,6,6	-	-	-		
92	OHX	5	4169	-	0,6,6	-	-	-		
92	OHX	n3	204	-	0,6,6	-	-	-		
92	OHX	5	4258	92	0,6,6	-	-	-		
92	OHX	5	4193	-	0,6,6	-	-	-		
92	OHX	6	2145	-	0,6,6	-	-	-		
92	OHX	1	4403	-	0,6,6	-	-	-		
92	OHX	2	2140	1	0,6,6	-	-	-		
92	OHX	1	4487	92	0,6,6	-	-	-		
92	OHX	5	4308	-	0,6,6	-	-	-		
92	OHX	5	4284	-	0,6,6	-	-	-		
92	OHX	5	4163	-	0,6,6	-	-	-		
92	OHX	6	2314	-	0,6,6	-	-	-		
92	OHX	C5	202	17	0,6,6	-	-	-		
92	OHX	1	4148	92	0,6,6	-	-	-		
92	OHX	5	4381	92	0,6,6	-	-	-		
92	OHX	5	4442	-	0,6,6	-	-	-		
92	OHX	1	4377	-	0,6,6	-	-	-		
92	OHX	5	4433	-	0,6,6	-	-	-		
92	OHX	5	4403	92	0,6,6	-	-	-		
92	OHX	6	2300	-	0,6,6	-	-	-		
92	OHX	4	246	92	0,6,6	-	-	-		
92	OHX	1	4415	-	0,6,6	-	-	-		
92	OHX	5	4453	92	0,6,6	-	-	-		
92	OHX	6	2182	-	0,6,6	-	-	-		
92	OHX	1	4107	-	0,6,6	-	-	-		
92	OHX	5	4201	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	1	4237	-	0,6,6	-	-	-		
92	OHX	1	4340	-	0,6,6	-	-	-		
92	OHX	6	2213	92	0,6,6	-	-	-		
92	OHX	3	226	92	0,6,6	-	-	-		
92	OHX	1	4454	-	0,6,6	-	-	-		
92	OHX	1	4162	-	0,6,6	-	-	-		
92	OHX	1	4138	-	0,6,6	-	-	-		
92	OHX	6	2185	-	0,6,6	-	-	-		
92	OHX	8	230	-	0,6,6	-	-	-		
92	OHX	2	2206	-	0,6,6	-	-	-		
92	OHX	5	4319	-	0,6,6	-	-	-		
92	OHX	5	4205	-	0,6,6	-	-	-		
92	OHX	5	4174	-	0,6,6	-	-	-		
92	OHX	1	4177	-	0,6,6	-	-	-		
92	OHX	1	4217	-	0,6,6	-	-	-		
92	OHX	2	2129	1,92	0,6,6	-	-	-		
92	OHX	1	4219	-	0,6,6	-	-	-		
92	OHX	1	4297	-	0,6,6	-	-	-		
92	OHX	1	4424	92	0,6,6	-	-	-		
92	OHX	1	4398	-	0,6,6	-	-	-		
92	OHX	6	2284	-	0,6,6	-	-	-		
92	OHX	o3	206	-	0,6,6	-	-	-		
92	OHX	1	4488	-	0,6,6	-	-	-		
92	OHX	5	4427	-	0,6,6	-	-	-		
92	OHX	7	234	-	0,6,6	-	-	-		
92	OHX	1	4386	92	0,6,6	-	-	-		
92	OHX	1	4442	92	0,6,6	-	-	-		
92	OHX	2	2105	-	0,6,6	-	-	-		
92	OHX	s8	305	-	0,6,6	-	-	-		
92	OHX	1	4310	-	0,6,6	-	-	-		
92	OHX	5	4357	-	0,6,6	-	-	-		
92	OHX	1	4189	-	0,6,6	-	-	-		
92	OHX	5	4391	92	0,6,6	-	-	-		
92	OHX	1	4411	92	0,6,6	-	-	-		
92	OHX	6	2272	1,92	0,6,6	-	-	-		
92	OHX	5	4486	92	0,6,6	-	-	-		
92	OHX	1	4439	92	0,6,6	-	-	-		
92	OHX	8	234	38	0,6,6	-	-	-		
92	OHX	5	4318	-	0,6,6	-	-	-		
92	OHX	6	2261	-	0,6,6	-	-	-		
92	OHX	1	4459	36,92	0,6,6	-	-	-		
92	OHX	5	4458	36	0,6,6	-	-	-		
92	OHX	2	2149	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
92	OHX	8	238	-	0,6,6	-	-	-		
92	OHX	5	4483	92	0,6,6	-	-	-		
92	OHX	2	2075	92	0,6,6	-	-	-		
92	OHX	5	4449	92	0,6,6	-	-	-		
92	OHX	1	4268	-	0,6,6	-	-	-		
92	OHX	1	4389	92	0,6,6	-	-	-		
92	OHX	1	4409	-	0,6,6	-	-	-		
92	OHX	6	2150	1	0,6,6	-	-	-		
92	OHX	5	4268	-	0,6,6	-	-	-		
92	OHX	1	4167	-	0,6,6	-	-	-		
92	OHX	2	2188	-	0,6,6	-	-	-		
92	OHX	6	2239	-	0,6,6	-	-	-		
92	OHX	2	2241	92	0,6,6	-	-	-		
92	OHX	1	4106	-	0,6,6	-	-	-		
92	OHX	5	4189	-	0,6,6	-	-	-		
92	OHX	2	2154	-	0,6,6	-	-	-		
92	OHX	5	4249	-	0,6,6	-	-	-		
92	OHX	2	2192	-	0,6,6	-	-	-		
92	OHX	6	2215	-	0,6,6	-	-	-		
92	OHX	5	4301	-	0,6,6	-	-	-		
92	OHX	1	4393	36	0,6,6	-	-	-		
92	OHX	6	2257	-	0,6,6	-	-	-		
92	OHX	5	4499	92	0,6,6	-	-	-		
92	OHX	M0	306	92	0,6,6	-	-	-		
92	OHX	5	4195	-	0,6,6	-	-	-		
92	OHX	5	4540	36	0,6,6	-	-	-		
92	OHX	5	4509	92	0,6,6	-	-	-		
92	OHX	5	4272	-	0,6,6	-	-	-		
92	OHX	2	2233	-	0,6,6	-	-	-		
92	OHX	8	232	-	0,6,6	-	-	-		
92	OHX	5	4274	-	0,6,6	-	-	-		
92	OHX	1	4349	-	0,6,6	-	-	-		
92	OHX	o2	204	-	0,6,6	-	-	-		
92	OHX	5	4315	92	0,6,6	-	-	-		
92	OHX	A	102	92,90	0,6,6	-	-	-		
92	OHX	5	4435	-	0,6,6	-	-	-		
92	OHX	l4	405	-	0,6,6	-	-	-		
92	OHX	1	4163	-	0,6,6	-	-	-		
92	OHX	1	4344	-	0,6,6	-	-	-		
92	OHX	l5	310	-	0,6,6	-	-	-		
92	OHX	6	2147	-	0,6,6	-	-	-		
92	OHX	1	4304	-	0,6,6	-	-	-		
92	OHX	3	224	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
92	OHX	2	2169	-	0,6,6	-	-	-		
92	OHX	1	4125	-	0,6,6	-	-	-		
92	OHX	5	4185	-	0,6,6	-	-	-		
92	OHX	c8	204	-	0,6,6	-	-	-		
92	OHX	6	2270	-	0,6,6	-	-	-		
92	OHX	m9	202	-	0,6,6	-	-	-		
92	OHX	1	4259	-	0,6,6	-	-	-		
92	OHX	1	4198	92	0,6,6	-	-	-		
92	OHX	1	4152	-	0,6,6	-	-	-		
92	OHX	1	4232	36	0,6,6	-	-	-		
92	OHX	2	2150	-	0,6,6	-	-	-		
92	OHX	2	2157	92	0,6,6	-	-	-		
92	OHX	2	2118	-	0,6,6	-	-	-		
92	OHX	2	2222	92	0,6,6	-	-	-		
92	OHX	6	2209	-	0,6,6	-	-	-		
92	OHX	1	4307	92	0,6,6	-	-	-		
92	OHX	5	4414	-	0,6,6	-	-	-		
92	OHX	2	2243	1,92	0,6,6	-	-	-		
92	OHX	1	4226	-	0,6,6	-	-	-		
92	OHX	5	4545	92	0,6,6	-	-	-		
92	OHX	1	4445	92	0,6,6	-	-	-		
92	OHX	6	2317	-	0,6,6	-	-	-		
92	OHX	1	4446	36,92	0,6,6	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

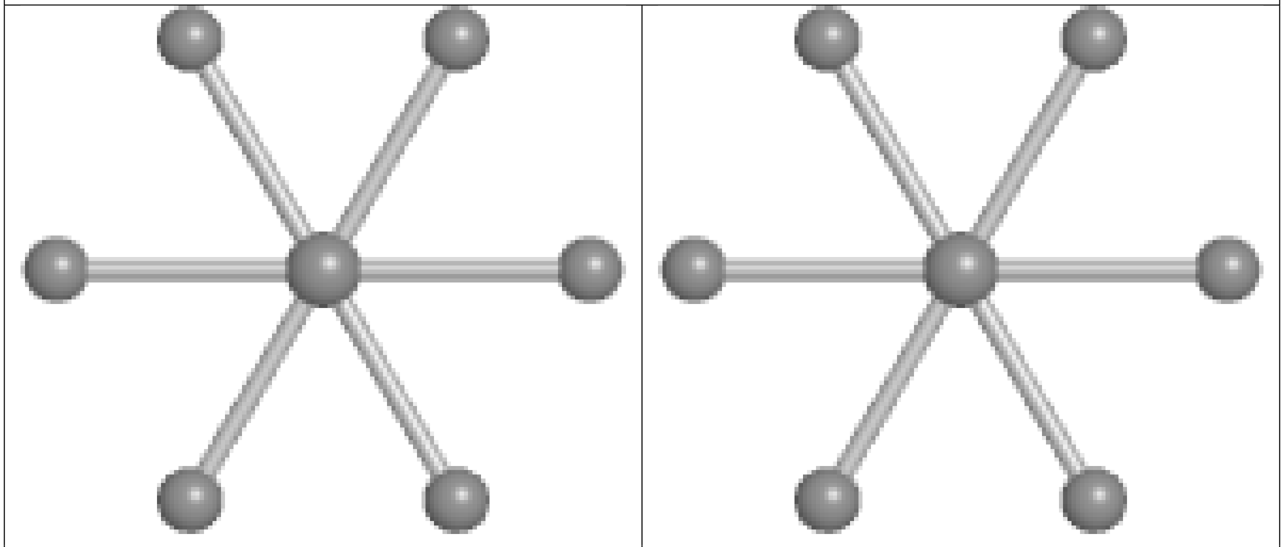
There are no ring outliers.

1 monomer is involved in 1 short contact:

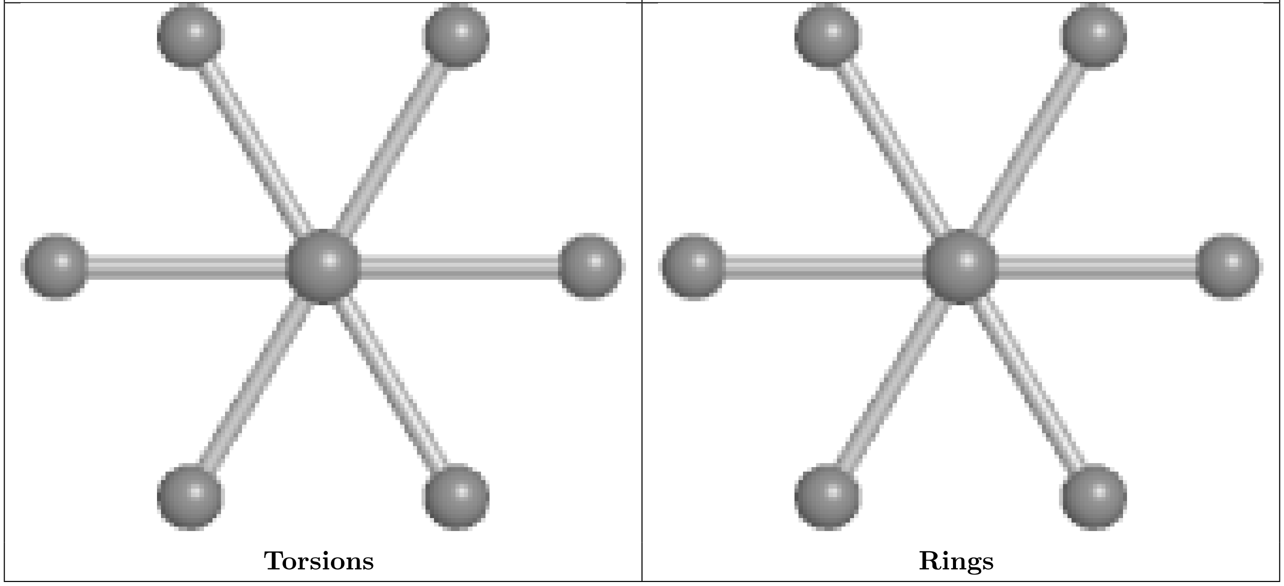
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	l9	204	OHX	0	1

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 OHX 5 4549

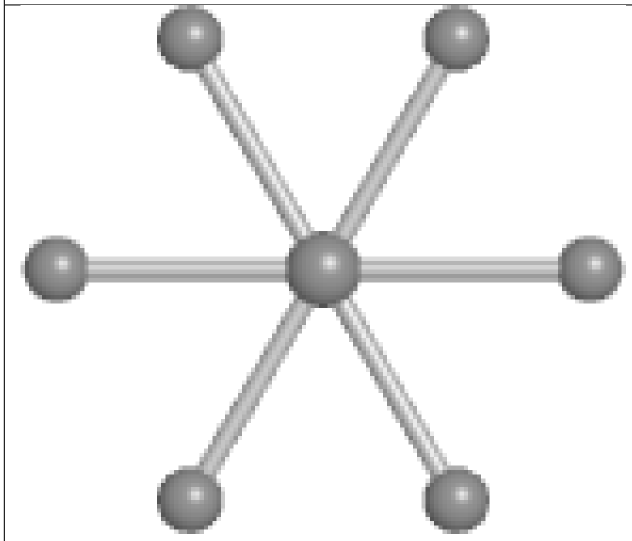


Bond lengths **Bond angles**

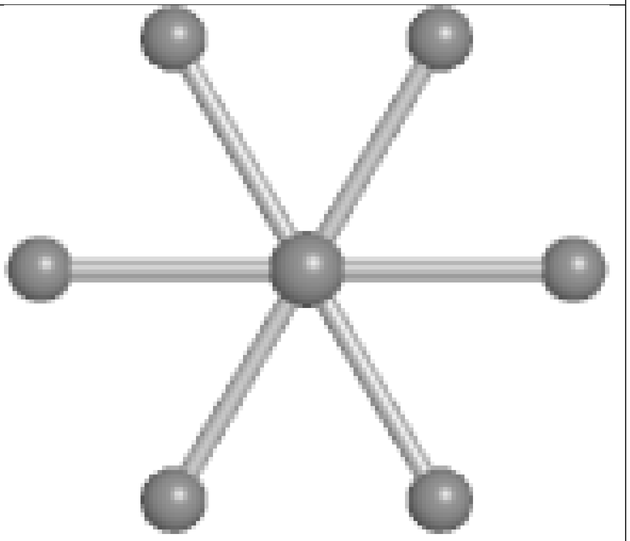


Torsions **Rings**

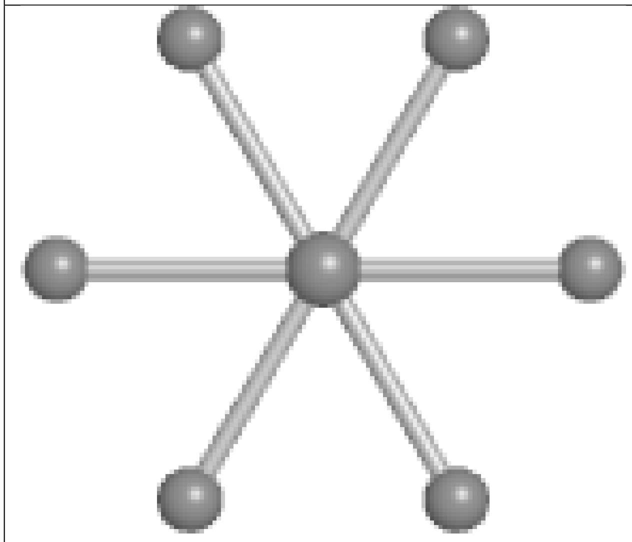
Ligand OHX 5 4495



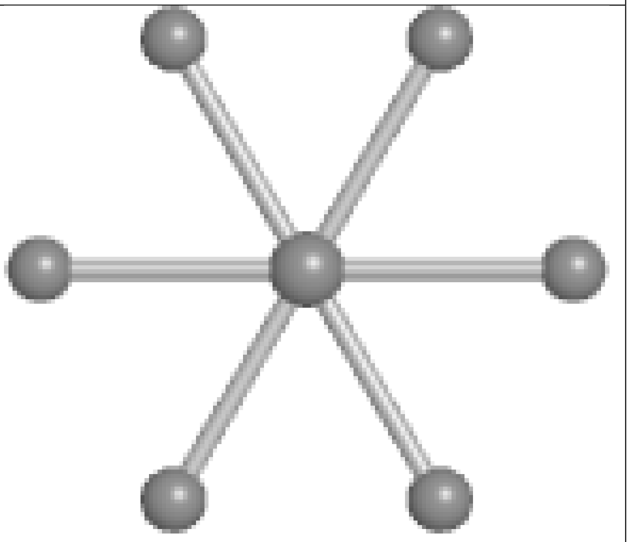
Bond lengths



Bond angles

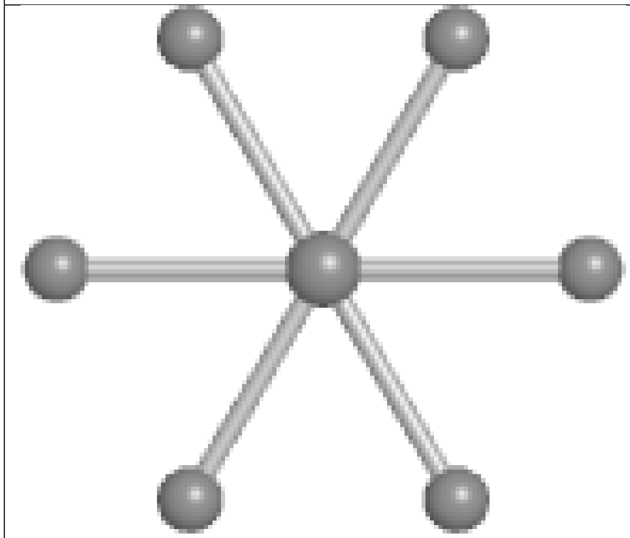


Torsions



Rings

Ligand OHX 2 2231



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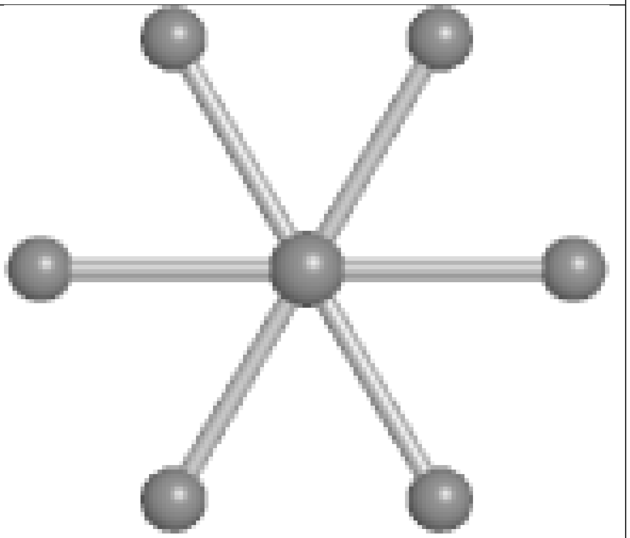

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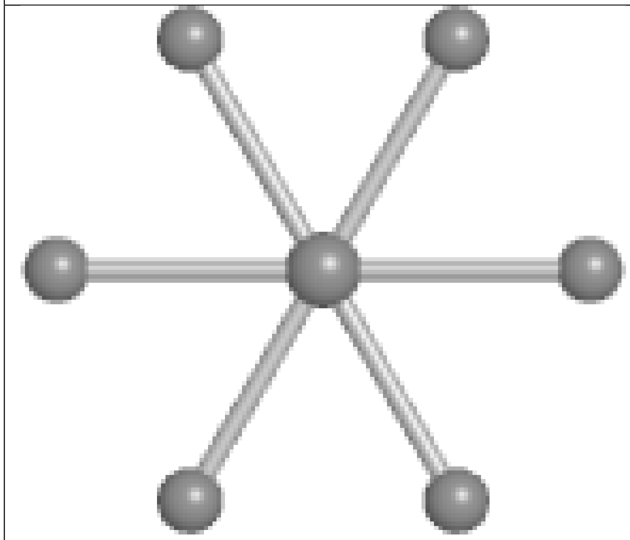

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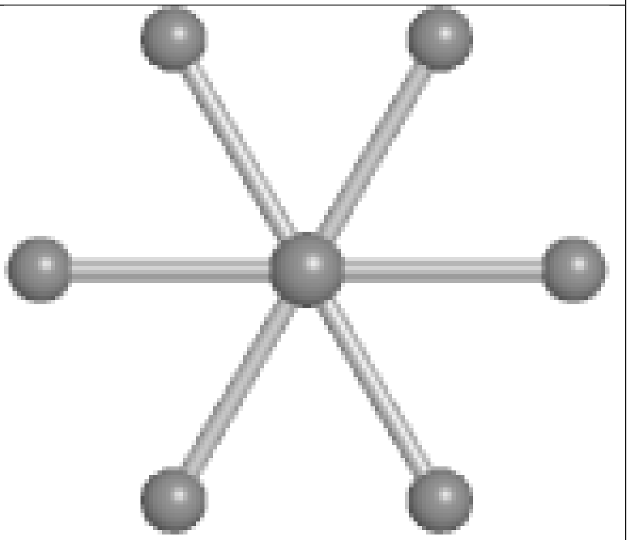
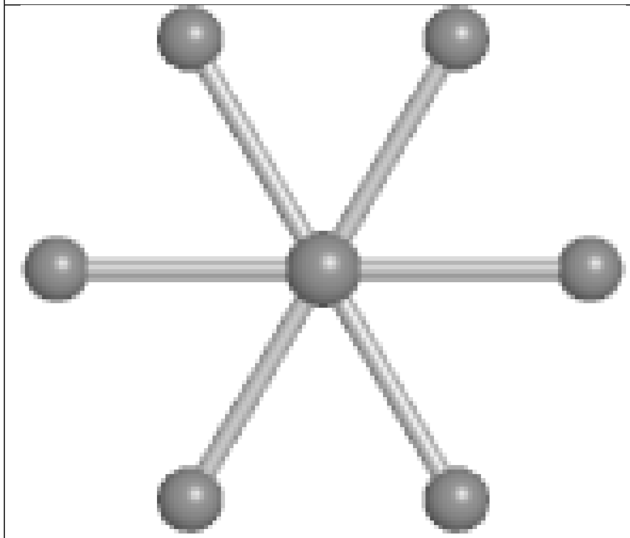


Rings

Ligand OHX 1 4429



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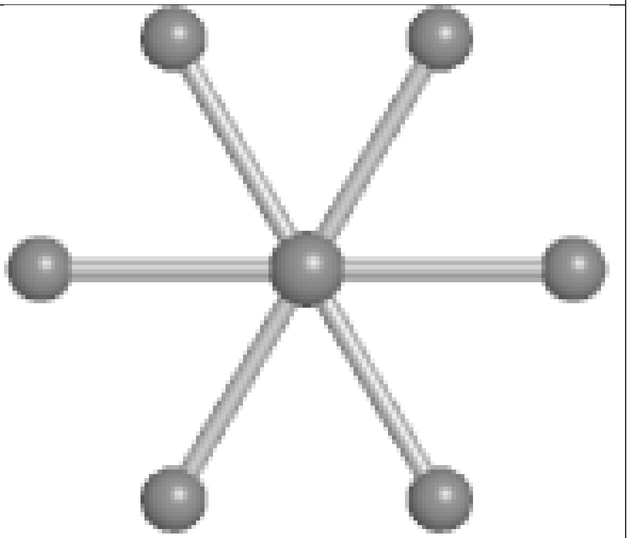
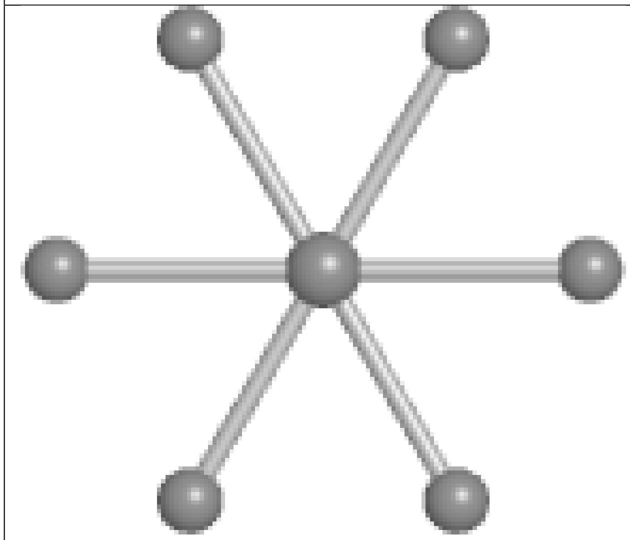


Bond angles



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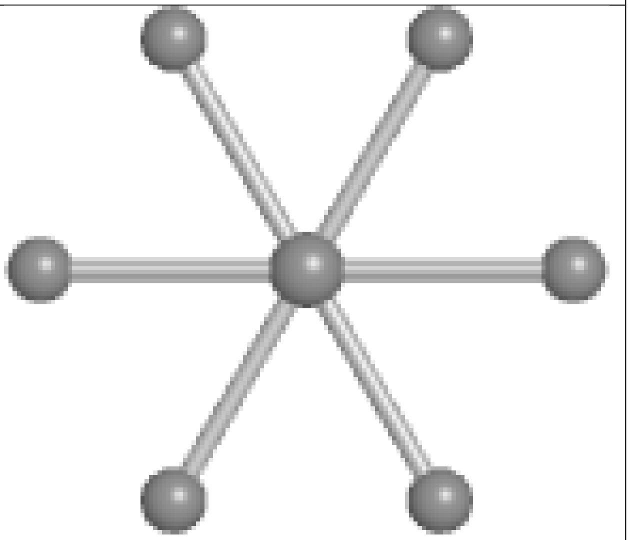
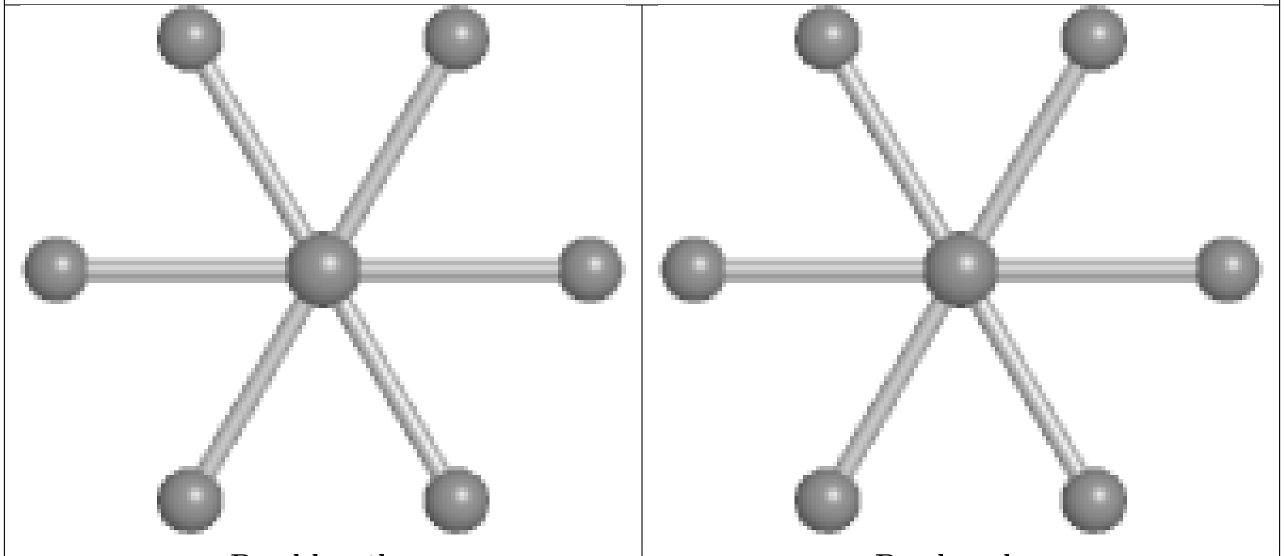
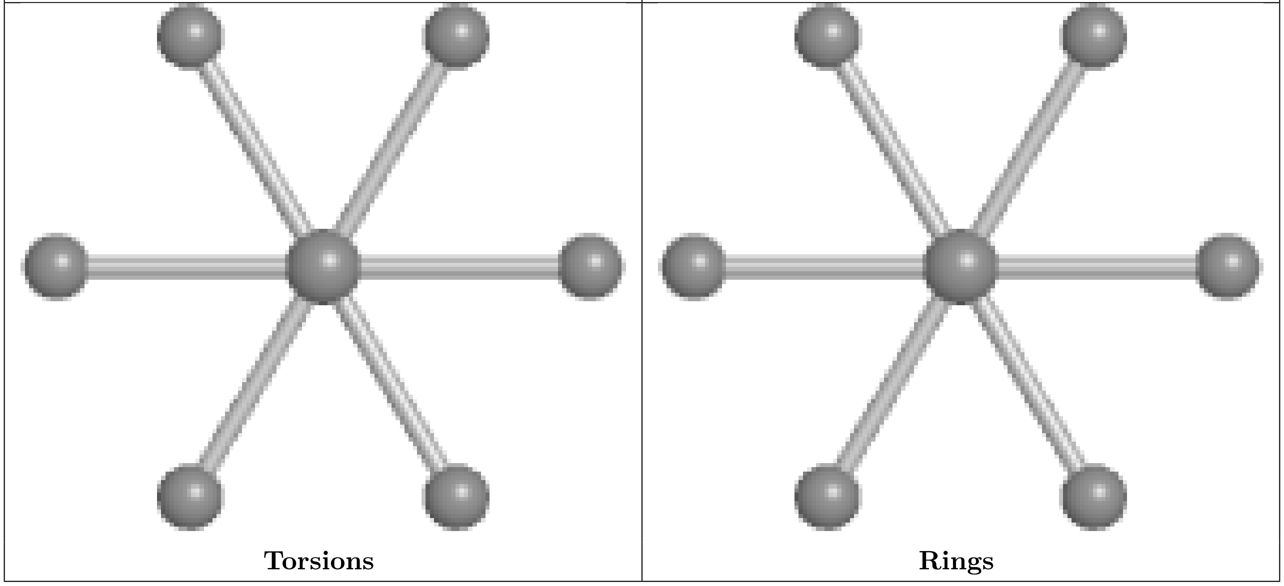


Rings

Ligand OHX 1 4434

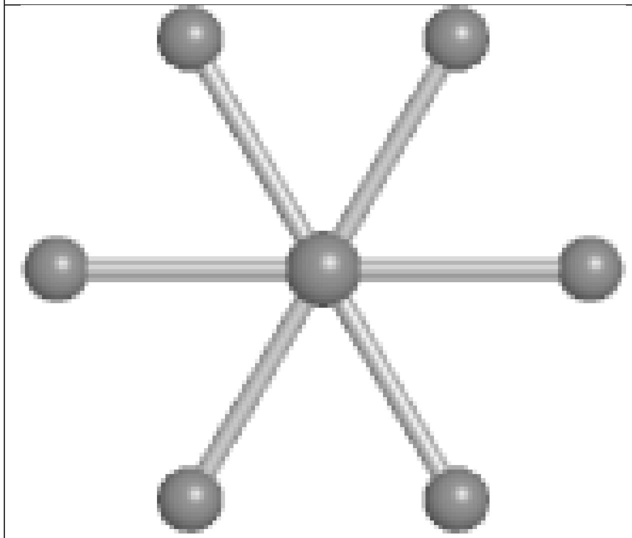


Bond lengths **Bond angles**



Torsions **Rings**

Ligand OHX 5 4520



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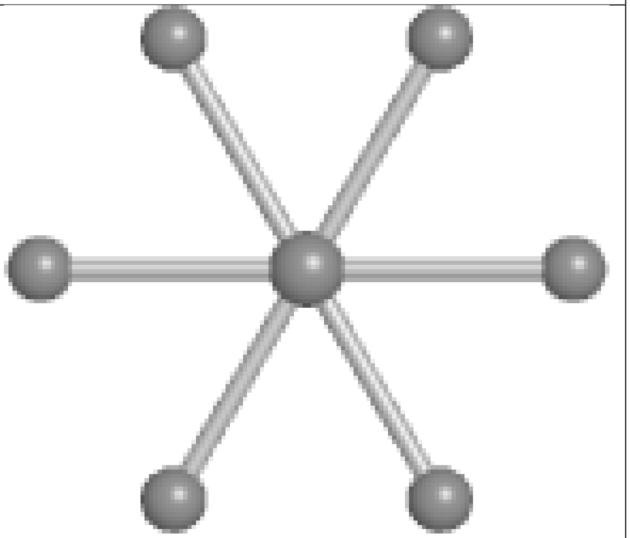
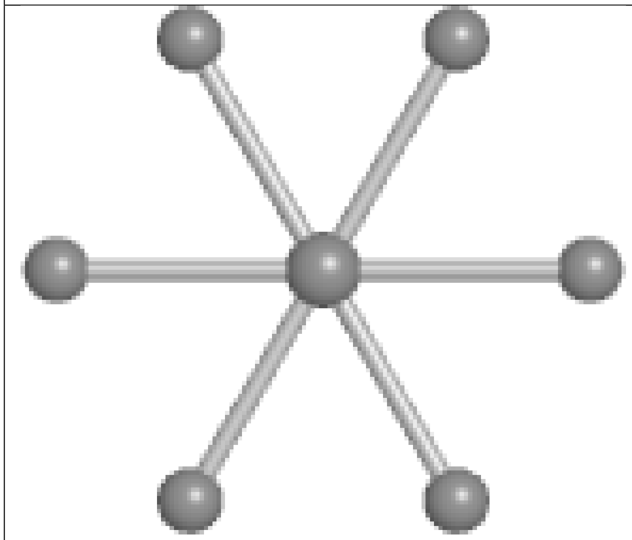


Bond angles



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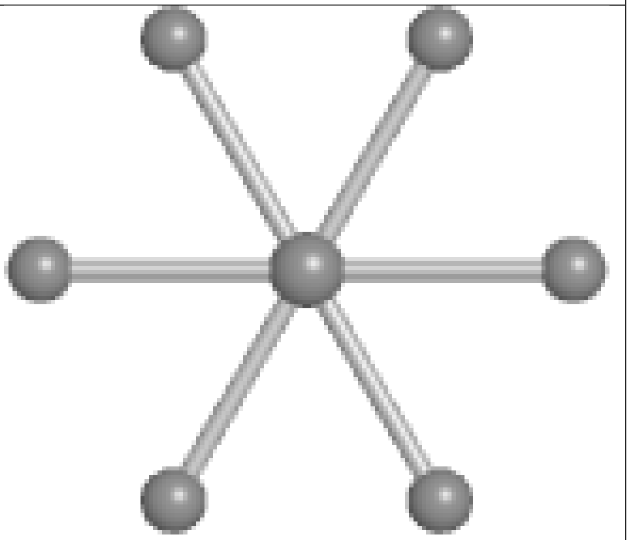
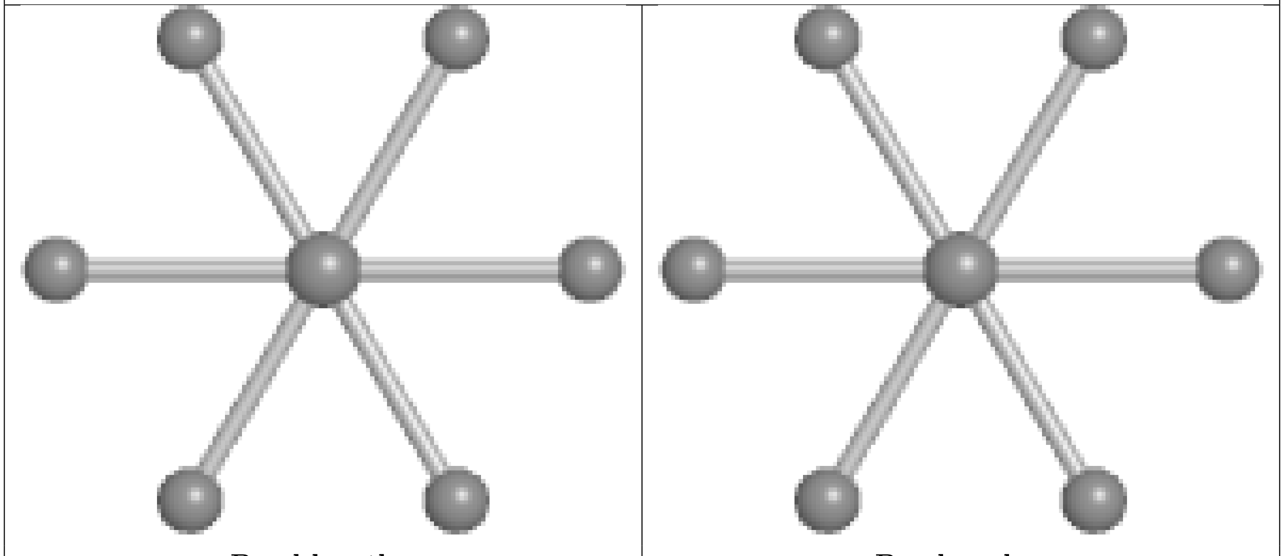


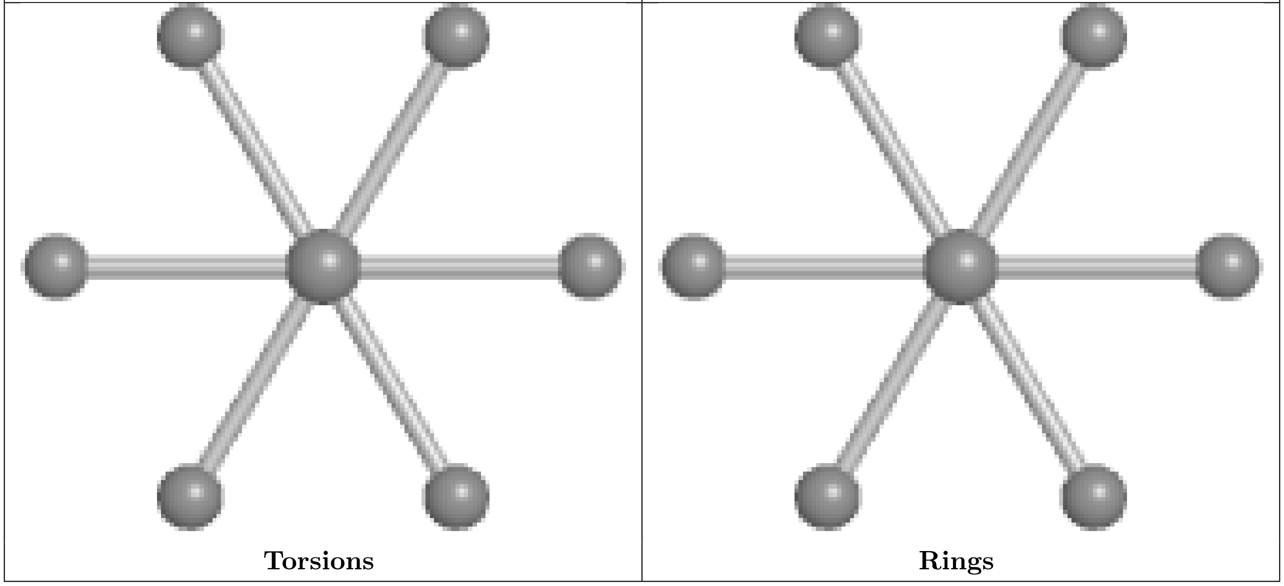
Rings

Ligand OHX 1 4463



Bond lengths

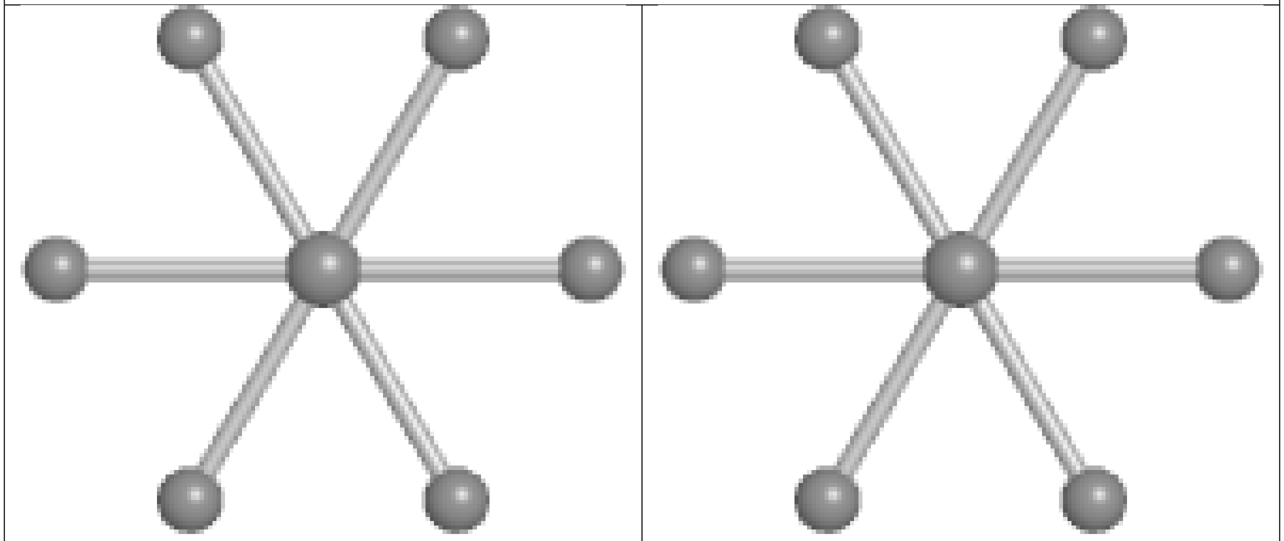
Bond angles



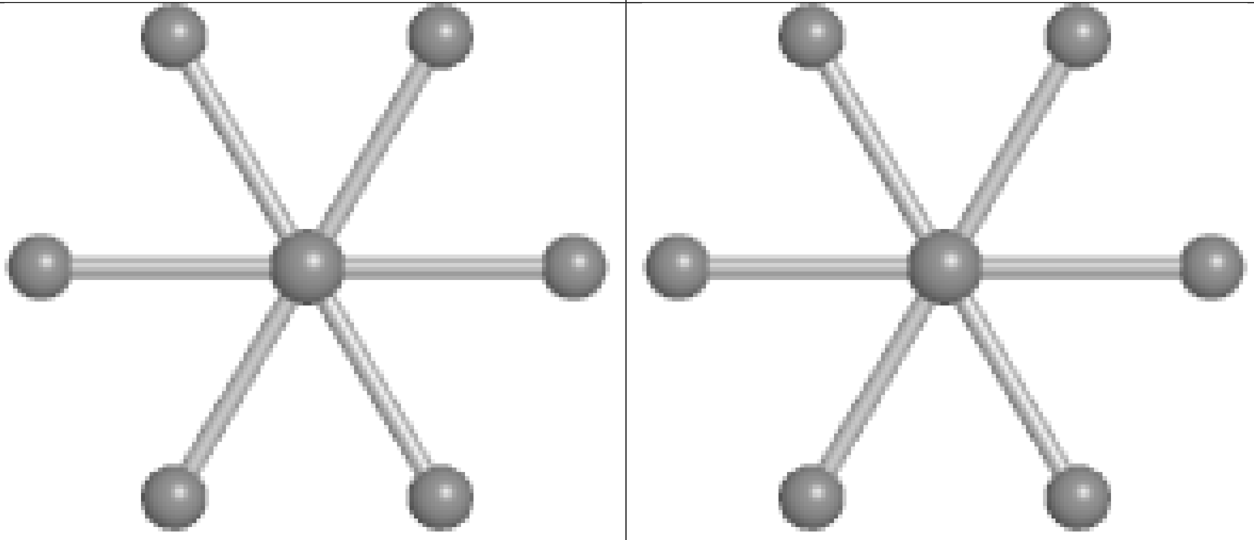
Torsions

Rings

Ligand OHX 1 4477

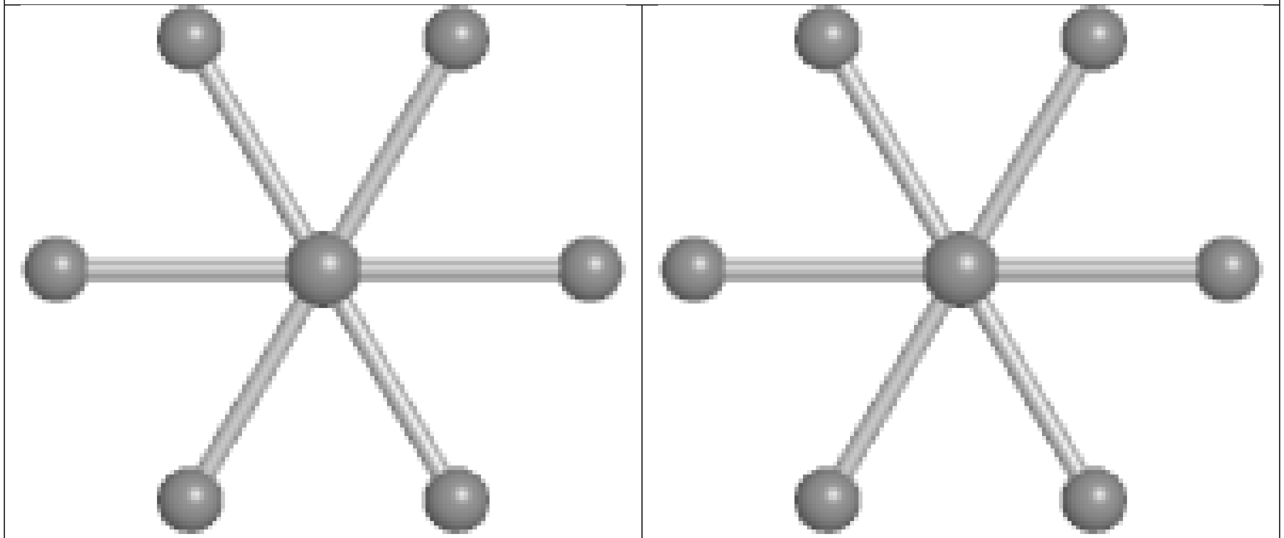


Bond lengths **Bond angles**



Torsions **Rings**

Ligand OHX 2 2197



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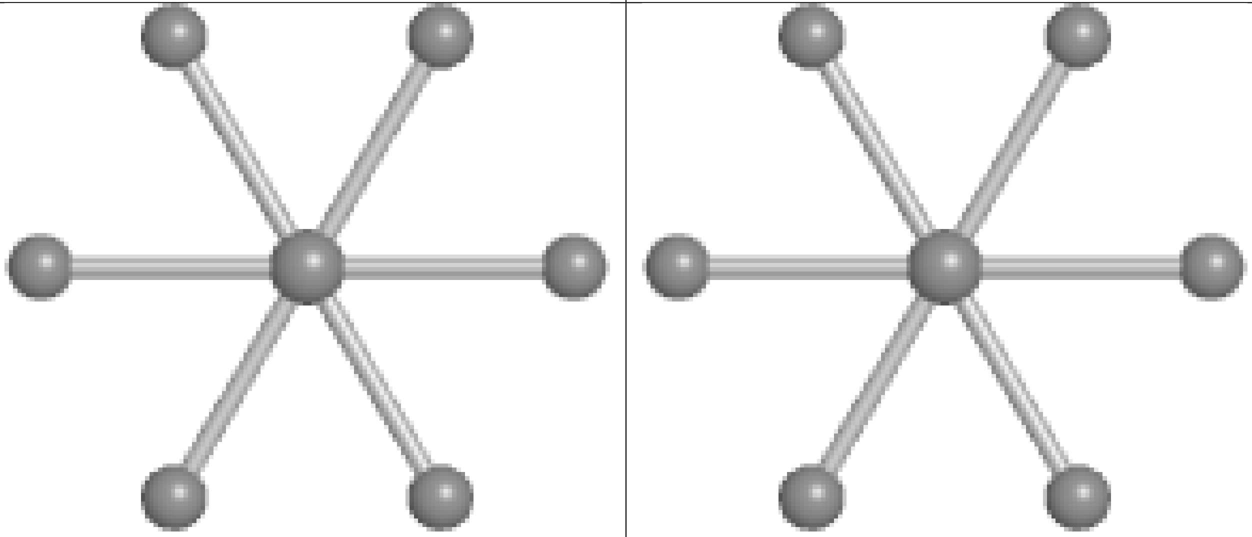

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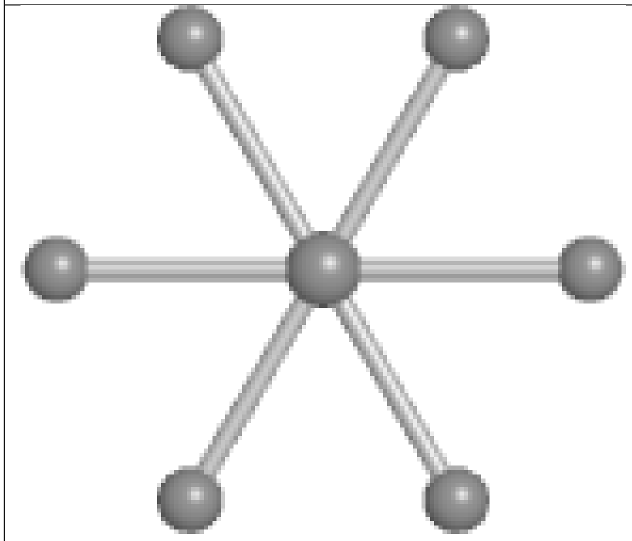
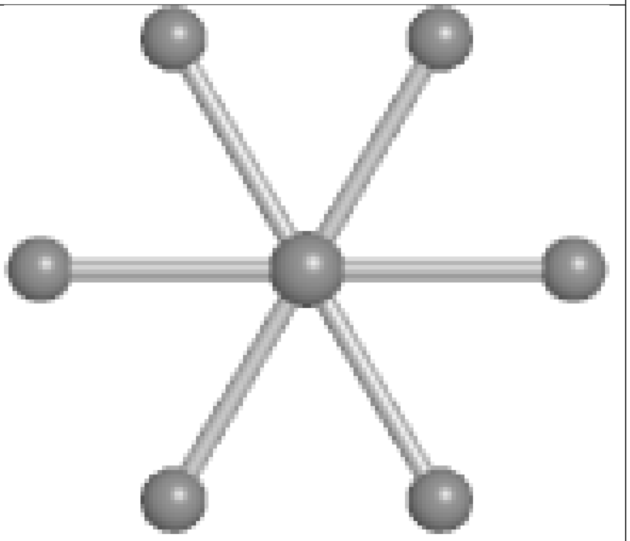
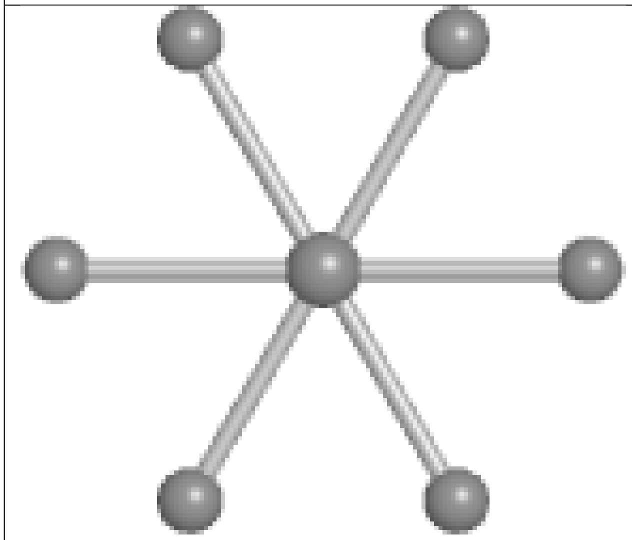
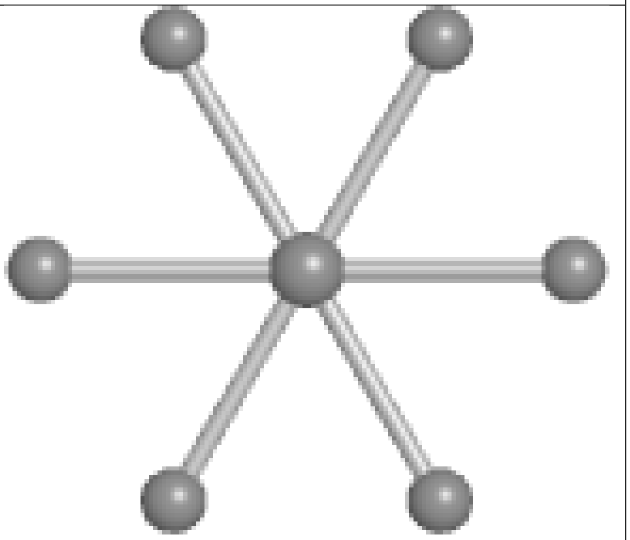
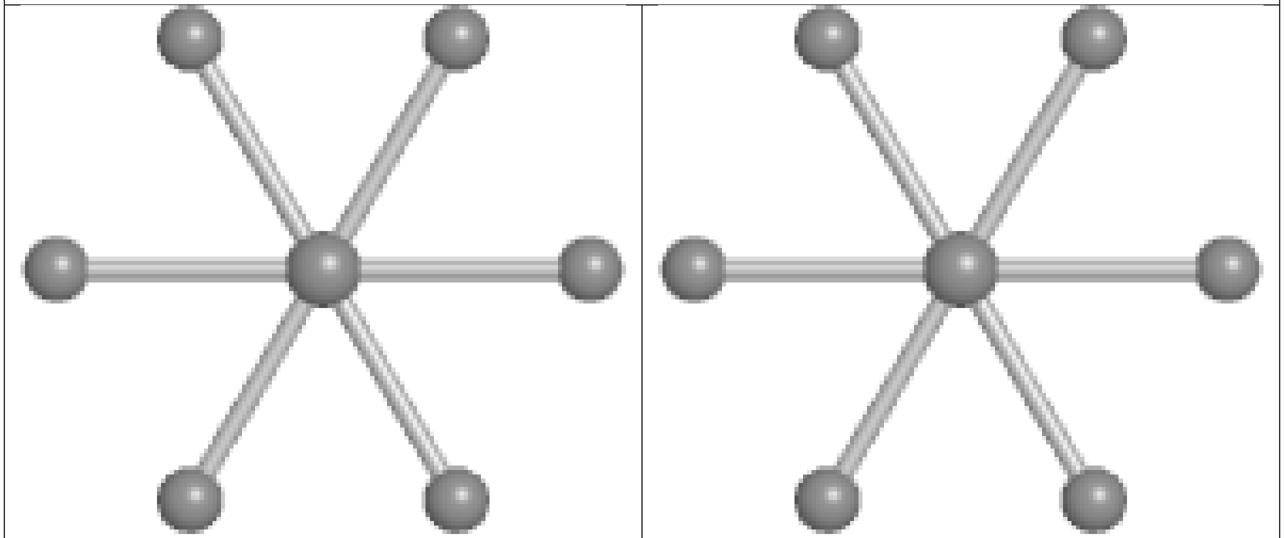
Ligand OHX 5 4536	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand OHX 5 4534



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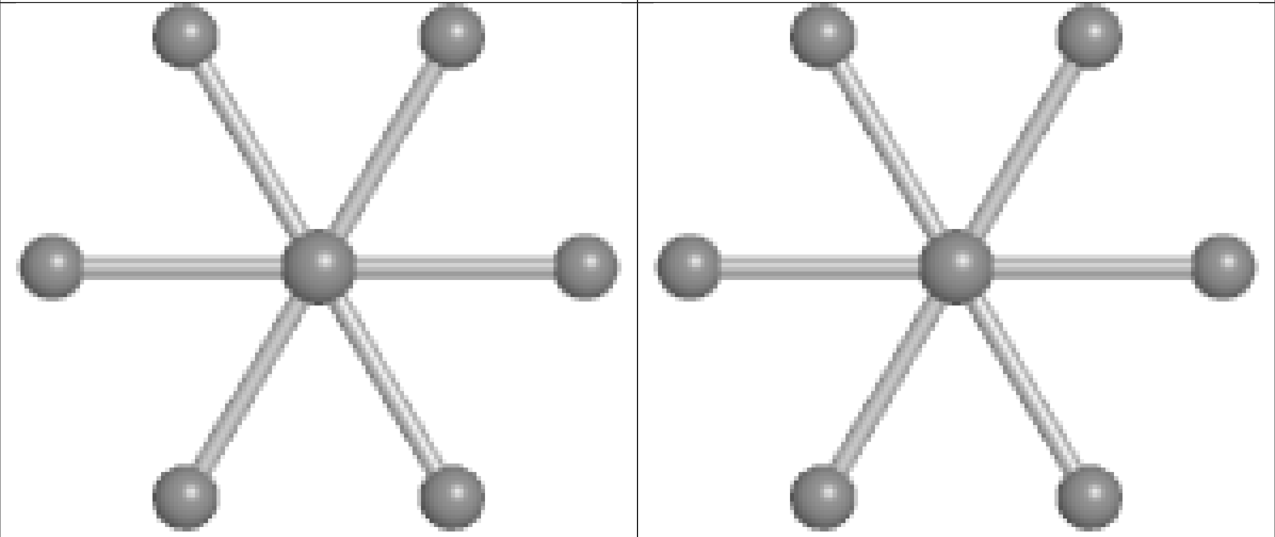

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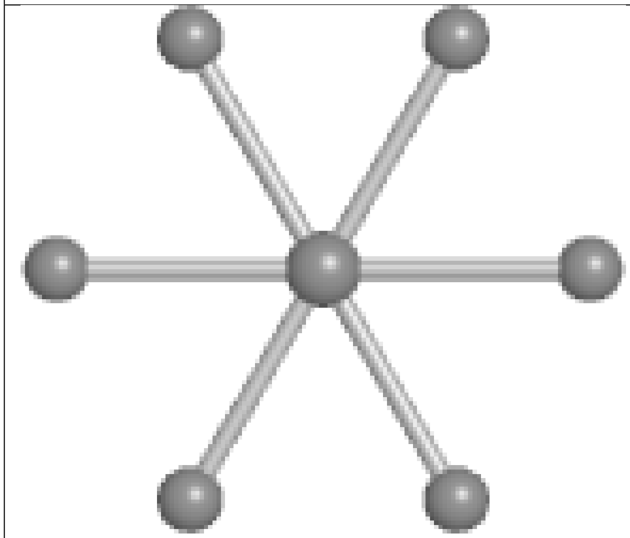
Ligand OHX 6 2322



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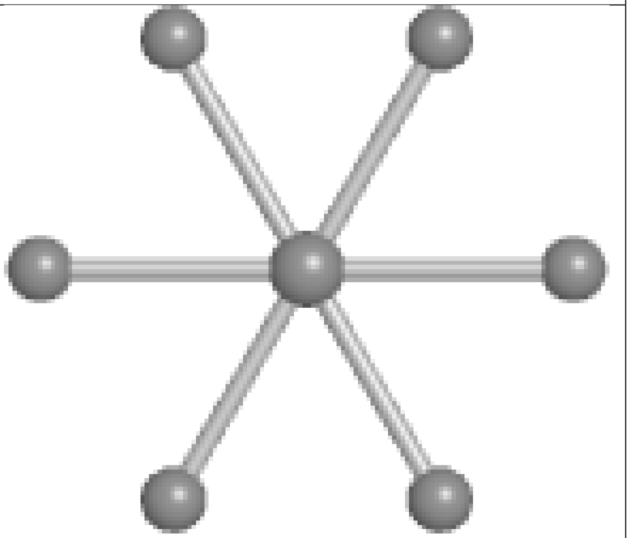

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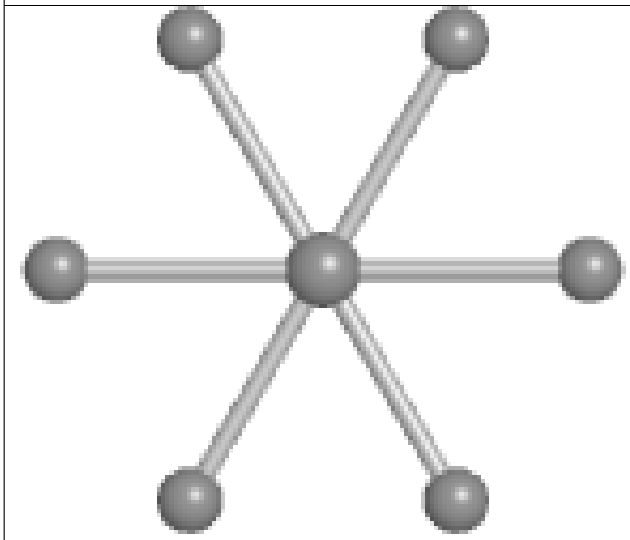

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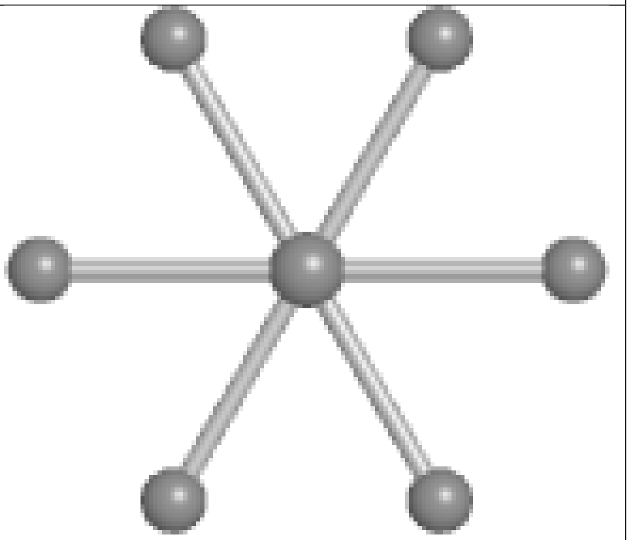
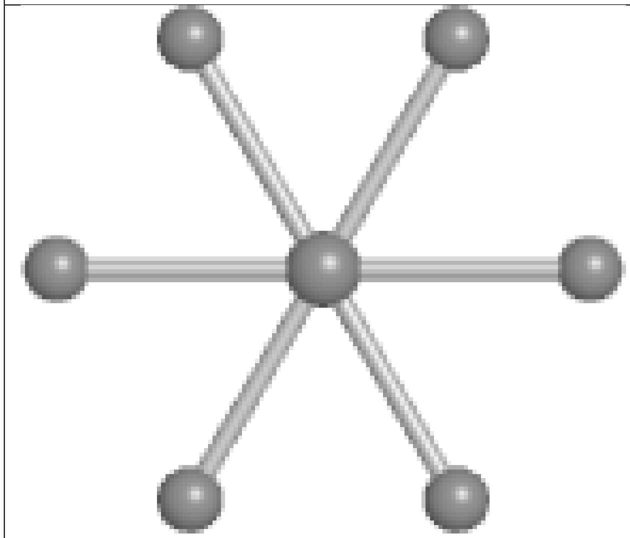


Rings

Ligand OHX 1 4485



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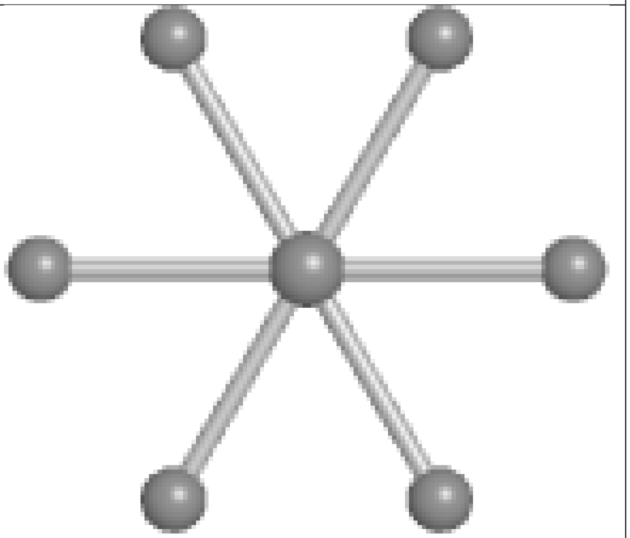
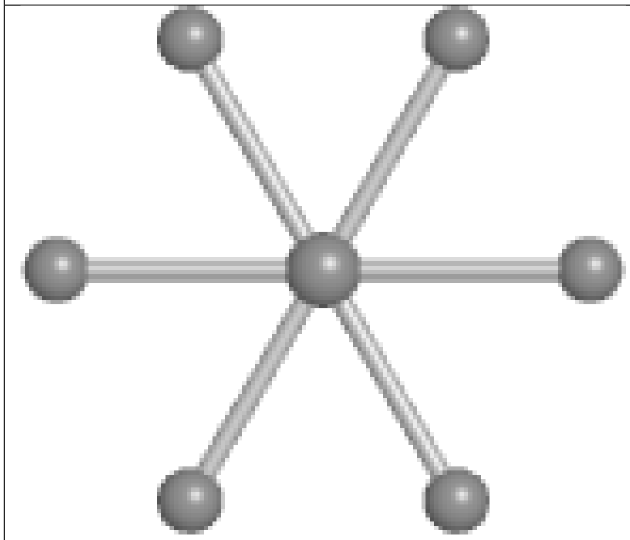


Bond angles



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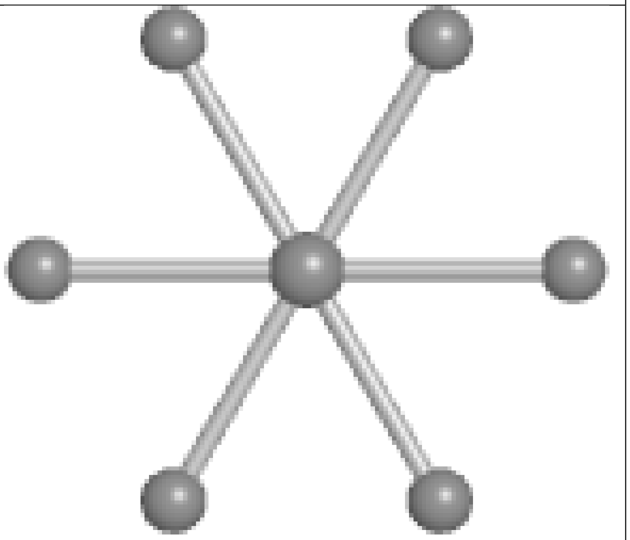
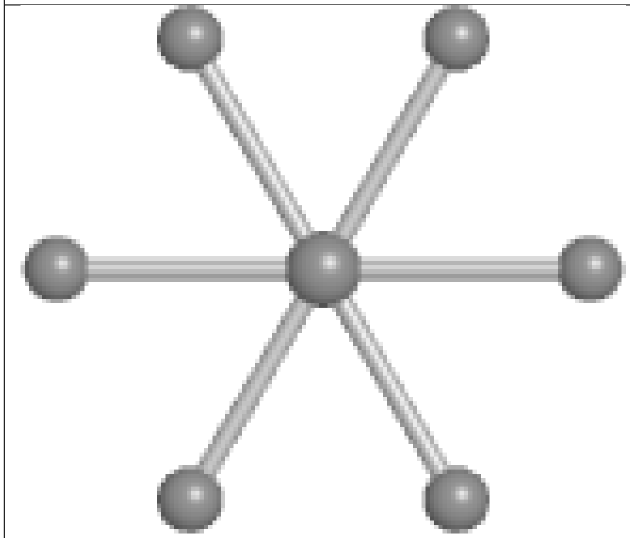


Rings

Ligand OHX 5 4541



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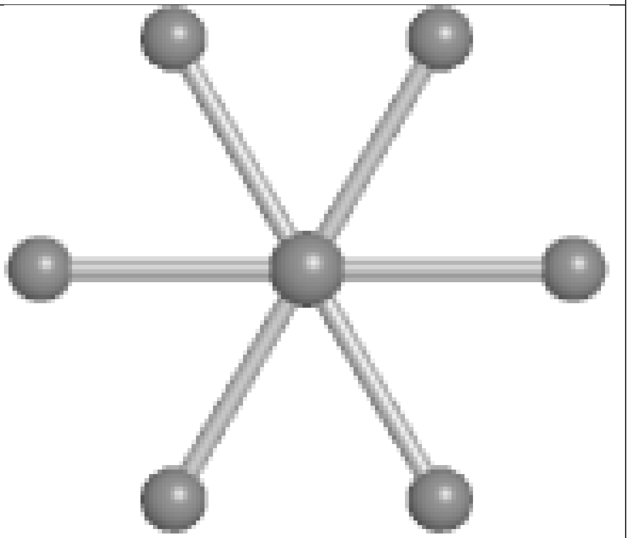
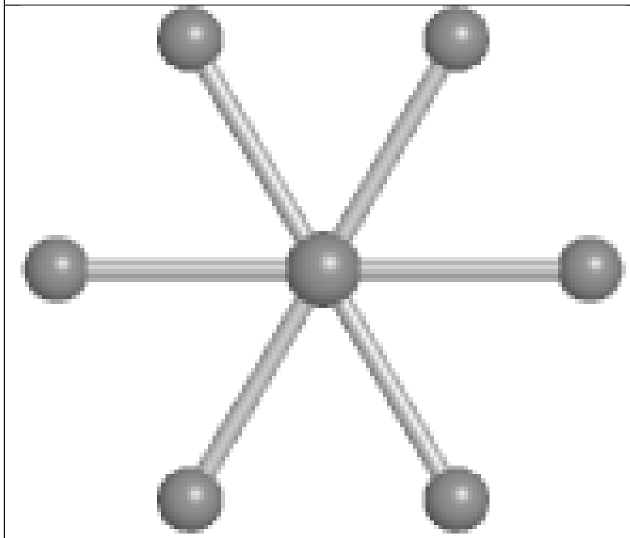


Bond angles



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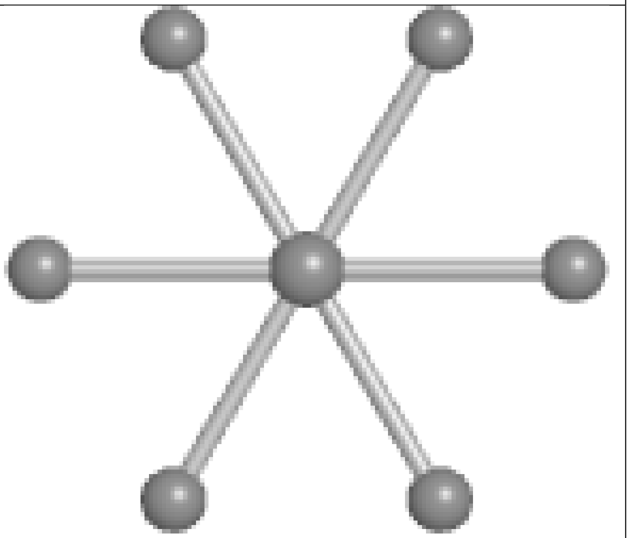
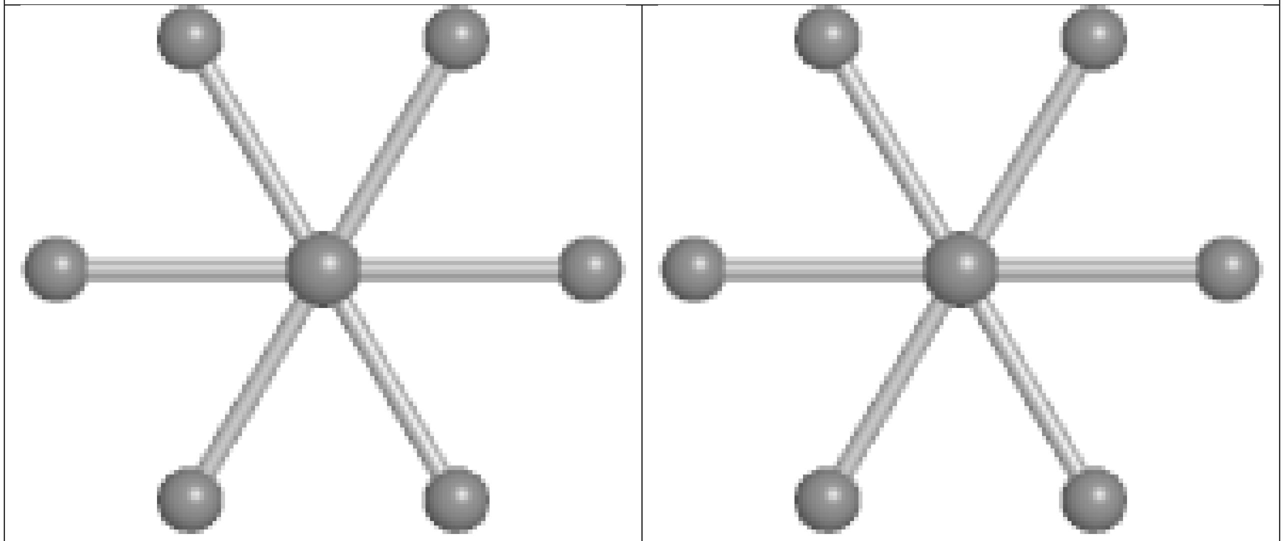
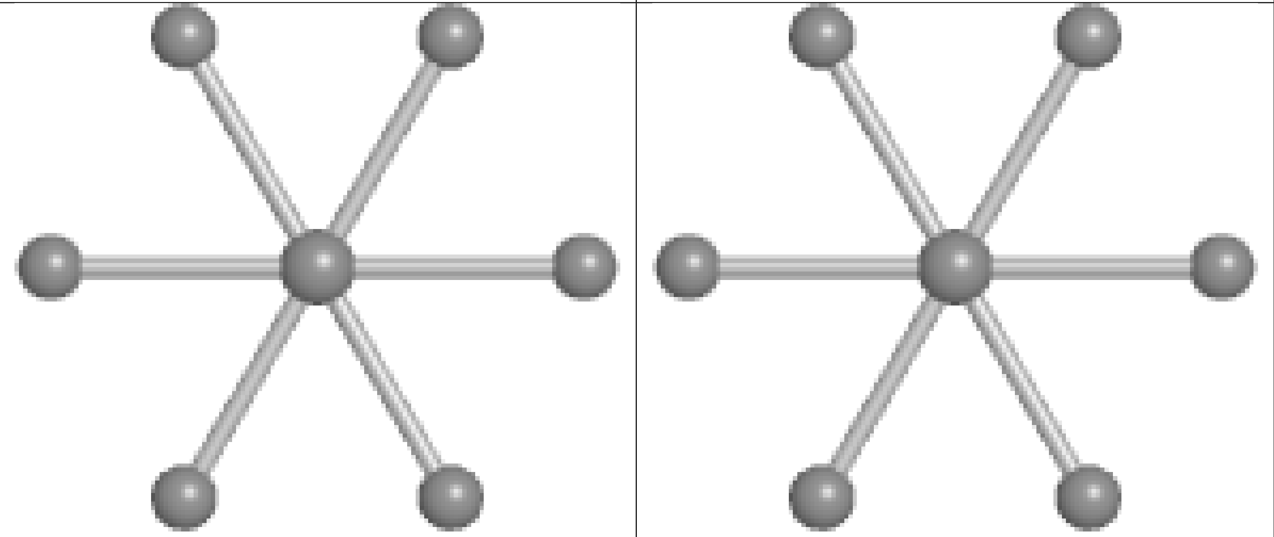


Rings

Ligand OHX 5 4562

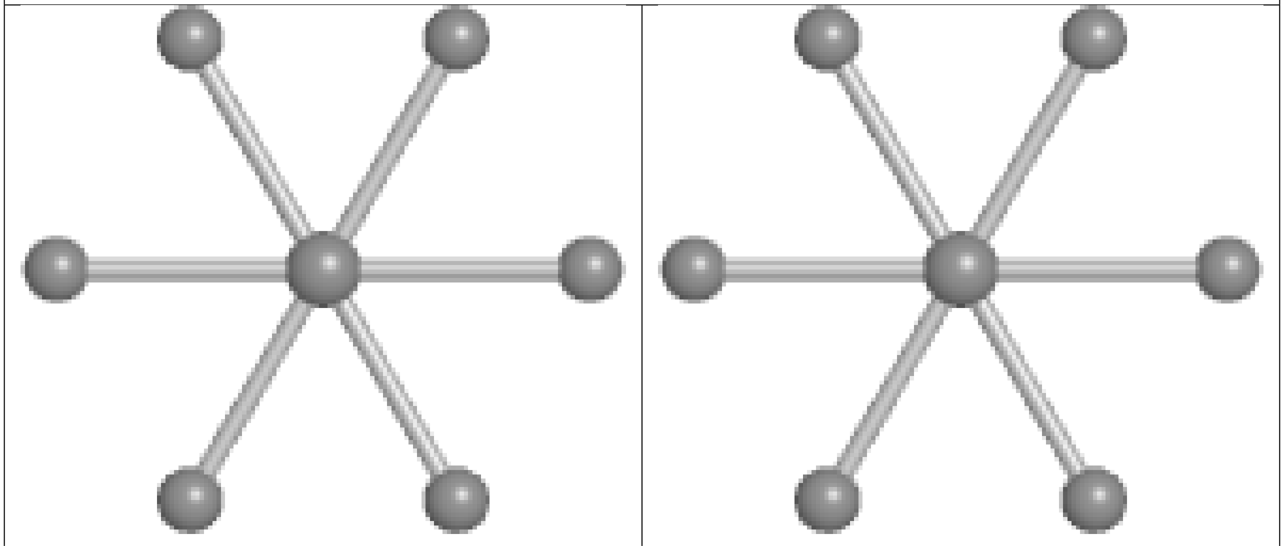


Bond lengths **Bond angles**



Torsions **Rings**

Ligand OHX 2 2246



Bond lengths

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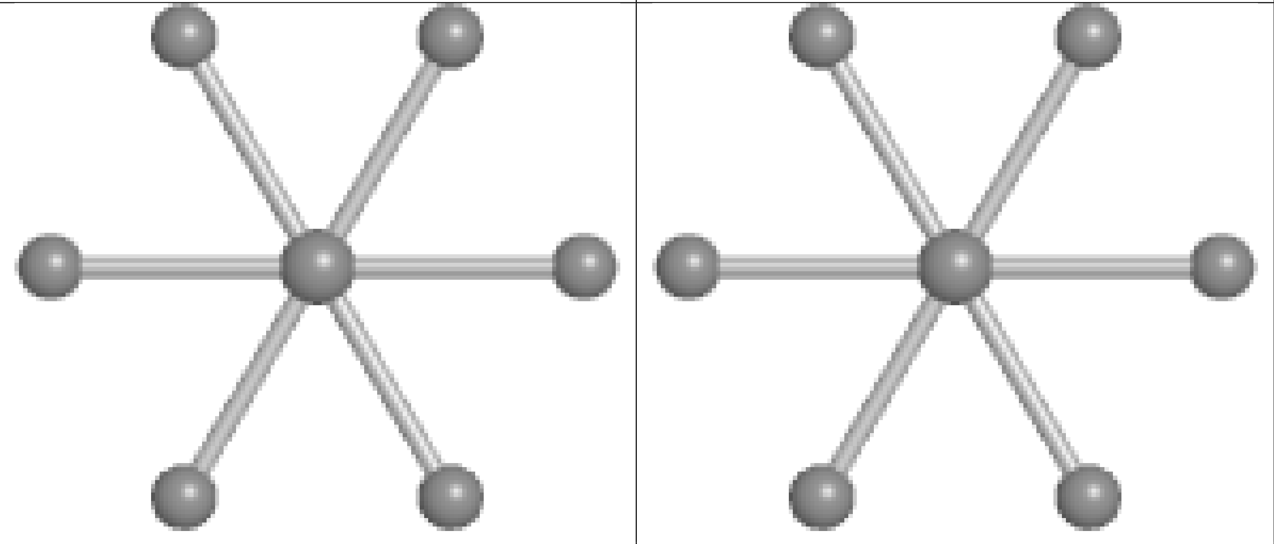
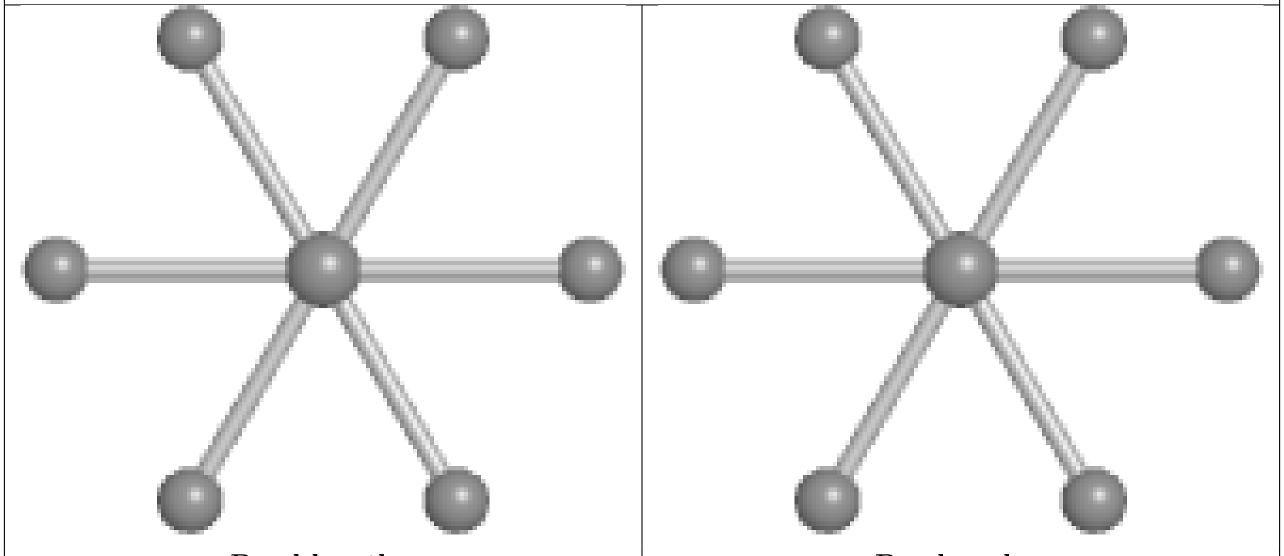


Torsions

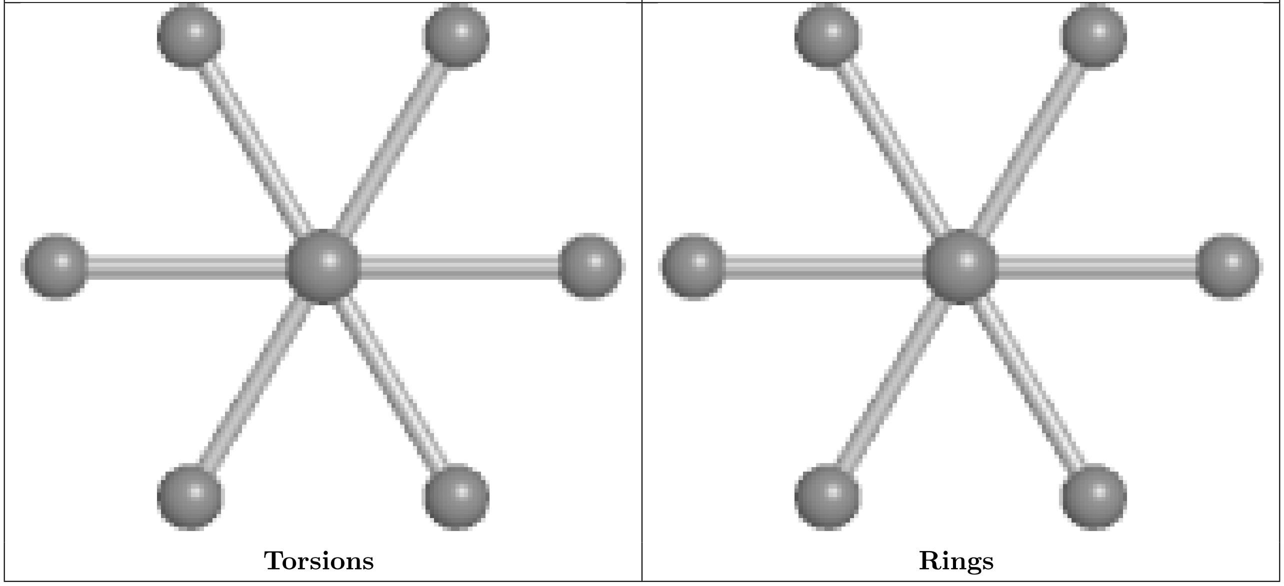
Rings

Ligand OHX 1 4423



Bond lengths

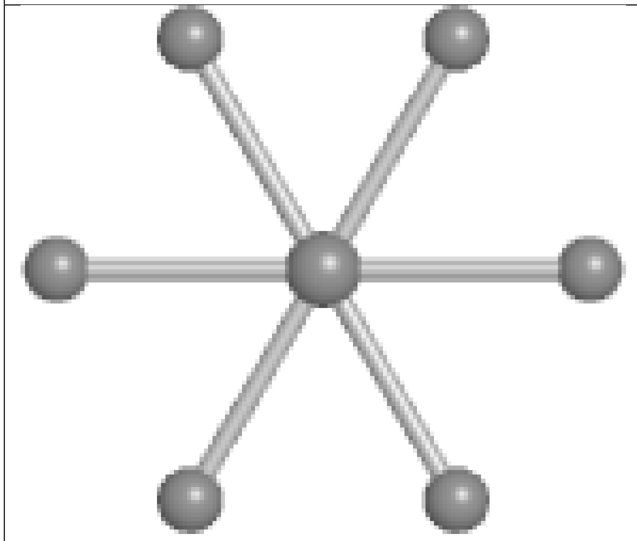
Bond angles



Torsions

Rings

Ligand OHX 6 2336



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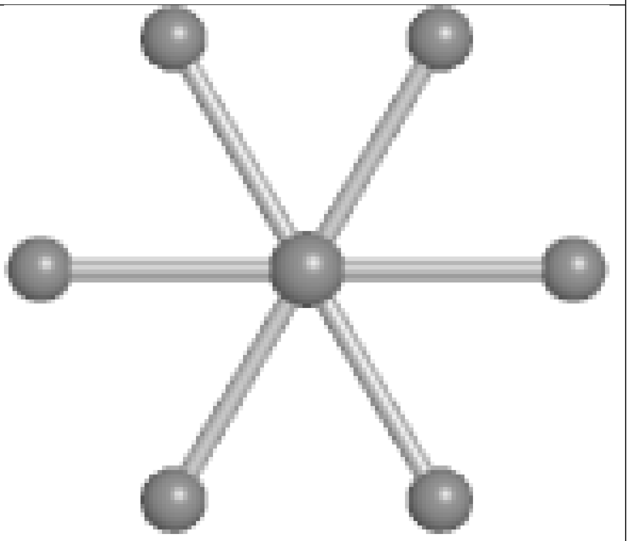

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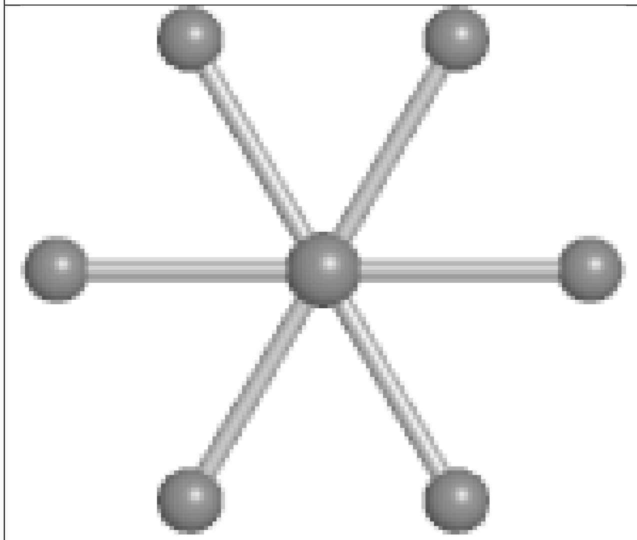

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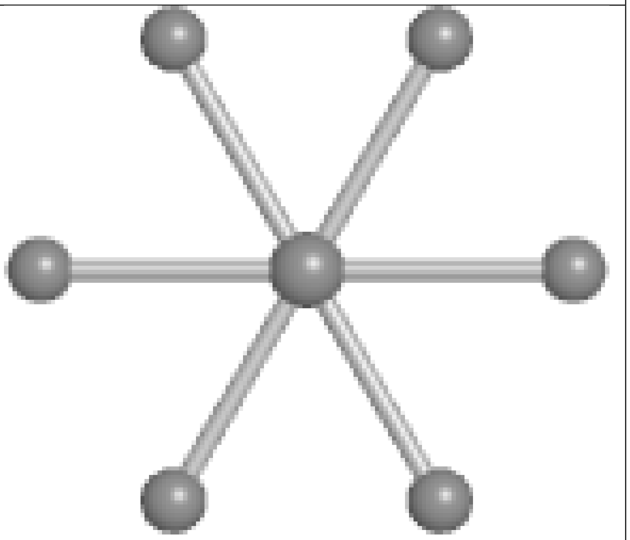
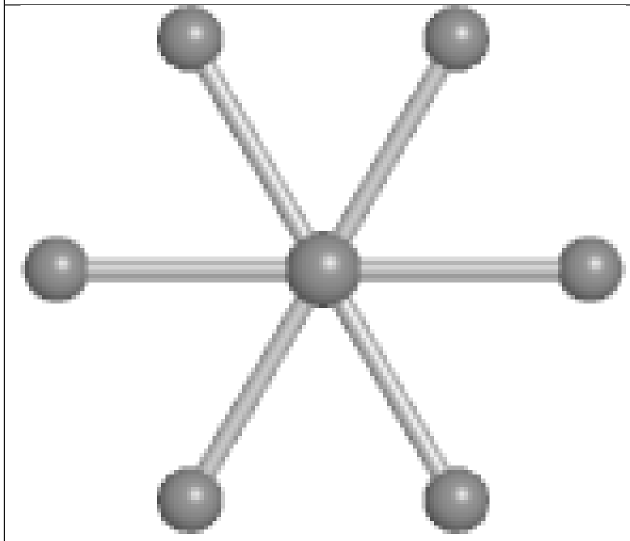


Rings

Ligand OHX 1 4450



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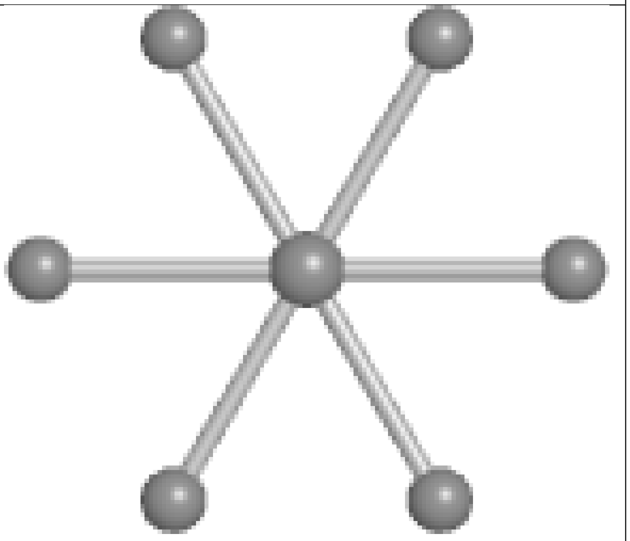
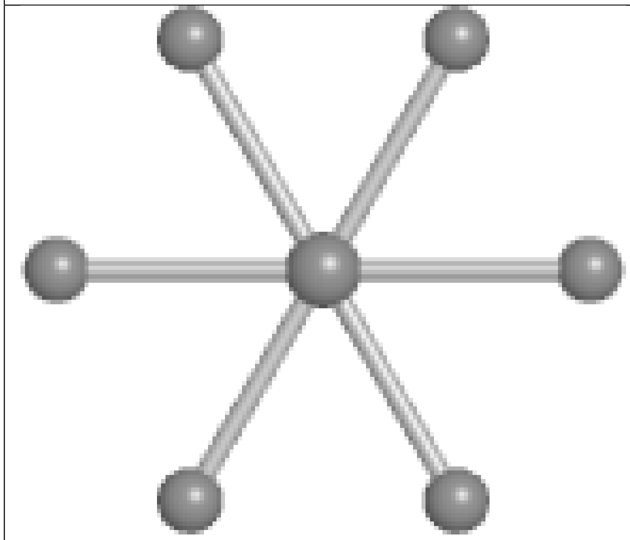


Bond angles



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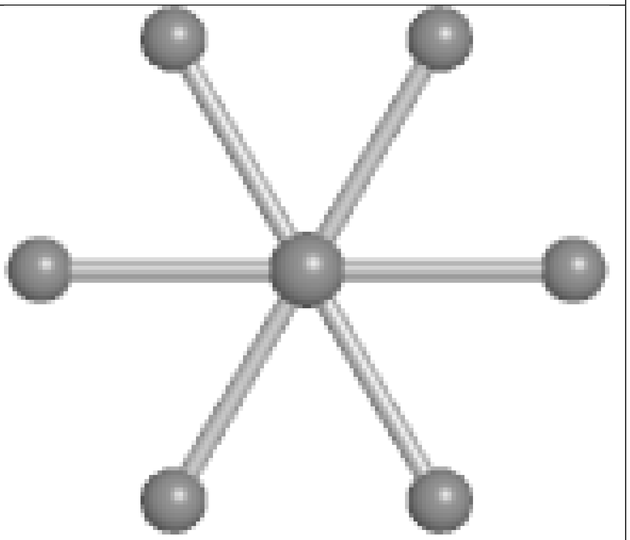
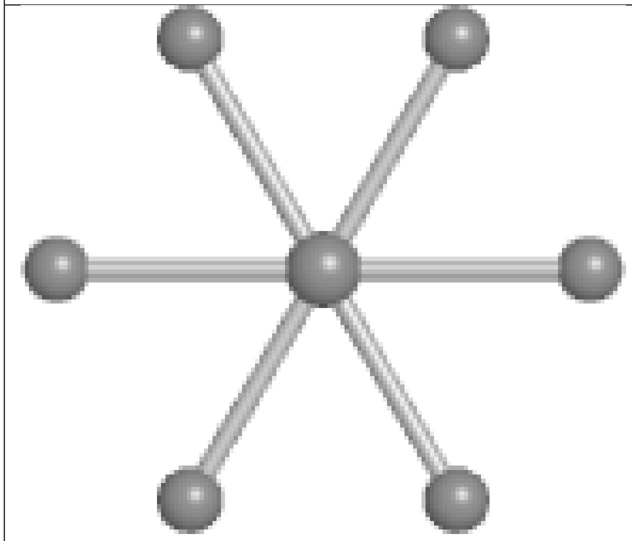


Rings

Ligand OHX 6 2305



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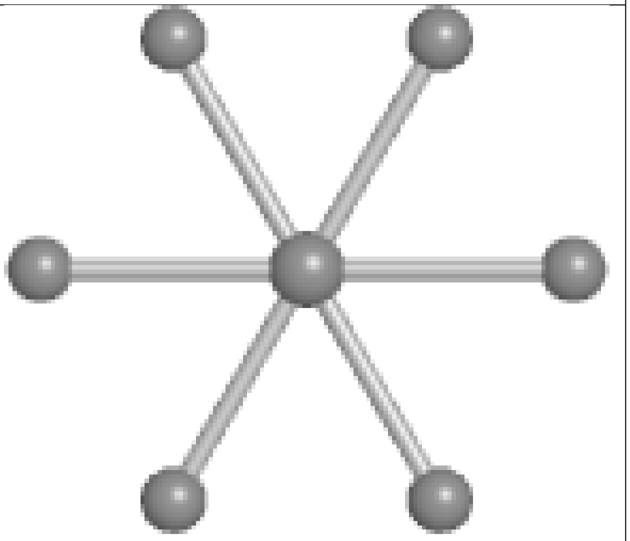
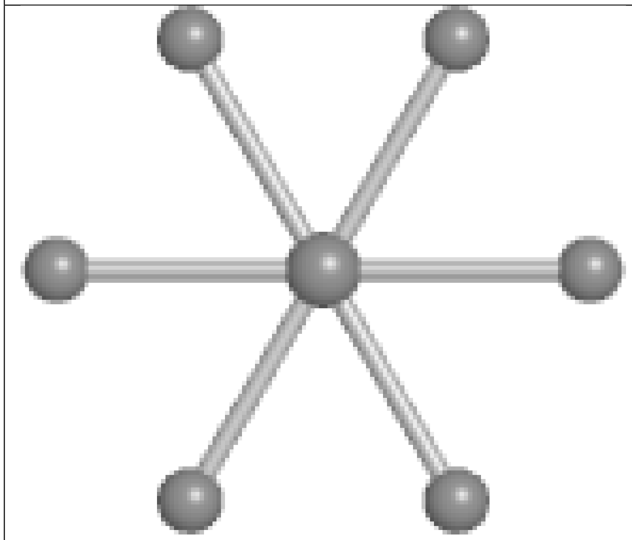


Bond angles



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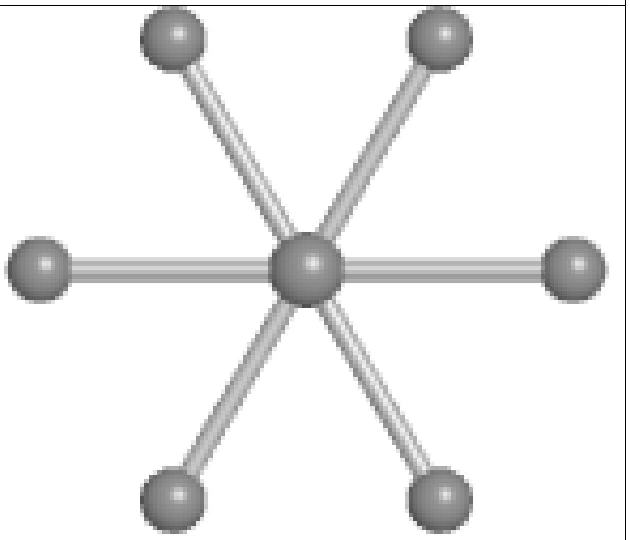
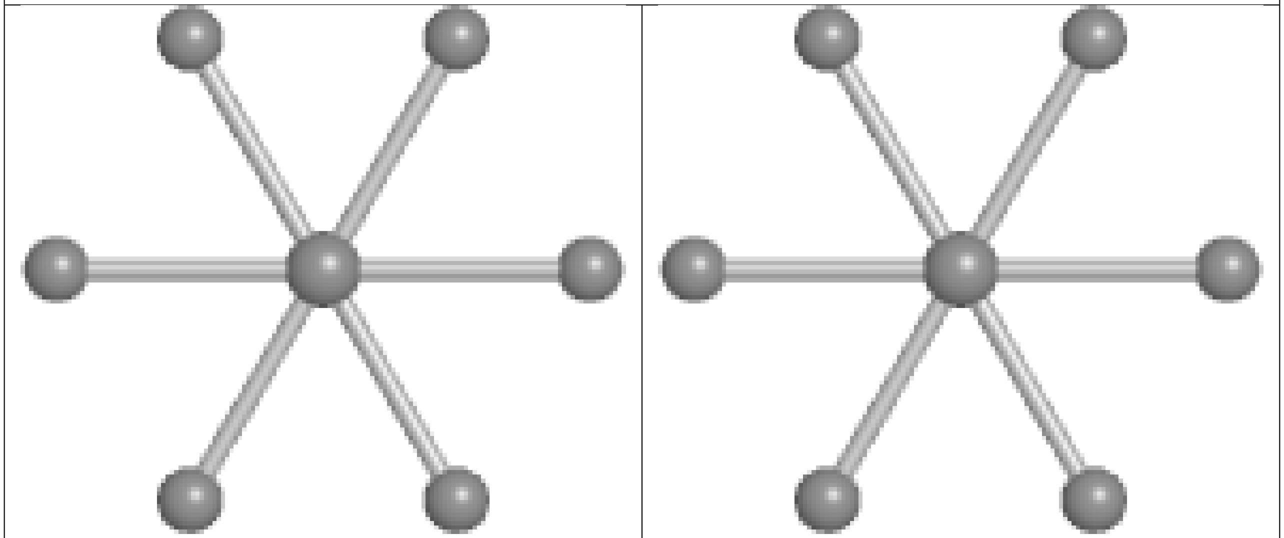


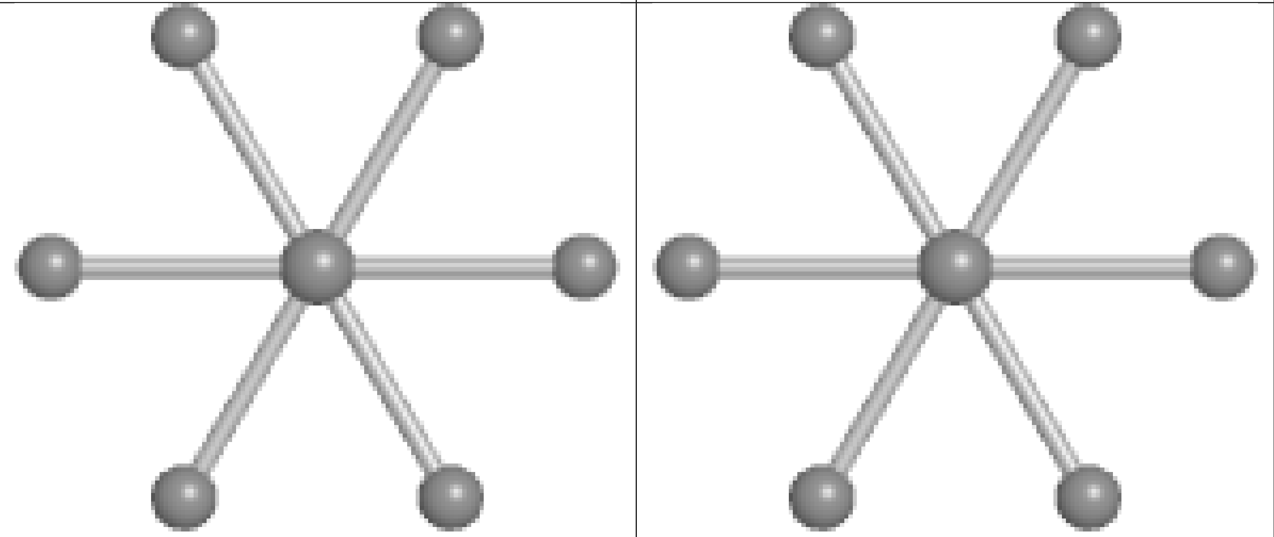
Rings

Ligand OHX 6 2328



Bond lengths

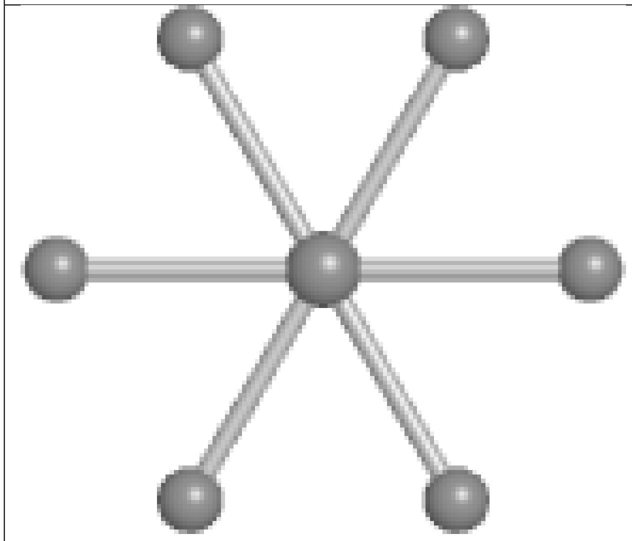
Bond angles



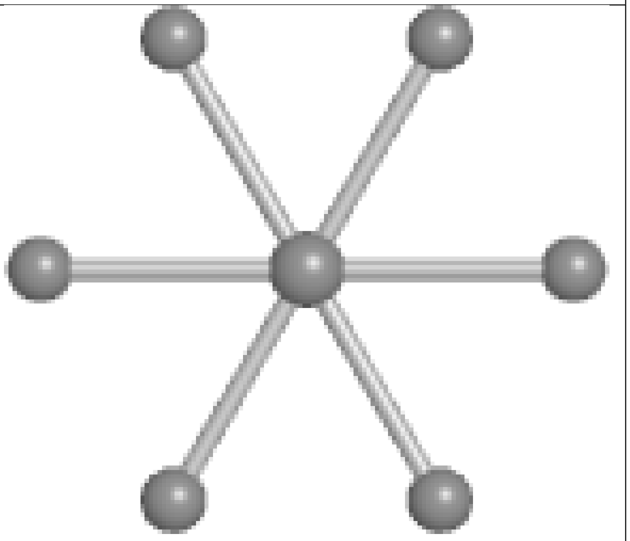
Torsions

Rings

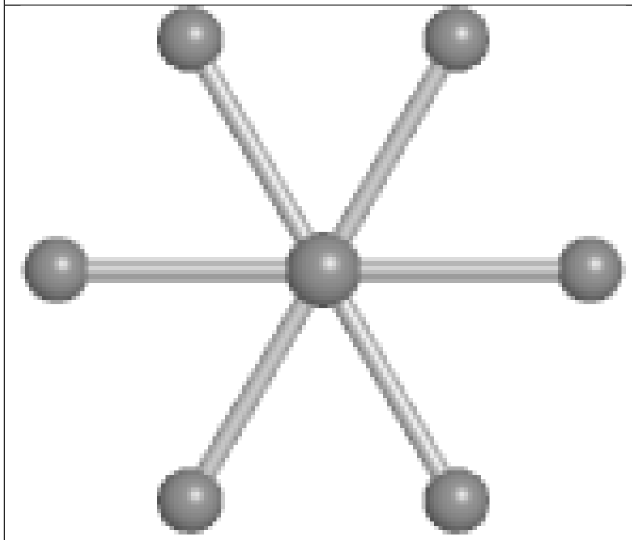
Ligand OHX 7 239



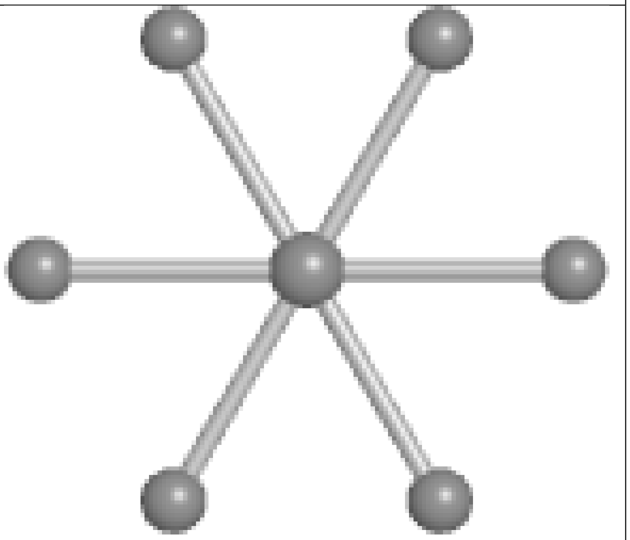
Bond lengths



Bond angles

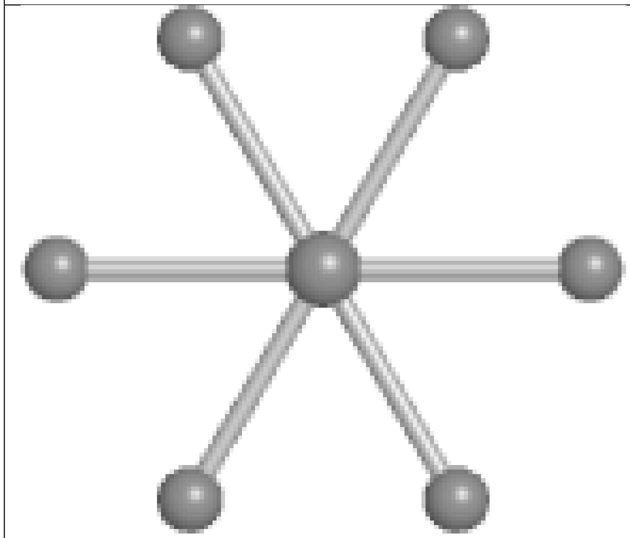


Torsions

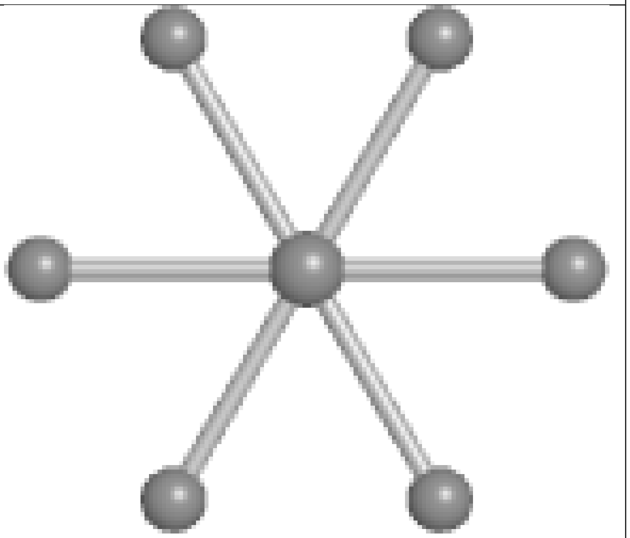


Rings

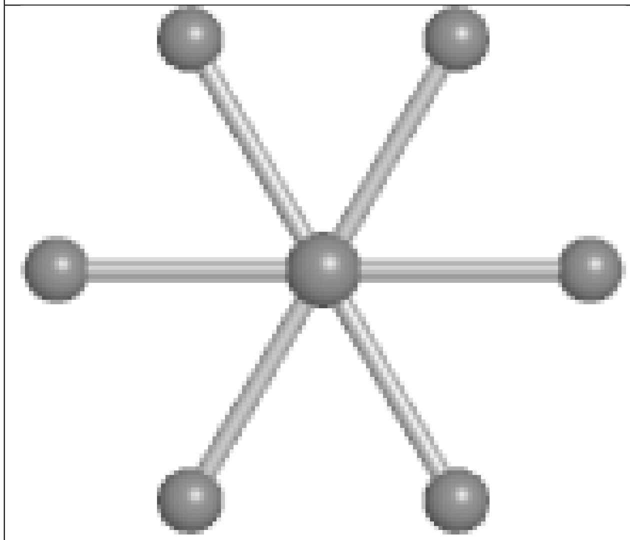
Ligand OHX 5 4528



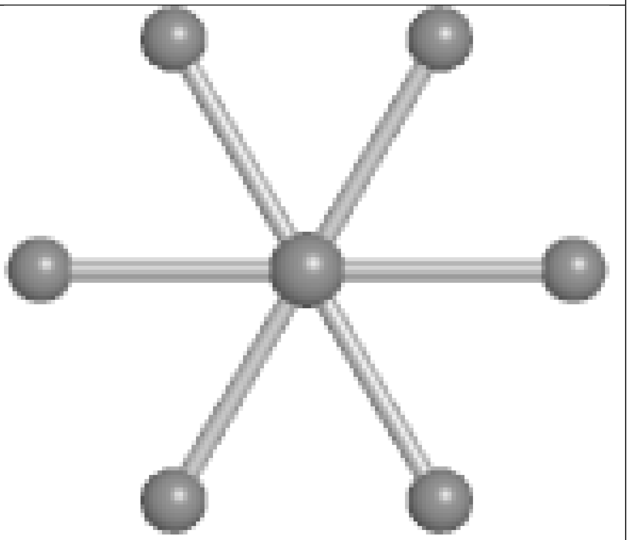
Bond lengths



Bond angles

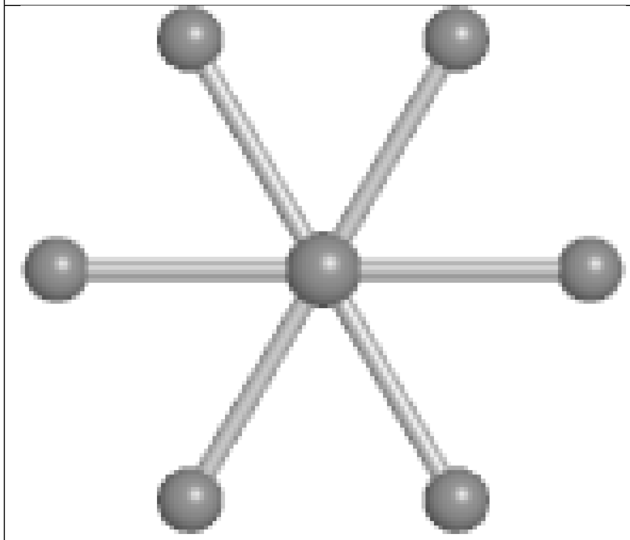


Torsions

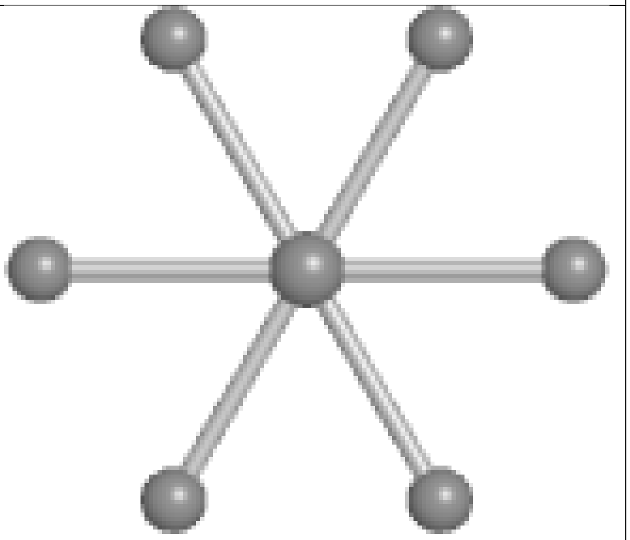


Rings

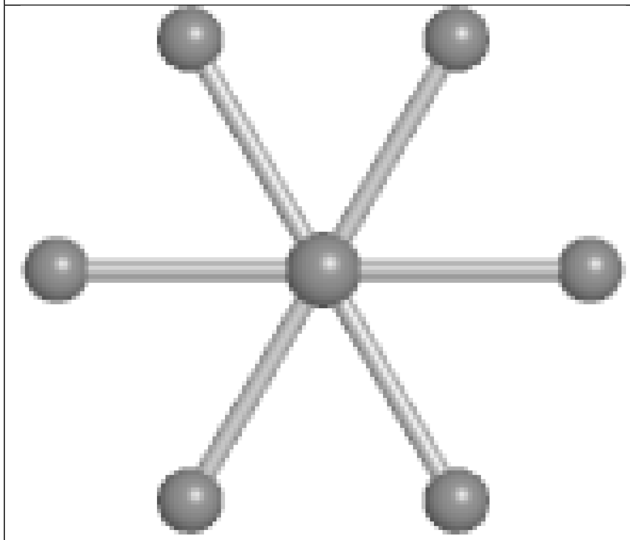
Ligand OHX 5 4513



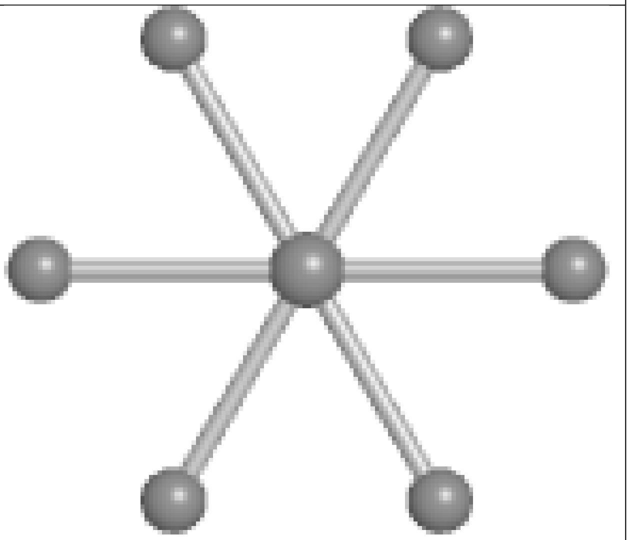
Bond lengths



Bond angles

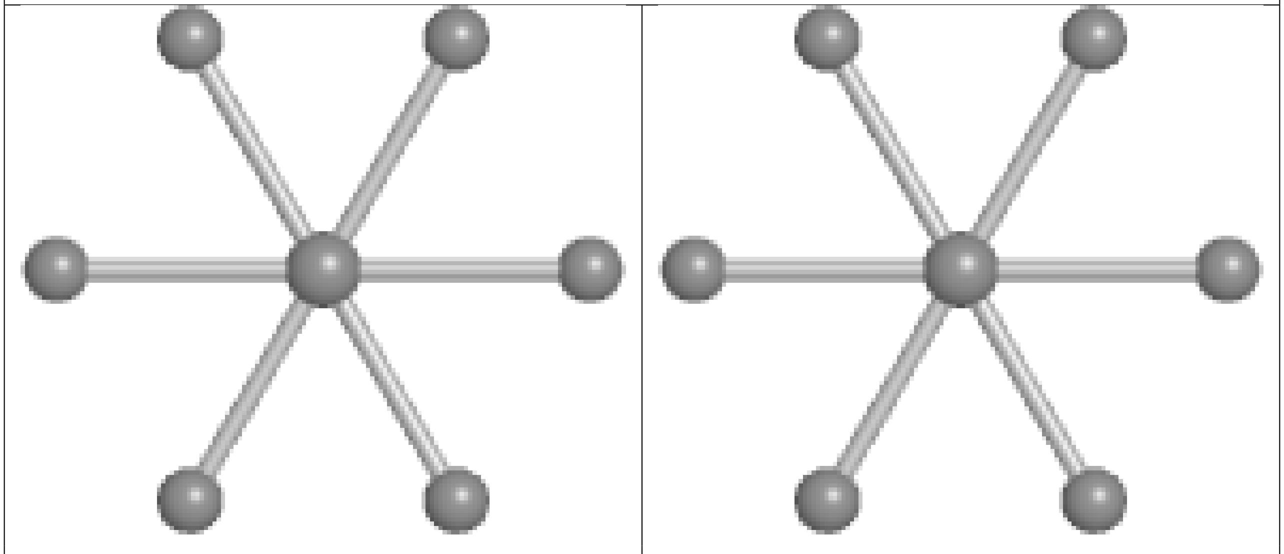


Torsions



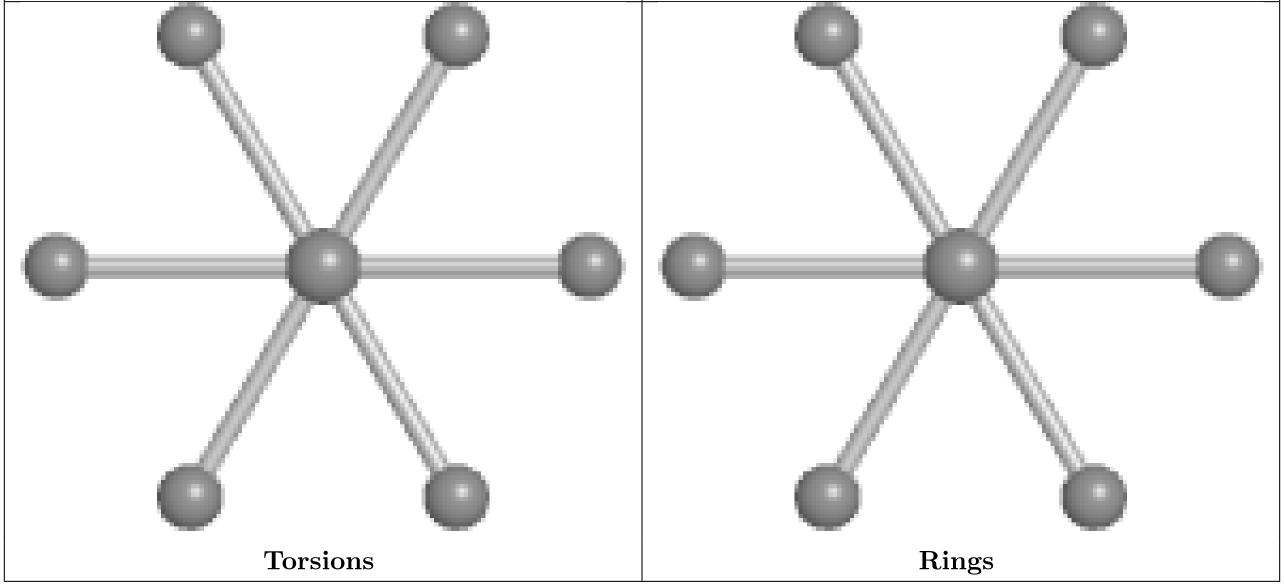
Rings

Ligand OHX 6 2314



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
84	sM	2
86	m2	2
35	SM	1

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Mol	Chain	Number of breaks
80	c0	1
1	2	1
6	s4	1
42	l5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	43.93
1	sM	139:UNK	C	155:UNK	N	38.21
1	SM	141:ALA	C	151:UNK	N	26.51
1	c0	84:UNK	C	87:UNK	N	7.82
1	2	1716:C	O3'	1717:G	P	3.78
1	m2	23:UNK	C	28:UNK	N	3.12
1	m2	52:UNK	C	54:UNK	N	3.12
1	s4	82:TYR	C	83:PRO	N	1.20
1	l5	179:ARG	C	180:PHE	N	1.18

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	2	1781/1800 (98%)	0.31	109 (6%)	21	20	66, 101, 181, 226	0
1	6	1795/1800 (99%)	0.20	78 (4%)	35	33	55, 93, 167, 227	0
2	S0	206/206 (100%)	2.12	109 (52%)	0	0	106, 120, 129, 135	0
2	s0	206/206 (100%)	1.46	57 (27%)	0	0	91, 107, 119, 120	0
3	S1	214/216 (99%)	0.60	29 (13%)	3	3	112, 144, 166, 170	0
3	s1	216/216 (100%)	0.99	36 (16%)	1	1	89, 100, 117, 126	0
4	S2	217/217 (100%)	2.11	100 (46%)	0	0	88, 100, 114, 121	0
4	s2	217/217 (100%)	1.25	45 (20%)	1	1	75, 90, 101, 110	0
5	S3	223/223 (100%)	1.08	53 (23%)	0	0	95, 105, 125, 136	0
5	s3	223/223 (100%)	0.28	12 (5%)	25	24	93, 115, 133, 138	0
6	S4	260/260 (100%)	1.19	60 (23%)	0	1	77, 102, 112, 131	0
6	s4	260/260 (100%)	0.84	27 (10%)	6	6	62, 90, 105, 125	0
7	S5	206/206 (100%)	1.33	46 (22%)	0	1	105, 121, 131, 140	0
7	s5	206/206 (100%)	1.03	41 (19%)	1	1	97, 116, 131, 137	0
8	S6	226/226 (100%)	1.01	45 (19%)	1	1	80, 112, 126, 133	0
8	s6	218/226 (96%)	1.00	35 (16%)	1	2	65, 92, 110, 121	0
9	S7	184/186 (98%)	0.37	11 (5%)	21	21	100, 124, 149, 154	0
9	s7	186/186 (100%)	0.91	29 (15%)	2	2	84, 115, 139, 144	0
10	S8	188/199 (94%)	1.32	44 (23%)	0	1	74, 89, 121, 132	0
10	s8	188/199 (94%)	0.84	26 (13%)	2	2	61, 83, 121, 139	0
11	S9	185/185 (100%)	1.47	61 (32%)	0	0	92, 109, 138, 156	0
11	s9	185/185 (100%)	0.36	16 (8%)	10	10	77, 95, 122, 136	0
12	C0	83/96 (86%)	-0.07	2 (2%)	59	55	98, 116, 126, 129	0
13	C1	146/155 (94%)	1.61	37 (25%)	0	0	76, 86, 106, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	c1	146/155 (94%)	1.58	36 (24%)	0	0	66, 81, 109, 129	0
14	C2	124/124 (100%)	0.48	12 (9%)	7	8	142, 150, 160, 162	0
15	C3	150/150 (100%)	0.29	6 (4%)	38	35	84, 99, 113, 118	0
15	c3	150/150 (100%)	0.39	8 (5%)	26	24	75, 88, 104, 107	0
16	C4	127/128 (99%)	0.59	20 (15%)	2	2	87, 145, 156, 158	0
16	c4	128/128 (100%)	1.75	56 (43%)	0	0	72, 104, 112, 117	0
17	C5	124/131 (94%)	0.75	14 (11%)	5	5	92, 105, 122, 138	0
18	C6	141/142 (99%)	1.31	37 (26%)	0	0	94, 114, 118, 121	0
18	c6	142/142 (100%)	1.30	42 (29%)	0	0	91, 111, 122, 135	0
19	C7	120/125 (96%)	1.43	39 (32%)	0	0	103, 116, 136, 138	0
19	c7	117/125 (93%)	0.65	12 (10%)	6	6	98, 111, 126, 134	0
20	C8	145/145 (100%)	0.91	24 (16%)	1	2	89, 109, 134, 139	0
20	c8	145/145 (100%)	0.91	26 (17%)	1	1	91, 105, 125, 130	0
21	C9	143/143 (100%)	1.26	27 (18%)	1	1	97, 109, 123, 130	0
21	c9	143/143 (100%)	1.20	36 (25%)	0	0	93, 105, 119, 128	0
22	D0	107/110 (97%)	1.12	24 (22%)	0	1	90, 117, 134, 136	0
22	d0	110/110 (100%)	1.43	33 (30%)	0	0	91, 121, 142, 148	0
23	D1	87/87 (100%)	2.20	47 (54%)	0	0	102, 110, 125, 131	0
23	d1	87/87 (100%)	1.56	28 (32%)	0	0	87, 96, 116, 122	0
24	D2	129/129 (100%)	1.52	39 (30%)	0	0	86, 97, 103, 115	0
24	d2	129/129 (100%)	1.54	39 (30%)	0	0	72, 82, 90, 98	0
25	D3	144/144 (100%)	0.81	12 (8%)	11	11	76, 81, 92, 104	0
25	d3	144/144 (100%)	0.62	11 (7%)	13	12	64, 69, 78, 90	0
26	D4	134/134 (100%)	0.24	6 (4%)	33	31	90, 110, 120, 125	0
26	d4	134/134 (100%)	0.33	7 (5%)	27	25	71, 94, 104, 110	0
27	D5	70/70 (100%)	0.56	5 (7%)	16	15	118, 130, 136, 138	0
27	d5	69/70 (98%)	0.80	9 (13%)	3	3	108, 121, 130, 131	0
28	D6	97/97 (100%)	2.17	42 (43%)	0	0	94, 110, 156, 157	0
28	d6	97/97 (100%)	2.94	72 (74%)	0	0	79, 92, 115, 120	0
29	D7	81/81 (100%)	0.43	5 (6%)	20	19	100, 113, 138, 141	0
29	d7	81/81 (100%)	0.73	12 (14%)	2	2	86, 100, 133, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
30	D8	63/63 (100%)	2.24	28 (44%) 0 0	115, 130, 137, 140	0
30	d8	63/63 (100%)	3.33	47 (74%) 0 0	111, 126, 132, 136	0
31	D9	53/53 (100%)	0.21	2 (3%) 40 37	89, 93, 112, 118	0
31	d9	53/53 (100%)	0.53	4 (7%) 14 13	90, 98, 126, 138	0
32	E0	60/62 (96%)	0.79	12 (20%) 1 1	82, 110, 134, 137	0
32	e0	62/62 (100%)	-0.09	1 (1%) 72 69	73, 97, 118, 122	0
33	E1	71/76 (93%)	1.05	15 (21%) 1 1	111, 138, 149, 152	0
33	e1	76/76 (100%)	1.89	31 (40%) 0 0	115, 163, 180, 182	0
34	SR	318/318 (100%)	1.62	109 (34%) 0 0	110, 122, 134, 155	0
35	SM	133/159 (83%)	1.47	34 (25%) 0 0	70, 100, 131, 138	0
36	1	3149/3394 (92%)	0.21	52 (1%) 70 67	44, 66, 136, 228	0
36	5	3150/3394 (92%)	0.20	39 (1%) 79 77	43, 64, 129, 201	0
37	3	121/121 (100%)	-0.19	0 100 100	52, 83, 98, 103	0
37	7	121/121 (100%)	-0.21	1 (0%) 86 86	48, 67, 79, 86	0
38	4	158/158 (100%)	0.09	2 (1%) 77 75	51, 67, 103, 140	0
38	8	158/158 (100%)	0.06	2 (1%) 77 75	53, 73, 107, 132	0
39	L2	252/252 (100%)	0.67	13 (5%) 27 25	51, 67, 83, 90	0
39	l2	252/252 (100%)	0.32	5 (1%) 65 63	52, 69, 84, 93	0
40	L3	386/386 (100%)	0.29	6 (1%) 72 69	49, 70, 82, 98	0
40	l3	386/386 (100%)	0.16	6 (1%) 72 69	44, 58, 71, 88	0
41	L4	361/361 (100%)	0.12	0 100 100	46, 62, 78, 81	0
41	l4	361/361 (100%)	0.27	10 (2%) 53 50	49, 66, 81, 90	0
42	L5	296/296 (100%)	0.98	54 (18%) 1 1	66, 90, 106, 125	0
42	l5	294/296 (99%)	0.28	6 (2%) 65 63	56, 70, 91, 107	0
43	L6	156/175 (89%)	0.36	1 (0%) 89 89	58, 66, 81, 92	0
43	l6	157/175 (89%)	0.31	3 (1%) 66 64	59, 66, 86, 97	0
44	L7	222/223 (99%)	0.10	2 (0%) 84 84	50, 58, 85, 115	0
44	l7	223/223 (100%)	0.01	0 100 100	49, 58, 91, 116	0
45	L8	233/233 (100%)	0.51	17 (7%) 15 14	74, 88, 117, 122	0
46	L9	191/191 (100%)	0.44	14 (7%) 15 14	68, 78, 88, 98	0
46	l9	191/191 (100%)	0.06	2 (1%) 82 82	54, 63, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
47	M0	211/220 (95%)	0.09	3 (1%)	75	74	55, 70, 100, 113	0
47	m0	213/220 (96%)	0.28	9 (4%)	36	33	51, 69, 89, 101	0
48	M1	169/169 (100%)	1.12	39 (23%)	0	1	78, 94, 104, 110	0
48	m1	169/169 (100%)	-0.18	0	100	100	61, 76, 85, 88	0
49	M3	193/194 (99%)	0.14	1 (0%)	91	90	49, 71, 105, 128	0
49	m3	194/194 (100%)	0.32	7 (3%)	42	39	52, 78, 112, 125	0
50	M4	136/137 (99%)	0.07	2 (1%)	73	71	62, 69, 79, 88	0
50	m4	137/137 (100%)	0.08	4 (2%)	51	50	57, 64, 81, 88	0
51	M5	203/203 (100%)	0.58	6 (2%)	50	48	50, 63, 74, 77	0
51	m5	203/203 (100%)	1.18	37 (18%)	1	1	54, 71, 82, 87	0
52	M6	197/197 (100%)	0.06	0	100	100	50, 58, 77, 81	0
52	m6	197/197 (100%)	0.02	0	100	100	44, 51, 77, 82	0
53	M7	183/183 (100%)	0.89	23 (12%)	3	3	53, 61, 108, 127	0
53	m7	155/183 (84%)	0.23	1 (0%)	89	89	49, 55, 67, 93	0
54	M8	185/185 (100%)	0.50	7 (3%)	40	37	51, 62, 78, 93	0
54	m8	185/185 (100%)	0.56	6 (3%)	47	45	51, 66, 77, 81	0
55	M9	188/188 (100%)	0.71	14 (7%)	14	14	70, 84, 147, 155	0
55	m9	188/188 (100%)	0.42	5 (2%)	54	51	63, 76, 134, 143	0
56	N0	172/172 (100%)	0.58	13 (7%)	13	12	59, 65, 77, 83	0
56	n0	172/172 (100%)	0.00	1 (0%)	89	89	52, 59, 70, 79	0
57	N1	159/159 (100%)	0.58	6 (3%)	40	37	51, 65, 104, 111	0
57	n1	159/159 (100%)	0.50	6 (3%)	40	37	51, 57, 95, 99	0
58	N2	100/100 (100%)	0.63	12 (12%)	4	4	100, 111, 117, 125	0
58	n2	98/100 (98%)	0.48	7 (7%)	16	15	88, 98, 103, 106	0
59	N3	136/136 (100%)	0.18	3 (2%)	62	59	57, 67, 77, 83	0
59	n3	136/136 (100%)	0.43	3 (2%)	62	59	45, 55, 65, 70	0
60	N4	98/98 (100%)	2.82	34 (34%)	0	0	66, 78, 138, 139	0
61	N5	121/121 (100%)	0.77	12 (9%)	7	7	63, 75, 90, 110	0
61	n5	120/121 (99%)	0.73	14 (11%)	4	4	66, 79, 95, 105	0
62	N6	126/126 (100%)	0.39	4 (3%)	47	45	56, 72, 81, 90	0
62	n6	126/126 (100%)	0.33	0	100	100	60, 76, 88, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
63	N7	135/135 (100%)	0.89	14 (10%)	6	6	88, 100, 110, 115	0
63	n7	135/135 (100%)	0.35	7 (5%)	27	25	93, 104, 116, 122	0
64	N8	148/148 (100%)	0.62	10 (6%)	17	16	44, 64, 84, 94	0
64	n8	148/148 (100%)	0.65	8 (5%)	25	24	44, 67, 84, 87	0
65	N9	58/58 (100%)	0.99	15 (25%)	0	0	48, 70, 103, 114	0
65	n9	58/58 (100%)	0.69	5 (8%)	10	10	48, 67, 86, 92	0
66	O0	97/100 (97%)	0.17	2 (2%)	63	61	87, 95, 113, 117	0
66	o0	100/100 (100%)	0.33	5 (5%)	28	26	84, 95, 111, 117	0
67	O1	109/109 (100%)	1.07	14 (12%)	3	3	67, 79, 99, 105	0
67	o1	109/109 (100%)	0.77	8 (7%)	15	14	57, 69, 96, 109	0
68	O2	127/127 (100%)	0.14	3 (2%)	59	55	46, 58, 72, 82	0
68	o2	127/127 (100%)	0.04	0	100	100	46, 62, 75, 82	0
69	O3	106/106 (100%)	0.27	0	100	100	49, 57, 77, 86	0
69	o3	106/106 (100%)	0.37	1 (0%)	84	84	49, 56, 80, 90	0
70	O4	112/112 (100%)	1.26	27 (24%)	0	0	63, 80, 115, 124	0
70	o4	112/112 (100%)	0.43	6 (5%)	25	24	62, 82, 116, 121	0
71	O5	119/119 (100%)	0.37	4 (3%)	45	42	61, 78, 86, 93	0
71	o5	119/119 (100%)	0.21	1 (0%)	86	86	68, 83, 96, 106	0
72	O6	99/99 (100%)	0.03	2 (2%)	65	63	68, 77, 102, 116	0
72	o6	99/99 (100%)	0.14	3 (3%)	50	48	76, 85, 101, 114	0
73	O7	87/87 (100%)	0.74	7 (8%)	12	11	51, 57, 76, 86	0
73	o7	87/87 (100%)	0.67	2 (2%)	60	58	49, 58, 85, 99	0
74	O8	77/77 (100%)	0.15	1 (1%)	77	75	89, 100, 114, 117	0
74	o8	77/77 (100%)	1.28	15 (19%)	1	1	88, 99, 108, 110	0
75	O9	50/50 (100%)	0.78	4 (8%)	12	11	60, 64, 69, 69	0
75	o9	50/50 (100%)	0.89	6 (12%)	4	4	59, 65, 72, 74	0
76	Q0	52/52 (100%)	0.68	6 (11%)	4	4	62, 67, 82, 91	0
76	q0	52/52 (100%)	-0.06	0	100	100	50, 54, 65, 68	0
77	Q1	25/25 (100%)	0.10	0	100	100	69, 74, 78, 79	0
77	q1	25/25 (100%)	0.03	0	100	100	62, 63, 65, 66	0
78	Q2	105/105 (100%)	1.41	27 (25%)	0	0	54, 67, 86, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
78	q2	105/105 (100%)	1.07	16 (15%) 2 2	54, 66, 80, 100	0
79	Q3	91/91 (100%)	0.38	2 (2%) 62 59	58, 71, 85, 91	0
79	q3	91/91 (100%)	0.23	3 (3%) 46 43	54, 69, 81, 89	0
80	c0	79/96 (82%)	0.52	8 (10%) 7 7	108, 133, 143, 145	0
81	c2	109/124 (87%)	1.77	44 (40%) 0 0	173, 185, 191, 194	0
82	c5	135/142 (95%)	0.41	9 (6%) 17 17	84, 110, 123, 125	0
83	sR	318/318 (100%)	1.63	104 (32%) 0 0	117, 131, 143, 156	0
84	sM	63/104 (60%)	0.85	9 (14%) 2 2	61, 111, 117, 122	0
85	l8	225/231 (97%)	0.94	25 (11%) 5 5	83, 95, 118, 123	0
86	m2	0/150	-	-	-	-
87	n4	135/135 (100%)	1.31	39 (28%) 0 0	54, 97, 121, 135	0
88	p0	120/219 (54%)	1.69	45 (37%) 0 0	103, 120, 135, 142	0
89	p1	0/47	-	-	-	-
89	p2	0/47	-	-	-	-
90	A	2/3 (66%)	1.12	0 100 100	106, 106, 106, 107	0
90	a	2/3 (66%)	1.24	0 100 100	100, 100, 100, 102	0
All	All	32948/34108 (96%)	0.58	3198 (9%) 7 8	43, 82, 136, 228	0

All (3198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	26.0
13	c1	3	THR	16.4
60	N4	75	THR	14.6
60	N4	84	GLY	14.3
60	N4	85	ALA	14.2
13	C1	145	ALA	13.4
35	SM	16	ASP	13.0
13	C1	146	ALA	12.2
60	N4	76	VAL	12.0
53	M7	162	GLU	11.7
78	Q2	106	PHE	11.7
1	2	1702	A	11.5
1	2	715	U	11.4
60	N4	88	ASP	11.2
13	c1	2	SER	11.1
60	N4	87	LEU	11.1

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Mol	Chain	Res	Type	RSRZ
40	L3	387	LEU	10.8
53	M7	160	ALA	10.8
60	N4	83	THR	10.8
53	M7	184	ALA	10.6
53	M7	161	ALA	10.6
1	2	656	G	10.5
1	2	719	U	10.3
36	1	1955	U	10.3
1	2	1693	A	10.1
1	2	1699	G	10.0
1	2	1698	G	10.0
1	6	663	U	9.7
28	D6	2	PRO	9.7
60	N4	78	ALA	9.6
4	s2	90	THR	9.5
82	c5	134	THR	9.3
30	d8	43	ASN	9.3
60	N4	90	ILE	9.1
1	6	678	A	9.0
33	E1	87	THR	9.0
1	2	1711	C	8.9
1	6	662	U	8.9
1	2	1696	G	8.8
7	s5	152	GLY	8.7
87	n4	70	LYS	8.7
13	c1	4	GLU	8.6
1	2	1697	G	8.6
34	SR	79	TYR	8.6
30	D8	67	ARG	8.5
36	1	1570	U	8.5
1	2	1694	A	8.4
78	Q2	105	GLN	8.3
7	s5	151	GLY	8.3
60	N4	89	LEU	8.3
22	D0	120	SER	8.2
1	2	1692	G	8.1
1	2	1709	C	8.0
28	D6	90	GLU	8.0
28	D6	91	ASP	7.8
13	C1	4	GLU	7.8
35	SM	87	THR	7.8
60	N4	73	ARG	7.8

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Mol	Chain	Res	Type	RSRZ
1	2	1710	U	7.7
61	N5	24	LEU	7.7
13	c1	145	ALA	7.6
30	d8	21	SER	7.5
60	N4	82	ILE	7.5
83	sR	252	LEU	7.5
33	e1	110	ALA	7.5
1	6	679	U	7.4
1	2	714	G	7.4
36	5	1567	U	7.4
1	2	658	C	7.4
28	d6	68	TYR	7.3
28	d6	11	ASN	7.3
1	2	718	U	7.3
1	2	1708	U	7.3
13	C1	2	SER	7.3
87	n4	69	LYS	7.3
7	s5	153	GLY	7.3
60	N4	81	PRO	7.1
35	SM	15	ALA	7.1
35	SM	88	ARG	7.1
34	SR	115	ILE	7.0
13	C1	147	ALA	7.0
81	c2	92	ALA	7.0
28	D6	85	ARG	7.0
81	c2	126	TRP	7.0
60	N4	77	LYS	6.9
35	SM	84	LYS	6.9
87	n4	67	VAL	6.9
1	2	1695	G	6.9
1	2	716	C	6.9
22	d0	98	GLN	6.9
30	d8	9	LEU	6.9
87	n4	66	GLU	6.9
60	N4	72	SER	6.8
35	SM	14	ASP	6.8
28	d6	44	ILE	6.8
13	c1	5	LEU	6.8
1	2	1703	C	6.7
7	S5	152	GLY	6.7
28	D6	8	ASN	6.7
60	N4	69	LYS	6.7

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Mol	Chain	Res	Type	RSRZ
33	e1	80	ARG	6.7
87	n4	68	ALA	6.7
35	SM	89	ARG	6.7
20	c8	18	LEU	6.7
1	2	657	U	6.7
4	s2	87	GLN	6.7
1	2	1700	C	6.6
35	SM	85	SER	6.6
6	S4	261	LEU	6.6
1	2	1707	A	6.6
30	d8	67	ARG	6.6
7	s5	37	GLN	6.6
22	d0	93	LEU	6.5
1	2	1701	A	6.5
1	6	658	C	6.5
13	C1	3	THR	6.5
30	d8	65	ARG	6.5
7	s5	145	ASP	6.5
10	S8	152	ILE	6.5
36	5	1569	U	6.5
4	S2	88	LYS	6.5
35	SM	18	VAL	6.4
60	N4	70	LYS	6.4
36	5	1350	A	6.4
28	D6	94	ASN	6.4
28	d6	69	ASN	6.4
2	S0	97	PRO	6.4
33	e1	111	GLU	6.4
5	S3	152	PHE	6.4
23	D1	10	GLU	6.4
2	S0	98	ILE	6.3
28	D6	89	ARG	6.3
1	2	1691	A	6.3
83	sR	214	ALA	6.3
35	SM	19	VAL	6.3
1	2	717	C	6.2
1	2	134	U	6.2
36	1	1569	U	6.2
11	S9	97	LEU	6.2
30	d8	66	LEU	6.2
81	c2	123	VAL	6.2
30	d8	13	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	2	1686	C	6.2
28	D6	88	SER	6.2
83	sR	24	ALA	6.1
1	6	676	G	6.1
56	N0	1	MET	6.1
5	S3	154	ASP	6.1
1	6	239	C	6.1
7	s5	150	GLY	6.1
36	5	1025	A	6.1
28	D6	86	VAL	6.0
3	S1	20	VAL	6.0
83	sR	314	GLN	6.0
28	D6	92	ARG	6.0
33	e1	85	TYR	6.0
48	M1	127	PHE	6.0
6	S4	253	ASP	6.0
7	s5	154	ALA	6.0
1	6	656	G	6.0
4	s2	88	LYS	5.9
3	S1	25	THR	5.9
30	D8	19	THR	5.9
47	m0	221	ALA	5.9
76	Q0	77	ILE	5.9
36	5	1349	G	5.9
34	SR	33	LEU	5.9
34	SR	72	THR	5.9
1	6	659	C	5.9
70	O4	23	VAL	5.8
13	c1	116	ARG	5.8
1	2	1690	G	5.8
36	5	1566	A	5.8
7	S5	153	GLY	5.8
1	2	1705	C	5.8
8	s6	169	TYR	5.8
30	D8	66	LEU	5.8
7	S5	154	ALA	5.8
23	D1	55	LEU	5.7
4	s2	89	GLN	5.7
10	S8	200	LYS	5.7
60	N4	74	LYS	5.7
36	1	1568	U	5.7
7	S5	151	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
30	d8	44	VAL	5.7
81	c2	65	SER	5.7
36	1	1350	A	5.7
21	c9	22	LEU	5.7
28	D6	84	VAL	5.7
35	SM	86	ASN	5.7
60	N4	71	ARG	5.7
45	L8	116	VAL	5.6
83	sR	316	MET	5.6
34	SR	43	ILE	5.6
32	E0	61	SER	5.6
7	s5	161	ASP	5.6
1	2	1706	C	5.6
31	d9	4	GLU	5.6
2	s0	46	HIS	5.5
8	S6	50	PHE	5.5
83	sR	7	LEU	5.5
7	S5	147	THR	5.5
1	6	677	G	5.5
28	D6	98	PRO	5.5
53	M7	157	VAL	5.5
4	S2	87	GLN	5.4
21	c9	55	TYR	5.4
1	6	1799	U	5.4
21	c9	18	TYR	5.4
82	c5	4	ALA	5.4
17	C5	50	THR	5.4
22	d0	99	ILE	5.4
82	c5	136	SER	5.4
1	2	723	G	5.4
36	1	1351	U	5.4
7	s5	155	ALA	5.4
83	sR	72	THR	5.4
11	S9	95	TYR	5.4
20	C8	2	SER	5.4
6	S4	256	ARG	5.4
53	M7	163	LYS	5.4
1	2	724	C	5.4
1	6	1710	U	5.4
67	O1	82	GLU	5.4
23	d1	87	ARG	5.3
7	S5	37	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	6	1711	C	5.3
1	6	1800	A	5.3
22	d0	18	GLN	5.3
4	S2	90	THR	5.3
8	s6	164	LYS	5.3
85	l8	120	LYS	5.3
1	6	668	C	5.3
11	S9	89	ASP	5.3
82	c5	135	THR	5.3
9	s7	58	LEU	5.3
28	d6	10	ARG	5.2
1	6	1695	G	5.2
1	6	666	U	5.2
20	c8	22	VAL	5.2
22	d0	97	VAL	5.2
58	N2	27	VAL	5.2
36	1	1349	G	5.2
28	D6	93	LYS	5.2
33	e1	77	GLY	5.2
46	L9	190	ASP	5.2
11	S9	60	LEU	5.1
67	o1	82	GLU	5.1
30	d8	33	LEU	5.1
34	SR	27	ALA	5.1
84	sM	84	LYS	5.1
28	d6	98	PRO	5.1
8	S6	175	ILE	5.1
34	SR	181	TRP	5.1
1	2	194	U	5.1
81	c2	41	LEU	5.0
8	S6	36	VAL	5.0
5	s3	151	LYS	5.0
30	d8	56	LEU	5.0
1	2	1704	U	5.0
62	N6	127	GLU	5.0
7	s5	158	GLN	5.0
2	S0	126	PRO	5.0
83	sR	121	MET	5.0
2	s0	170	ILE	5.0
60	N4	66	GLU	5.0
53	M7	183	ALA	5.0
35	SM	17	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	6	664	U	5.0
36	5	1351	U	5.0
78	q2	106	PHE	5.0
23	D1	53	TYR	5.0
4	S2	64	LYS	5.0
2	S0	146	LEU	5.0
1	2	711	U	5.0
60	N4	68	ALA	5.0
42	L5	95	TRP	5.0
28	d6	41	ILE	5.0
36	5	2503	G	5.0
30	D8	28	VAL	5.0
78	Q2	99	GLN	5.0
4	S2	146	THR	5.0
34	SR	34	LEU	5.0
7	S5	222	LYS	5.0
36	5	1568	U	5.0
4	S2	69	ILE	4.9
23	D1	33	GLN	4.9
2	S0	122	ILE	4.9
78	Q2	102	GLN	4.9
24	D2	18	GLU	4.9
13	C1	144	ALA	4.9
11	S9	87	SER	4.9
23	D1	8	LEU	4.9
7	s5	225	ARG	4.9
9	s7	187	SER	4.9
36	5	1580	A	4.9
9	s7	52	ALA	4.9
1	6	675	U	4.9
1	2	1712	A	4.9
18	C6	20	ALA	4.9
23	D1	24	ILE	4.9
2	S0	107	PHE	4.9
83	sR	3	SER	4.9
33	e1	112	GLY	4.9
28	D6	3	LYS	4.9
83	sR	157	VAL	4.8
4	S2	94	GLN	4.8
7	S5	70	VAL	4.8
83	sR	158	PRO	4.8
16	c4	102	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
2	S0	170	ILE	4.8
33	E1	86	THR	4.8
78	Q2	92	GLU	4.8
78	Q2	104	LEU	4.8
1	6	1702	A	4.8
34	SR	81	LEU	4.8
1	6	660	G	4.8
1	6	794	U	4.8
28	d6	71	LEU	4.8
30	D8	16	LEU	4.8
4	S2	57	PHE	4.8
4	S2	55	GLU	4.8
36	5	2507	C	4.8
10	s8	200	LYS	4.8
28	d6	73	TYR	4.8
42	L5	146	LEU	4.8
83	sR	123	ILE	4.8
33	e1	87	THR	4.8
23	D1	1	MET	4.8
2	S0	158	VAL	4.8
13	c1	117	VAL	4.8
48	M1	83	GLY	4.7
84	sM	75	ASP	4.7
16	c4	48	VAL	4.7
6	S4	251	GLU	4.7
7	S5	71	ALA	4.7
18	c6	49	TYR	4.7
34	SR	32	LEU	4.7
53	M7	159	LYS	4.7
19	c7	2	GLY	4.7
16	C4	47	LYS	4.7
28	d6	86	VAL	4.7
30	D8	21	SER	4.7
1	6	653	C	4.7
45	L8	121	SER	4.7
7	S5	148	ARG	4.7
83	sR	251	TRP	4.7
1	2	677	G	4.7
83	sR	25	THR	4.7
2	S0	110	TYR	4.7
11	S9	86	LEU	4.7
67	o1	112	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
33	e1	98	VAL	4.7
36	5	2506	U	4.7
2	S0	102	PHE	4.7
2	s0	165	ARG	4.6
88	p0	192	ASP	4.6
23	D1	34	ILE	4.6
84	sM	83	LYS	4.6
1	6	1707	A	4.6
34	SR	46	LYS	4.6
4	S2	162	CYS	4.6
81	c2	59	LEU	4.6
28	d6	90	GLU	4.6
33	e1	86	THR	4.6
20	c8	17	LEU	4.6
2	S0	127	ARG	4.6
4	S2	141	ARG	4.6
26	D4	70	VAL	4.6
83	sR	168	THR	4.6
28	d6	88	SER	4.6
20	c8	73	MET	4.6
1	6	665	U	4.6
16	c4	53	ASP	4.6
18	c6	52	LEU	4.6
28	d6	85	ARG	4.6
30	D8	27	GLN	4.6
7	S5	165	LEU	4.6
28	d6	42	ARG	4.6
40	L3	386	ASP	4.6
8	s6	162	VAL	4.6
28	d6	45	VAL	4.6
42	L5	159	VAL	4.6
7	s5	137	ILE	4.5
83	sR	79	TYR	4.5
83	sR	254	ALA	4.5
30	D8	44	VAL	4.5
83	sR	92	TRP	4.5
66	o0	7	GLN	4.5
79	q3	2	ALA	4.5
1	6	232	U	4.5
20	C8	18	LEU	4.5
4	S2	62	PRO	4.5
7	S5	155	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
78	Q2	2	VAL	4.5
16	C4	76	ILE	4.5
87	n4	134	GLN	4.5
2	S0	201	LEU	4.5
11	S9	64	GLU	4.5
87	n4	135	SER	4.5
3	S1	26	ARG	4.5
30	d8	57	MET	4.5
16	c4	98	GLY	4.5
28	d6	9	GLY	4.5
23	D1	32	VAL	4.5
30	d8	63	ALA	4.5
53	M7	182	ILE	4.4
28	d6	64	LEU	4.4
1	2	913	G	4.4
30	D8	43	ASN	4.4
16	C4	15	GLY	4.4
16	c4	97	GLY	4.4
81	c2	43	ARG	4.4
85	l8	109	LEU	4.4
2	S0	174	TRP	4.4
30	d8	42	ARG	4.4
16	c4	55	SER	4.4
42	L5	127	GLY	4.4
81	c2	64	SER	4.4
87	n4	72	SER	4.4
59	n3	2	SER	4.4
83	sR	32	LEU	4.4
60	N4	79	GLN	4.4
1	2	132	U	4.4
30	d8	45	LYS	4.4
83	sR	315	VAL	4.4
84	sM	85	SER	4.4
2	S0	99	ALA	4.4
4	s2	64	LYS	4.4
7	s5	156	ARG	4.4
83	sR	6	VAL	4.4
16	c4	117	ASP	4.4
22	D0	20	ILE	4.4
13	c1	146	ALA	4.4
42	L5	189	GLU	4.4
2	s0	186	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
4	S2	45	VAL	4.4
30	D8	15	VAL	4.4
2	S0	198	MET	4.4
28	D6	7	SER	4.4
34	SR	52	GLN	4.4
46	L9	189	GLU	4.4
25	d3	2	GLY	4.4
87	n4	84	GLY	4.4
78	Q2	15	LYS	4.4
61	N5	23	ALA	4.4
6	S4	54	TYR	4.4
70	O4	21	LYS	4.4
3	s1	152	ARG	4.4
28	d6	91	ASP	4.4
33	E1	148	TYR	4.3
24	D2	70	ASN	4.3
33	E1	124	PRO	4.3
83	sR	82	SER	4.3
16	c4	60	ALA	4.3
34	SR	44	SER	4.3
30	D8	45	LYS	4.3
6	S4	252	ARG	4.3
18	C6	5	PRO	4.3
36	1	1352	A	4.3
32	E0	54	ARG	4.3
4	s2	92	ALA	4.3
7	S5	150	GLY	4.3
75	o9	51	ILE	4.3
1	6	194	U	4.3
24	D2	92	ASN	4.3
6	s4	183	VAL	4.3
11	S9	80	LEU	4.3
1	6	1701	A	4.3
4	S2	222	TYR	4.3
83	sR	245	PHE	4.3
16	c4	99	GLN	4.3
28	D6	6	ALA	4.3
81	c2	121	VAL	4.3
36	1	1567	U	4.3
18	C6	52	LEU	4.3
2	S0	144	ILE	4.3
35	SM	20	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
83	sR	33	LEU	4.3
30	d8	59	SER	4.3
20	c8	146	ALA	4.3
30	d8	48	VAL	4.3
83	sR	227	ALA	4.3
85	l8	121	SER	4.2
11	S9	156	ILE	4.2
34	SR	103	PHE	4.2
8	s6	147	LEU	4.2
2	S0	104	PRO	4.2
28	D6	9	GLY	4.2
63	N7	70	PRO	4.2
83	sR	166	SER	4.2
10	S8	179	CYS	4.2
1	6	657	U	4.2
4	s2	118	ALA	4.2
5	S3	135	GLU	4.2
34	SR	102	ARG	4.2
83	sR	81	LEU	4.2
23	d1	82	VAL	4.2
34	SR	25	THR	4.2
83	sR	313	TRP	4.2
11	s9	184	SER	4.2
21	C9	2	PRO	4.2
22	d0	64	LYS	4.2
53	M7	168	LEU	4.2
74	o8	69	LEU	4.2
20	c8	14	ILE	4.2
24	D2	41	MET	4.2
35	SM	21	PRO	4.2
46	L9	191	LEU	4.2
30	D8	6	PRO	4.2
81	c2	104	ALA	4.2
33	e1	145	HIS	4.2
2	S0	29	VAL	4.2
83	sR	319	ASN	4.2
1	2	1713	G	4.2
28	D6	87	ARG	4.2
19	C7	2	GLY	4.2
6	S4	257	ALA	4.2
24	d2	2	THR	4.2
4	s2	84	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
21	C9	39	THR	4.2
28	d6	66	LYS	4.2
30	D8	41	VAL	4.2
81	c2	103	LEU	4.2
4	S2	223	GLY	4.2
30	d8	12	VAL	4.2
18	c6	29	ILE	4.2
7	S5	161	ASP	4.1
16	c4	92	LYS	4.1
28	D6	83	ILE	4.1
30	d8	61	ARG	4.1
23	D1	31	SER	4.1
36	1	1581	C	4.1
18	c6	142	TYR	4.1
35	SM	99	LYS	4.1
4	S2	144	TRP	4.1
24	D2	81	VAL	4.1
13	C1	30	ARG	4.1
5	S3	185	LYS	4.1
34	SR	117	LYS	4.1
28	D6	80	HIS	4.1
42	L5	51	LEU	4.1
7	s5	159	ALA	4.1
4	s2	93	GLY	4.1
23	D1	23	ILE	4.1
1	2	1688	U	4.1
18	c6	19	VAL	4.1
88	p0	187	VAL	4.1
18	C6	6	SER	4.1
83	sR	116	ASP	4.1
16	C4	41	ARG	4.1
1	6	1709	C	4.1
4	S2	86	VAL	4.1
60	N4	67	VAL	4.1
88	p0	27	VAL	4.1
21	c9	37	VAL	4.1
4	s2	95	ARG	4.1
5	S3	184	ILE	4.1
16	c4	108	SER	4.1
21	c9	19	ALA	4.1
28	d6	40	ALA	4.1
2	S0	141	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
28	d6	70	LYS	4.1
33	E1	85	TYR	4.1
27	d5	51	LEU	4.1
58	N2	28	PHE	4.1
6	S4	254	ARG	4.1
71	O5	120	ALA	4.1
30	d8	27	GLN	4.1
8	s6	171	LYS	4.0
30	d8	22	ARG	4.0
30	d8	15	VAL	4.0
40	l3	387	LEU	4.0
36	5	2505	U	4.0
11	S9	65	LYS	4.0
13	C1	13	PHE	4.0
78	Q2	100	LYS	4.0
29	d7	24	LEU	4.0
58	N2	92	TRP	4.0
3	S1	94	LYS	4.0
2	S0	153	SER	4.0
2	s0	146	LEU	4.0
18	C6	143	ARG	4.0
16	c4	103	ARG	4.0
18	C6	57	LEU	4.0
75	O9	2	ALA	4.0
83	sR	4	ASN	4.0
87	n4	131	ALA	4.0
55	M9	50	ILE	4.0
6	S4	255	ARG	4.0
28	d6	17	HIS	4.0
2	s0	98	ILE	4.0
42	L5	190	ILE	4.0
8	s6	116	LYS	4.0
30	d8	14	LYS	4.0
4	S2	154	LEU	4.0
2	S0	155	PHE	4.0
4	S2	82	ASN	4.0
19	C7	71	PHE	4.0
7	s5	144	GLU	4.0
1	2	1398	U	4.0
82	c5	133	ALA	4.0
33	e1	83	LYS	4.0
33	E1	145	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
4	S2	224	PHE	4.0
58	N2	93	ILE	4.0
2	S0	83	GLN	4.0
2	S0	157	ASP	4.0
18	c6	28	LEU	4.0
8	S6	145	PHE	4.0
23	d1	34	ILE	4.0
28	d6	93	LYS	4.0
83	sR	244	ALA	4.0
2	S0	138	TYR	3.9
18	C6	92	TYR	3.9
58	N2	108	TYR	3.9
35	SM	106	VAL	3.9
4	S2	240	LEU	3.9
34	SR	49	GLY	3.9
24	D2	37	PHE	3.9
34	SR	92	TRP	3.9
63	N7	92	PHE	3.9
42	L5	221	GLU	3.9
4	S2	63	VAL	3.9
10	s8	80	GLY	3.9
21	c9	119	LYS	3.9
28	d6	7	SER	3.9
45	L8	120	LYS	3.9
70	O4	113	LYS	3.9
21	c9	101	ASN	3.9
3	S1	50	LYS	3.9
7	s5	83	ARG	3.9
11	s9	148	VAL	3.9
16	c4	79	VAL	3.9
18	C6	7	VAL	3.9
1	2	720	G	3.9
4	S2	66	PHE	3.9
28	d6	8	ASN	3.9
36	1	2502	A	3.9
2	s0	110	TYR	3.9
18	C6	142	TYR	3.9
2	S0	156	VAL	3.9
3	s1	54	LEU	3.9
11	S9	76	LEU	3.9
45	L8	119	GLY	3.9
83	sR	13	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
22	d0	22	ILE	3.9
25	d3	3	LYS	3.9
28	D6	49	ALA	3.9
1	6	1712	A	3.9
5	S3	218	LEU	3.9
30	D8	7	VAL	3.9
4	S2	164	SER	3.9
34	SR	121	MET	3.9
88	p0	188	VAL	3.9
18	c6	64	ASP	3.9
3	s1	111	ARG	3.9
30	d8	26	THR	3.9
87	n4	95	SER	3.9
1	2	709	C	3.9
36	1	1239	C	3.9
33	e1	134	ASN	3.9
10	S8	72	ILE	3.9
10	S8	96	LEU	3.9
23	d1	43	GLY	3.9
1	6	1700	C	3.9
83	sR	263	PHE	3.9
2	S0	76	ILE	3.9
24	D2	130	TYR	3.9
28	d6	3	LYS	3.9
83	sR	138	GLY	3.9
1	6	655	G	3.9
28	D6	48	ALA	3.9
88	p0	80	VAL	3.9
16	c4	44	GLY	3.9
21	C9	80	TYR	3.9
30	D8	65	ARG	3.9
2	S0	203	PHE	3.9
60	N4	98	PRO	3.9
22	d0	14	GLN	3.9
22	d0	54	GLY	3.8
8	s6	35	GLU	3.8
1	6	661	A	3.8
4	S2	41	LEU	3.8
30	d8	10	ALA	3.8
65	N9	55	ALA	3.8
2	S0	175	TYR	3.8
6	S4	208	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
30	D8	25	VAL	3.8
24	d2	85	ASP	3.8
1	2	135	A	3.8
49	m3	189	GLU	3.8
13	c1	139	VAL	3.8
53	M7	165	VAL	3.8
35	SM	101	ASP	3.8
4	S2	95	ARG	3.8
50	M4	138	ALA	3.8
4	S2	151	PRO	3.8
6	s4	207	LEU	3.8
1	2	1370	U	3.8
3	s1	114	VAL	3.8
20	c8	15	LEU	3.8
23	D1	40	ASP	3.8
8	S6	157	VAL	3.8
84	sM	52	PRO	3.8
73	o7	88	ALA	3.8
1	2	678	A	3.8
28	d6	80	HIS	3.8
36	1	1571	A	3.8
21	C9	108	LEU	3.8
28	d6	19	LYS	3.8
31	d9	5	ASN	3.8
33	e1	79	LYS	3.8
49	m3	190	LYS	3.8
70	O4	33	GLN	3.8
81	c2	57	ALA	3.8
50	m4	2	SER	3.8
48	M1	79	ILE	3.8
42	l5	296	GLN	3.8
16	c4	58	TYR	3.8
25	d3	18	HIS	3.8
76	Q0	85	LEU	3.8
2	s0	166	GLY	3.8
6	S4	260	GLY	3.8
78	Q2	93	LEU	3.8
1	2	712	G	3.8
11	S9	96	VAL	3.8
21	c9	23	GLN	3.7
42	L5	226	TYR	3.7
19	C7	60	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
28	d6	35	ALA	3.7
74	o8	32	ASN	3.7
23	d1	39	VAL	3.7
34	SR	74	THR	3.7
1	6	1708	U	3.7
81	c2	133	LEU	3.7
16	C4	16	VAL	3.7
28	d6	81	ALA	3.7
53	M7	156	ALA	3.7
1	2	793	A	3.7
2	S0	149	LEU	3.7
3	S1	54	LEU	3.7
1	2	238	U	3.7
13	C1	116	ARG	3.7
58	N2	94	ARG	3.7
88	p0	88	PHE	3.7
32	E0	6	GLY	3.7
19	C7	62	GLN	3.7
24	D2	126	LEU	3.7
70	o4	33	GLN	3.7
22	D0	121	ASN	3.7
30	D8	17	GLY	3.7
36	5	1573	G	3.7
21	C9	28	LEU	3.7
46	L9	178	GLY	3.7
85	l8	155	ASN	3.7
2	S0	162	CYS	3.7
2	s0	162	CYS	3.7
4	S2	169	LEU	3.7
4	S2	137	ILE	3.7
2	S0	139	VAL	3.7
25	d3	11	SER	3.7
28	d6	2	PRO	3.7
84	sM	69	ARG	3.7
4	S2	179	VAL	3.7
7	S5	149	VAL	3.7
8	S6	156	PHE	3.7
28	d6	67	THR	3.7
5	S3	183	GLY	3.7
83	sR	292	LEU	3.7
30	d8	7	VAL	3.7
42	l5	135	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	S0	22	THR	3.7
2	S0	147	THR	3.7
18	C6	141	SER	3.7
58	N2	89	LEU	3.7
83	sR	301	LEU	3.7
24	D2	128	PHE	3.7
81	c2	56	GLU	3.7
81	c2	96	GLN	3.7
36	5	252	U	3.7
23	D1	68	SER	3.7
30	d8	19	THR	3.7
4	S2	84	LYS	3.7
18	c6	44	LEU	3.7
18	c6	117	LEU	3.7
10	S8	198	ALA	3.7
88	p0	104	ARG	3.7
8	s6	1	MET	3.6
10	S8	143	TRP	3.6
17	C5	51	SER	3.6
28	D6	79	ILE	3.6
1	6	1228	G	3.6
2	s0	101	ARG	3.6
4	s2	164	SER	3.6
21	c9	17	ALA	3.6
56	N0	2	ALA	3.6
8	S6	41	VAL	3.6
22	d0	92	ASP	3.6
81	c2	93	ASP	3.6
4	S2	220	ASN	3.6
4	S2	231	ALA	3.6
5	S3	153	ALA	3.6
16	c4	101	ALA	3.6
9	s7	142	TYR	3.6
36	1	1764	U	3.6
88	p0	69	ASP	3.6
18	c6	11	GLY	3.6
7	S5	175	LEU	3.6
81	c2	28	LEU	3.6
1	6	1694	A	3.6
2	S0	20	ALA	3.6
30	d8	41	VAL	3.6
35	SM	22	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
61	N5	30	ALA	3.6
78	q2	79	THR	3.6
9	s7	93	LEU	3.6
34	SR	55	GLY	3.6
53	M7	174	GLY	3.6
36	1	3275	U	3.6
21	C9	38	LYS	3.6
10	s8	61	GLU	3.6
2	s0	185	ARG	3.6
23	D1	69	LEU	3.6
3	s1	153	HIS	3.6
4	S2	65	GLU	3.6
13	c1	138	ASN	3.6
1	6	669	G	3.6
75	O9	51	ILE	3.6
25	d3	10	ASN	3.6
34	SR	80	ALA	3.6
1	2	729	G	3.6
33	e1	100	LEU	3.6
85	l8	162	LEU	3.6
2	S0	28	ASN	3.6
18	C6	66	ARG	3.6
18	c6	143	ARG	3.6
42	L5	158	ARG	3.6
5	S3	188	ILE	3.6
28	D6	78	ALA	3.6
40	l3	386	ASP	3.6
58	n2	14	THR	3.6
87	n4	132	GLY	3.6
34	SR	186	PHE	3.6
1	6	1699	G	3.6
9	s7	184	GLU	3.6
81	c2	85	LYS	3.6
34	SR	78	ALA	3.6
3	s1	110	LEU	3.6
83	sR	135	THR	3.6
1	2	710	U	3.5
2	S0	161	PRO	3.5
33	e1	81	LYS	3.5
30	d8	55	VAL	3.5
36	5	1762	C	3.5
11	s9	183	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
19	C7	68	GLY	3.5
19	C7	100	LEU	3.5
1	2	1687	U	3.5
5	S3	186	VAL	3.5
6	s4	199	GLU	3.5
9	s7	48	GLU	3.5
18	C6	39	VAL	3.5
71	O5	3	GLY	3.5
53	M7	164	LYS	3.5
7	S5	198	LEU	3.5
18	C6	60	PHE	3.5
13	c1	101	GLU	3.5
72	o6	2	THR	3.5
7	S5	69	PHE	3.5
4	S2	96	THR	3.5
19	C7	78	ARG	3.5
30	d8	28	VAL	3.5
10	S8	199	LYS	3.5
22	D0	93	LEU	3.5
42	L5	131	LEU	3.5
48	M1	167	TYR	3.5
2	S0	164	ASN	3.5
31	D9	4	GLU	3.5
1	6	1696	G	3.5
2	S0	50	VAL	3.5
34	SR	252	LEU	3.5
4	s2	94	GLN	3.5
51	m5	39	ALA	3.5
70	O4	20	ILE	3.5
23	d1	47	PRO	3.5
1	6	674	C	3.5
19	C7	63	LYS	3.5
65	N9	25	LYS	3.5
4	S2	115	ILE	3.5
67	O1	14	ILE	3.5
22	d0	67	THR	3.5
83	sR	302	PHE	3.5
23	D1	5	LYS	3.5
6	s4	208	VAL	3.5
2	s0	173	ILE	3.5
16	C4	75	GLY	3.5
17	C5	49	MET	3.5

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Mol	Chain	Res	Type	RSRZ
24	D2	85	ASP	3.5
36	1	1269	U	3.5
6	S4	110	ALA	3.5
8	s6	115	LYS	3.5
23	D1	25	LYS	3.5
39	L2	252	THR	3.5
4	S2	103	VAL	3.5
24	D2	68	ARG	3.5
28	d6	39	MET	3.5
30	d8	17	GLY	3.5
34	SR	137	LYS	3.5
81	c2	127	GLY	3.5
1	2	1795	U	3.5
34	SR	24	ALA	3.5
34	SR	73	LEU	3.5
34	SR	202	LEU	3.5
2	S0	116	LYS	3.5
2	s0	100	GLY	3.5
11	S9	90	LYS	3.5
28	d6	63	ALA	3.5
16	c4	20	TYR	3.4
36	5	1352	A	3.4
61	n5	31	THR	3.4
83	sR	134	TRP	3.4
79	Q3	86	LEU	3.4
83	sR	115	ILE	3.4
2	S0	143	VAL	3.4
4	S2	134	LEU	3.4
5	S3	151	LYS	3.4
55	M9	51	VAL	3.4
8	S6	52	ILE	3.4
23	d1	83	TRP	3.4
65	N9	54	LEU	3.4
81	c2	119	SER	3.4
13	C1	118	GLN	3.4
18	C6	21	HIS	3.4
87	n4	103	ALA	3.4
18	C6	96	TYR	3.4
80	c0	22	VAL	3.4
78	Q2	94	GLY	3.4
4	S2	178	ILE	3.4
22	d0	91	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
21	c9	69	LYS	3.4
36	1	2205	U	3.4
46	l9	191	LEU	3.4
74	o8	54	LEU	3.4
1	2	1689	A	3.4
2	s0	48	ILE	3.4
4	s2	201	ASN	3.4
64	n8	120	ASN	3.4
82	c5	132	GLY	3.4
33	e1	89	LYS	3.4
14	C2	119	SER	3.4
10	S8	148	ALA	3.4
16	C4	101	ALA	3.4
87	n4	75	THR	3.4
30	D8	30	VAL	3.4
36	1	1564	U	3.4
36	5	1582	C	3.4
4	S2	78	ASP	3.4
4	s2	97	ARG	3.4
16	c4	23	PHE	3.4
10	S8	63	GLY	3.4
18	c6	114	ARG	3.4
21	c9	21	PHE	3.4
88	p0	86	PHE	3.4
42	L5	177	GLU	3.4
34	SR	262	VAL	3.4
78	q2	21	THR	3.4
25	d3	4	GLY	3.4
51	m5	58	GLY	3.4
59	n3	3	GLY	3.4
4	S2	236	PRO	3.4
54	m8	186	VAL	3.4
61	N5	124	VAL	3.4
34	SR	263	PHE	3.4
2	s0	25	GLY	3.4
11	S9	5	PRO	3.4
34	SR	313	TRP	3.4
3	S1	91	VAL	3.4
83	sR	253	ALA	3.4
4	S2	51	THR	3.4
27	d5	50	ILE	3.4
2	S0	120	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
19	C7	73	LEU	3.4
34	SR	116	ASP	3.4
53	M7	158	ALA	3.4
87	n4	85	ALA	3.4
11	S9	104	PHE	3.4
24	d2	16	ASN	3.4
88	p0	85	GLY	3.4
22	D0	84	MET	3.4
87	n4	97	LYS	3.4
20	c8	53	ASP	3.4
34	SR	199	ILE	3.4
49	m3	192	GLU	3.4
15	c3	5	HIS	3.4
30	D8	5	THR	3.4
78	q2	54	THR	3.4
19	C7	99	VAL	3.3
34	SR	221	MET	3.4
8	s6	50	PHE	3.3
21	c9	66	TYR	3.3
3	S1	92	GLN	3.3
6	S4	250	GLU	3.3
87	n4	104	ASN	3.3
1	2	1796	C	3.3
6	s4	225	VAL	3.3
8	S6	1	MET	3.3
36	1	1563	C	3.3
1	6	234	G	3.3
16	C4	27	PHE	3.3
36	1	1954	G	3.3
30	d8	18	ARG	3.3
7	S5	158	GLN	3.3
23	D1	56	SER	3.3
24	d2	122	SER	3.3
5	S3	144	ALA	3.3
53	M7	181	ARG	3.3
8	S6	66	GLY	3.3
23	D1	7	GLN	3.3
22	d0	26	LEU	3.3
78	Q2	3	ASN	3.3
88	p0	70	LEU	3.3
17	C5	89	MET	3.3
8	s6	163	THR	3.3

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Mol	Chain	Res	Type	RSRZ
16	c4	119	THR	3.3
34	SR	213	SER	3.3
24	d2	108	ALA	3.3
85	l8	154	ALA	3.3
8	s6	133	LEU	3.3
20	c8	61	LEU	3.3
24	d2	126	LEU	3.3
75	o9	36	ARG	3.3
8	S6	148	SER	3.3
11	S9	77	ILE	3.3
87	n4	64	THR	3.3
1	2	653	C	3.3
2	S0	150	ASP	3.3
4	s2	162	CYS	3.3
7	S5	160	VAL	3.3
8	S6	18	ILE	3.3
27	D5	88	ILE	3.3
34	SR	91	LEU	3.3
2	S0	181	VAL	3.3
30	d8	32	PHE	3.3
2	s0	49	ASN	3.3
7	s5	130	ILE	3.3
28	d6	79	ILE	3.3
6	s4	15	PRO	3.3
7	S5	194	LEU	3.3
8	S6	77	LEU	3.3
25	d3	15	LEU	3.3
42	L5	185	PHE	3.3
84	sM	78	ASP	3.3
5	S3	217	ILE	3.3
6	S4	71	LYS	3.3
2	S0	128	SER	3.3
46	L9	188	THR	3.3
56	N0	135	VAL	3.3
81	c2	116	VAL	3.3
8	S6	37	ASP	3.3
8	s6	113	ILE	3.3
18	C6	29	ILE	3.3
22	D0	19	ILE	3.3
78	Q2	96	GLU	3.3
6	S4	48	LEU	3.3
18	C6	116	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
25	d3	22	ASN	3.3
28	d6	31	PRO	3.3
29	D7	38	PRO	3.3
7	s5	34	GLN	3.3
10	s8	67	TRP	3.3
83	sR	186	PHE	3.3
42	L5	126	GLU	3.3
3	S1	131	ASP	3.3
35	SM	90	ALA	3.3
36	1	1259	A	3.3
2	s0	54	TRP	3.3
26	d4	99	LYS	3.3
4	S2	156	THR	3.3
28	D6	67	THR	3.3
3	S1	140	ILE	3.3
9	S7	98	ILE	3.3
18	c6	89	LEU	3.3
21	c9	33	TYR	3.3
55	m9	184	LEU	3.3
4	S2	59	HIS	3.3
7	S5	41	LYS	3.3
2	S0	101	ARG	3.2
20	c8	82	PRO	3.2
70	O4	24	LYS	3.2
83	sR	61	PHE	3.2
11	s9	64	GLU	3.2
19	C7	79	GLU	3.2
87	n4	65	GLU	3.2
23	D1	6	GLY	3.2
6	S4	103	TYR	3.2
6	S4	246	LEU	3.2
48	M1	66	ALA	3.2
4	S2	140	ARG	3.2
28	D6	5	ARG	3.2
28	d6	18	VAL	3.2
33	e1	135	HIS	3.2
2	S0	199	PRO	3.2
4	S2	150	GLN	3.2
87	n4	130	SER	3.2
13	c1	97	TYR	3.2
5	S3	136	VAL	3.2
3	S1	28	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
56	N0	93	GLU	3.2
24	D2	69	LEU	3.2
19	c7	3	ARG	3.2
49	m3	193	ALA	3.2
50	m4	138	ALA	3.2
3	s1	107	THR	3.2
7	s5	149	VAL	3.2
18	c6	6	SER	3.2
24	D2	101	TYR	3.2
21	C9	114	VAL	3.2
36	1	1555	U	3.2
2	s0	199	PRO	3.2
4	S2	113	LEU	3.2
13	c1	113	PRO	3.2
53	M7	167	ARG	3.2
2	S0	21	ASN	3.2
42	L5	183	TRP	3.2
3	S1	46	THR	3.2
74	o8	26	LYS	3.2
16	c4	45	GLY	3.2
6	S4	55	ALA	3.2
28	d6	49	ALA	3.2
70	O4	7	PHE	3.2
81	c2	42	ALA	3.2
18	c6	4	VAL	3.2
2	S0	134	LYS	3.2
32	E0	53	LYS	3.2
24	D2	83	ILE	3.2
20	C8	146	ALA	3.2
8	S6	149	LYS	3.2
21	C9	71	VAL	3.2
18	c6	68	ARG	3.2
66	o0	6	SER	3.2
3	S1	47	LEU	3.2
3	s1	89	ASP	3.2
5	S3	150	MET	3.2
7	S5	217	LEU	3.2
11	S9	54	ARG	3.2
1	2	713	A	3.2
11	S9	116	LEU	3.2
20	c8	54	LEU	3.2
24	D2	104	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
34	SR	211	ILE	3.2
56	N0	76	GLY	3.2
1	6	682	C	3.2
83	sR	48	THR	3.2
8	s6	112	VAL	3.2
11	S9	85	VAL	3.2
23	D1	87	ARG	3.2
4	S2	230	TRP	3.2
2	S0	105	GLY	3.2
33	e1	113	LYS	3.2
35	SM	83	LYS	3.2
2	S0	75	ALA	3.2
11	S9	3	ARG	3.2
83	sR	50	ASP	3.2
9	S7	48	GLU	3.2
5	S3	216	PRO	3.2
2	S0	30	GLN	3.2
24	D2	25	VAL	3.2
21	C9	29	GLU	3.2
63	N7	2	ALA	3.2
85	l8	117	ALA	3.2
23	D1	17	CYS	3.2
36	5	1565	G	3.2
88	p0	44	GLU	3.2
36	5	1571	A	3.2
4	s2	236	PRO	3.1
19	C7	14	LYS	3.1
78	q2	72	LEU	3.1
1	6	681	U	3.1
36	1	1572	U	3.1
21	C9	54	PHE	3.1
2	s0	26	ALA	3.1
9	S7	33	GLU	3.1
21	c9	25	GLN	3.1
25	D3	27	ASN	3.1
42	L5	176	SER	3.1
9	s7	123	ASP	3.1
22	D0	87	HIS	3.1
2	S0	24	LEU	3.1
18	C6	89	LEU	3.1
1	2	1797	A	3.1
28	d6	5	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
36	5	1103	A	3.1
42	L5	247	ILE	3.1
1	6	235	G	3.1
48	M1	125	MET	3.1
22	D0	53	LYS	3.1
35	SM	137	GLU	3.1
34	SR	319	ASN	3.1
2	s0	161	PRO	3.1
10	S8	67	TRP	3.1
34	SR	296	ALA	3.1
58	n2	13	LYS	3.1
21	c9	24	ARG	3.1
34	SR	122	ILE	3.1
34	SR	169	ILE	3.1
16	c4	27	PHE	3.1
87	n4	133	THR	3.1
8	S6	118	GLU	3.1
81	c2	132	GLU	3.1
2	S0	84	ARG	3.1
50	m4	9	ALA	3.1
66	o0	105	ALA	3.1
4	S2	197	TYR	3.1
1	6	654	C	3.1
2	S0	18	LEU	3.1
13	C1	40	LEU	3.1
16	c4	137	LEU	3.1
28	d6	62	TYR	3.1
39	L2	253	GLN	3.1
5	S3	208	ILE	3.1
2	s0	92	HIS	3.1
25	D3	28	ASN	3.1
5	S3	122	VAL	3.1
28	D6	82	ARG	3.1
17	C5	17	TYR	3.1
4	S2	139	ILE	3.1
8	s6	145	PHE	3.1
57	n1	66	ASN	3.1
28	d6	33	ASP	3.1
67	O1	83	GLU	3.1
15	C3	15	ALA	3.1
34	SR	45	TRP	3.1
36	1	1762	C	3.1

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Mol	Chain	Res	Type	RSRZ
51	m5	6	TYR	3.1
4	S2	199	GLN	3.1
2	s0	160	ILE	3.1
6	s4	162	ILE	3.1
22	d0	20	ILE	3.1
28	d6	36	ILE	3.1
1	2	1362	U	3.1
23	d1	81	ASN	3.1
42	L5	203	HIS	3.1
5	s3	148	LYS	3.1
34	SR	253	ALA	3.1
44	L7	23	ALA	3.1
1	6	1693	A	3.1
20	c8	42	TYR	3.1
85	l8	65	LEU	3.1
61	n5	142	ILE	3.1
88	p0	26	PHE	3.1
22	D0	97	VAL	3.1
28	D6	46	GLU	3.1
30	d8	31	GLU	3.1
43	l6	129	GLU	3.1
78	Q2	6	LYS	3.1
6	S4	123	LEU	3.1
10	S8	168	CYS	3.1
14	C2	88	LEU	3.1
2	s0	96	THR	3.1
16	C4	39	ILE	3.1
4	s2	165	VAL	3.1
83	sR	309	VAL	3.1
19	C7	16	LEU	3.1
24	d2	26	LEU	3.1
4	S2	50	ILE	3.1
13	c1	127	GLN	3.1
5	s3	138	VAL	3.1
21	c9	110	LYS	3.1
5	S3	190	ARG	3.1
30	D8	56	LEU	3.1
13	c1	144	ALA	3.1
2	S0	106	SER	3.0
19	C7	53	TYR	3.0
36	5	2097	U	3.0
83	sR	139	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
78	q2	75	VAL	3.0
1	2	722	G	3.0
18	C6	109	PHE	3.0
15	C3	14	SER	3.0
22	D0	92	ASP	3.0
4	S2	198	THR	3.0
30	d8	25	VAL	3.0
33	e1	125	THR	3.0
18	C6	28	LEU	3.0
5	S3	156	PHE	3.0
23	d1	37	ALA	3.0
34	SR	180	ALA	3.0
34	SR	318	ALA	3.0
1	6	651	G	3.0
9	s7	181	ILE	3.0
45	L8	130	TYR	3.0
87	n4	82	ILE	3.0
29	d7	46	VAL	3.0
53	M7	166	VAL	3.0
3	S1	97	LEU	3.0
7	S5	146	THR	3.0
64	N8	98	THR	3.0
34	SR	71	CYS	3.0
83	sR	122	ILE	3.0
28	D6	95	ARG	3.0
42	L5	63	GLN	3.0
70	O4	5	VAL	3.0
18	c6	12	LYS	3.0
36	5	1579	C	3.0
36	1	1763	U	3.0
83	sR	303	ALA	3.0
87	n4	128	ALA	3.0
88	p0	18	TYR	3.0
88	p0	49	ALA	3.0
8	s6	166	GLU	3.0
2	s0	97	PRO	3.0
3	s1	217	LEU	3.0
4	S2	161	LYS	3.0
21	c9	27	LYS	3.0
34	SR	89	LEU	3.0
83	sR	202	LEU	3.0
5	S3	25	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
4	s2	202	GLY	3.0
23	D1	20	THR	3.0
10	S8	169	ILE	3.0
4	S2	85	PRO	3.0
24	d2	124	LYS	3.0
27	d5	46	LYS	3.0
64	n8	89	GLN	3.0
3	s1	141	ALA	3.0
19	c7	87	GLU	3.0
39	L2	78	ALA	3.0
83	sR	211	ILE	3.0
88	p0	100	ILE	3.0
2	S0	23	HIS	3.0
36	5	1764	U	3.0
64	n8	121	VAL	3.0
16	c4	96	PRO	3.0
11	S9	79	ARG	3.0
41	l4	65	TRP	3.0
42	L5	145	PHE	3.0
88	p0	38	MET	3.0
18	c6	3	ALA	3.0
39	L2	195	SER	3.0
27	d5	105	THR	3.0
6	s4	101	LEU	3.0
18	c6	21	HIS	3.0
28	D6	31	PRO	3.0
28	d6	72	HIS	3.0
29	D7	41	LEU	3.0
67	O1	71	LEU	3.0
1	2	679	U	3.0
33	E1	88	PRO	3.0
58	n2	15	PHE	3.0
2	S0	171	GLY	3.0
5	S3	223	LYS	3.0
4	S2	155	ALA	3.0
23	d1	41	GLU	3.0
34	SR	83	ALA	3.0
2	S0	123	VAL	3.0
23	D1	9	VAL	3.0
28	d6	94	ASN	3.0
48	M1	54	VAL	3.0
56	N0	74	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
81	c2	63	VAL	3.0
32	E0	60	PRO	3.0
63	N7	61	LYS	3.0
1	2	1794	A	3.0
1	2	676	G	3.0
2	s0	107	PHE	3.0
39	l2	253	GLN	3.0
1	6	238	U	3.0
19	C7	122	ILE	3.0
24	D2	27	ILE	3.0
27	d5	89	ILE	3.0
36	5	2504	U	3.0
1	2	1306	C	3.0
36	1	1574	C	3.0
1	6	225	A	3.0
5	S3	148	LYS	3.0
13	c1	137	PHE	3.0
22	d0	121	ASN	3.0
33	e1	151	ASN	3.0
51	m5	101	THR	3.0
78	Q2	22	GLN	3.0
55	M9	179	GLU	3.0
7	S5	137	ILE	2.9
2	s0	158	VAL	2.9
7	s5	160	VAL	2.9
28	d6	34	LYS	2.9
74	o8	51	LEU	2.9
6	s4	73	ASP	2.9
6	S4	226	PHE	2.9
18	c6	141	SER	2.9
60	N4	95	SER	2.9
16	c4	46	MET	2.9
78	q2	22	GLN	2.9
34	SR	244	ALA	2.9
71	O5	2	ALA	2.9
88	p0	96	ILE	2.9
16	c4	105	LEU	2.9
1	2	696	C	2.9
4	S2	93	GLY	2.9
24	d2	39	GLN	2.9
81	c2	25	GLU	2.9
5	s3	184	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
6	S4	162	ILE	2.9
8	S6	5	ILE	2.9
10	s8	165	LEU	2.9
51	m5	64	VAL	2.9
85	l8	198	ALA	2.9
9	s7	104	ARG	2.9
23	D1	4	ASP	2.9
36	1	1095	U	2.9
87	n4	71	ARG	2.9
7	S5	91	GLU	2.9
35	SM	98	GLY	2.9
88	p0	47	GLY	2.9
4	s2	154	LEU	2.9
6	S4	70	VAL	2.9
24	d2	25	VAL	2.9
28	d6	65	PRO	2.9
34	SR	23	LEU	2.9
59	N3	137	VAL	2.9
6	S4	99	PHE	2.9
24	d2	41	MET	2.9
8	s6	175	ILE	2.9
11	S9	70	LEU	2.9
11	S9	148	VAL	2.9
19	C7	69	ILE	2.9
19	C7	101	ASN	2.9
23	D1	11	LEU	2.9
23	D1	39	VAL	2.9
83	sR	156	VAL	2.9
23	D1	58	TYR	2.9
25	d3	6	PRO	2.9
5	S3	200	LYS	2.9
87	n4	74	LYS	2.9
13	C1	16	GLN	2.9
13	C1	109	VAL	2.9
24	d2	38	LEU	2.9
6	s4	14	ALA	2.9
10	S8	69	SER	2.9
21	C9	5	SER	2.9
22	d0	95	ALA	2.9
28	D6	10	ARG	2.9
48	M1	163	PHE	2.9
6	S4	91	THR	2.9

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Mol	Chain	Res	Type	RSRZ
11	S9	94	ASP	2.9
11	S9	118	LEU	2.9
14	C2	59	LEU	2.9
24	D2	129	VAL	2.9
72	o6	58	ILE	2.9
83	sR	71	CYS	2.9
16	c4	85	ALA	2.9
1	2	133	U	2.9
63	n7	56	LYS	2.9
30	D8	26	THR	2.9
3	s1	20	VAL	2.9
24	d2	47	ILE	2.9
66	o0	100	ILE	2.9
88	p0	25	LEU	2.9
6	s4	235	TYR	2.9
7	S5	209	TYR	2.9
1	6	667	U	2.9
1	6	680	U	2.9
36	5	1763	U	2.9
6	S4	207	LEU	2.9
13	C1	91	LEU	2.9
13	c1	122	ILE	2.9
20	C8	17	LEU	2.9
65	N9	58	LYS	2.9
65	n9	25	LYS	2.9
70	o4	21	LYS	2.9
85	l8	34	PHE	2.9
1	2	1059	U	2.9
4	s2	209	ASN	2.9
51	m5	65	ARG	2.9
2	S0	172	LEU	2.9
6	S4	180	LEU	2.9
20	C8	73	MET	2.9
20	c8	20	THR	2.9
83	sR	89	LEU	2.9
6	S4	109	PHE	2.9
85	l8	192	GLN	2.9
2	s0	2	SER	2.9
4	S2	145	GLY	2.9
20	C8	48	LYS	2.9
1	2	1307	U	2.9
8	S6	102	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
33	E1	151	ASN	2.9
34	SR	113	VAL	2.9
49	m3	6	ASN	2.9
38	4	82	U	2.9
2	S0	81	PHE	2.9
3	s1	142	PHE	2.9
10	s8	65	PHE	2.9
34	SR	61	PHE	2.9
16	c4	135	ARG	2.9
28	d6	46	GLU	2.9
4	s2	161	LYS	2.9
76	Q0	128	LYS	2.9
4	s2	59	HIS	2.9
18	c6	5	PRO	2.9
4	S2	218	ILE	2.8
17	C5	41	VAL	2.8
83	sR	224	ASN	2.8
4	S2	158	THR	2.8
34	SR	212	ALA	2.8
38	8	81	U	2.8
58	N2	33	TYR	2.8
1	2	1152	A	2.8
1	2	1714	A	2.8
34	SR	76	ASP	2.8
36	1	1566	A	2.8
83	sR	49	GLY	2.8
42	L5	181	PRO	2.8
61	N5	107	VAL	2.8
35	SM	95	SER	2.8
39	L2	72	ARG	2.8
11	S9	16	LYS	2.8
11	S9	98	ALA	2.8
18	c6	26	LYS	2.8
74	o8	33	LYS	2.8
16	c4	26	THR	2.8
34	SR	201	THR	2.8
81	c2	68	GLU	2.8
6	S4	190	GLY	2.8
13	C1	5	LEU	2.8
3	s1	189	ILE	2.8
24	D2	102	VAL	2.8
10	S8	109	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
32	E0	44	PHE	2.8
6	S4	249	ALA	2.8
10	S8	192	TYR	2.8
34	SR	189	GLU	2.8
34	SR	214	ALA	2.8
11	s9	80	LEU	2.8
16	C4	102	LEU	2.8
21	c9	112	GLY	2.8
26	D4	18	LEU	2.8
88	p0	185	LEU	2.8
2	S0	74	VAL	2.8
11	S9	6	ARG	2.8
16	c4	28	VAL	2.8
39	l2	60	LYS	2.8
51	m5	66	VAL	2.8
81	c2	33	ARG	2.8
10	S8	167	ALA	2.8
13	c1	147	ALA	2.8
16	c4	22	SER	2.8
20	c8	66	LEU	2.8
20	c8	48	LYS	2.8
22	d0	104	THR	2.8
70	O4	78	GLY	2.8
34	SR	165	ASP	2.8
34	SR	192	PHE	2.8
18	c6	124	PRO	2.8
19	c7	65	PRO	2.8
23	d1	42	GLU	2.8
85	l8	134	TYR	2.8
7	s5	148	ARG	2.8
11	s9	90	LYS	2.8
20	C8	101	LEU	2.8
23	D1	62	ARG	2.8
50	m4	8	LYS	2.8
3	s1	84	ILE	2.8
7	S5	140	THR	2.8
7	s5	134	VAL	2.8
51	m5	43	THR	2.8
63	n7	68	ILE	2.8
88	p0	73	PHE	2.8
2	s0	34	GLU	2.8
36	1	2522	G	2.8

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Mol	Chain	Res	Type	RSRZ
36	5	1572	U	2.8
11	s9	65	LYS	2.8
21	c9	122	ARG	2.8
23	D1	37	ALA	2.8
23	D1	54	ALA	2.8
87	n4	94	ARG	2.8
5	S3	21	LEU	2.8
24	D2	26	LEU	2.8
22	d0	100	VAL	2.8
88	p0	79	PHE	2.8
88	p0	58	MET	2.8
1	6	1398	U	2.8
13	C1	92	HIS	2.8
34	SR	51	ASP	2.8
40	l3	146	ARG	2.8
87	n4	88	ASP	2.8
11	s9	93	LEU	2.8
21	c9	105	LEU	2.8
1	2	1685	G	2.8
16	c4	112	ILE	2.8
42	L5	148	ILE	2.8
88	p0	63	ILE	2.8
20	C8	21	ASN	2.8
7	s5	143	ARG	2.8
23	D1	15	ARG	2.8
23	D1	60	ARG	2.8
83	sR	10	ARG	2.8
6	s4	261	LEU	2.8
28	d6	96	ALA	2.8
34	SR	226	ALA	2.8
38	4	158	U	2.8
83	sR	167	VAL	2.8
10	S8	104	ILE	2.8
2	S0	119	ARG	2.8
2	s0	106	SER	2.8
10	s8	123	LYS	2.8
48	M1	26	SER	2.8
25	d3	21	ASN	2.8
36	1	1255	C	2.8
85	l8	137	ASN	2.8
4	S2	112	GLY	2.8
5	s3	3	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
8	s6	22	HIS	2.8
47	m0	111	LEU	2.8
4	s2	63	VAL	2.8
8	S6	81	VAL	2.8
21	C9	4	VAL	2.8
45	L8	58	VAL	2.8
51	M5	60	VAL	2.8
51	M5	66	VAL	2.8
74	o8	45	VAL	2.8
88	p0	30	VAL	2.8
2	S0	185	ARG	2.8
4	S2	91	ARG	2.8
6	S4	90	ILE	2.8
5	S3	213	GLU	2.8
24	D2	88	LYS	2.8
26	d4	96	LEU	2.8
81	c2	125	ASN	2.8
5	S3	120	TYR	2.8
2	S0	72	ASP	2.8
4	S2	111	VAL	2.8
25	D3	18	HIS	2.8
8	S6	164	LYS	2.8
27	D5	71	ILE	2.8
32	E0	55	ARG	2.8
74	o8	43	PHE	2.8
83	sR	54	PHE	2.8
2	s0	40	ALA	2.8
5	S3	187	LYS	2.8
7	s5	33	VAL	2.8
28	d6	89	ARG	2.8
13	C1	14	GLN	2.7
13	C1	121	ASP	2.8
88	p0	87	VAL	2.8
4	S2	163	GLY	2.7
7	S5	182	ALA	2.7
7	s5	157	ARG	2.7
24	d2	73	GLY	2.7
36	1	2207	A	2.7
41	l4	62	ALA	2.7
75	O9	46	ARG	2.7
80	c0	64	TYR	2.7
81	c2	124	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
8	s6	156	PHE	2.7
22	d0	116	VAL	2.7
28	d6	21	VAL	2.7
2	S0	131	GLN	2.7
4	S2	53	ILE	2.7
8	S6	32	ILE	2.7
9	S7	150	GLN	2.7
30	d8	36	THR	2.7
18	c6	98	ASP	2.7
34	SR	114	ASP	2.7
34	SR	136	ILE	2.7
36	5	2098	C	2.7
34	SR	225	LEU	2.7
61	n5	40	LEU	2.7
4	s2	181	SER	2.7
18	c6	18	ALA	2.7
28	D6	18	VAL	2.7
2	s0	164	ASN	2.7
6	S4	239	PRO	2.7
45	L8	240	ASN	2.7
75	o9	11	GLN	2.7
3	S1	45	LYS	2.7
8	S6	115	LYS	2.7
17	C5	9	LYS	2.7
61	n5	113	LEU	2.7
83	sR	90	ARG	2.7
85	l8	152	LEU	2.7
87	n4	73	ARG	2.7
1	2	1145	U	2.7
2	S0	187	ALA	2.7
8	S6	33	GLY	2.7
23	d1	51	VAL	2.7
24	d2	63	VAL	2.7
47	m0	217	PHE	2.7
83	sR	104	VAL	2.7
15	c3	14	SER	2.7
9	S7	108	GLN	2.7
3	s1	116	LYS	2.7
3	s1	119	THR	2.7
20	C8	40	ARG	2.7
30	d8	8	THR	2.7
48	M1	28	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
48	M1	55	ARG	2.7
67	O1	112	ASP	2.7
42	l5	125	VAL	2.7
24	d2	61	ILE	2.7
60	N4	92	GLU	2.7
63	N7	46	ILE	2.7
65	N9	24	PRO	2.7
78	q2	19	LYS	2.7
34	SR	144	LEU	2.7
34	SR	198	ASN	2.7
39	L2	71	LEU	2.7
61	n5	82	LEU	2.7
16	C4	97	GLY	2.7
34	SR	54	PHE	2.7
7	s5	133	VAL	2.7
83	sR	285	ALA	2.7
85	l8	199	ALA	2.7
4	S2	97	ARG	2.7
6	s4	161	LYS	2.7
48	M1	63	GLU	2.7
55	M9	72	GLU	2.7
1	6	744	U	2.7
6	S4	101	LEU	2.7
63	N7	42	LEU	2.7
35	SM	97	THR	2.7
3	s1	83	LYS	2.7
3	s1	115	ARG	2.7
29	D7	70	LYS	2.7
53	M7	180	LYS	2.7
65	N9	52	LYS	2.7
78	Q2	71	ARG	2.7
1	6	226	A	2.7
42	L5	195	LEU	2.7
47	M0	200	LEU	2.7
4	S2	119	LYS	2.7
10	S8	112	TRP	2.7
25	D3	2	GLY	2.7
2	S0	19	ALA	2.7
2	S0	26	ALA	2.7
13	c1	121	ASP	2.7
34	SR	190	ALA	2.7
35	SM	92	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
48	M1	85	LYS	2.7
22	d0	119	ALA	2.7
65	n9	27	TYR	2.7
68	O2	127	ALA	2.7
82	c5	131	ALA	2.7
5	S3	142	LEU	2.7
20	C8	15	LEU	2.7
9	s7	92	PHE	2.7
16	c4	56	SER	2.7
16	c4	57	PRO	2.7
19	c7	59	LYS	2.7
51	m5	130	PHE	2.7
87	n4	1	MET	2.7
4	S2	196	VAL	2.7
8	S6	49	VAL	2.7
23	D1	82	VAL	2.7
36	1	1243	G	2.7
36	5	1570	U	2.7
51	m5	147	ARG	2.7
8	S6	80	ASN	2.7
8	S6	73	ILE	2.7
34	SR	36	ALA	2.7
34	SR	131	ILE	2.7
34	SR	310	ILE	2.7
9	s7	24	PHE	2.7
2	s0	73	VAL	2.7
11	S9	101	VAL	2.7
81	c2	122	VAL	2.7
83	sR	65	SER	2.7
83	sR	171	SER	2.7
83	sR	213	SER	2.7
28	d6	48	ALA	2.7
36	5	1028	U	2.7
1	2	655	G	2.7
1	2	1082	C	2.7
30	d8	16	LEU	2.7
36	1	1237	G	2.7
36	1	1577	G	2.7
6	S4	259	GLN	2.7
16	C4	103	ARG	2.7
19	C7	83	GLN	2.7
22	D0	15	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
4	s2	138	PRO	2.7
8	s6	173	PRO	2.7
42	L5	217	GLU	2.7
3	s1	140	ILE	2.7
5	S3	50	ILE	2.7
13	C1	38	ALA	2.7
67	o1	76	SER	2.7
1	2	721	U	2.7
34	SR	118	LYS	2.7
76	Q0	83	LYS	2.7
88	p0	103	ASN	2.7
18	c6	8	GLN	2.7
9	s7	32	PRO	2.7
2	S0	48	ILE	2.7
16	c4	125	SER	2.6
22	D0	86	ILE	2.7
51	m5	129	TYR	2.6
29	d7	33	LEU	2.6
40	l3	47	LEU	2.6
4	S2	166	THR	2.6
28	D6	77	CYS	2.6
20	C8	22	VAL	2.6
57	N1	127	GLN	2.6
2	s0	41	ARG	2.6
2	s0	122	ILE	2.6
8	S6	172	ALA	2.6
18	c6	36	ILE	2.6
34	SR	188	ILE	2.6
36	1	1238	C	2.6
80	c0	23	ALA	2.6
1	2	1717	G	2.6
18	C6	54	LEU	2.6
9	s7	43	PHE	2.6
18	C6	10	PHE	2.6
24	d2	55	ASP	2.6
83	sR	272	ASP	2.6
5	S3	105	MET	2.6
33	e1	150	VAL	2.6
35	SM	105	LYS	2.6
3	s1	120	LEU	2.6
11	S9	93	LEU	2.6
21	c9	111	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
30	D8	53	ILE	2.6
30	d8	29	ARG	2.6
43	L6	130	ILE	2.6
67	O1	101	ALA	2.6
1	6	136	C	2.6
29	d7	32	PHE	2.6
5	S3	206	VAL	2.6
5	S3	210	GLU	2.6
13	c1	125	VAL	2.6
21	C9	51	GLU	2.6
7	S5	61	TYR	2.6
10	s8	58	LEU	2.6
14	C2	41	LEU	2.6
19	c7	24	LEU	2.6
20	C8	72	ILE	2.6
21	c9	28	LEU	2.6
21	c9	107	ALA	2.6
28	d6	30	ILE	2.6
83	sR	170	ILE	2.6
23	D1	14	PRO	2.6
3	s1	117	TRP	2.6
4	s2	144	TRP	2.6
8	s6	16	PHE	2.6
37	7	73	C	2.6
4	S2	89	GLN	2.6
11	s9	63	ASP	2.6
51	M5	135	VAL	2.6
2	S0	160	ILE	2.6
1	2	1314	U	2.6
4	S2	217	ALA	2.6
7	S5	172	ILE	2.6
7	S5	211	ILE	2.6
33	E1	91	ILE	2.6
76	Q0	78	ILE	2.6
6	s4	122	LYS	2.6
13	C1	46	LYS	2.6
4	s2	86	VAL	2.6
18	C6	55	VAL	2.6
19	C7	80	ARG	2.6
55	M9	181	ARG	2.6
60	N4	80	ARG	2.6
56	N0	96	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
15	c3	125	LEU	2.6
18	C6	36	ILE	2.6
19	c7	57	LEU	2.6
24	d2	27	ILE	2.6
53	M7	176	ILE	2.6
4	s2	203	LYS	2.6
41	l4	67	THR	2.6
48	M1	104	PHE	2.6
55	m9	21	LYS	2.6
2	s0	58	VAL	2.6
4	S2	246	GLU	2.6
11	S9	27	GLU	2.6
73	O7	4	GLY	2.6
85	l8	197	VAL	2.6
2	S0	176	LEU	2.6
25	D3	133	LEU	2.6
42	l5	290	ILE	2.6
48	M1	17	LEU	2.6
19	C7	123	ASN	2.6
21	C9	55	TYR	2.6
23	D1	50	TYR	2.6
26	d4	133	ASN	2.6
23	D1	22	ARG	2.6
34	SR	317	THR	2.6
63	n7	92	PHE	2.6
8	S6	8	PRO	2.6
28	d6	20	PRO	2.6
4	s2	208	GLU	2.6
5	S3	214	GLU	2.6
8	s6	9	VAL	2.6
11	S9	88	GLU	2.6
42	L5	216	GLU	2.6
46	L9	15	GLY	2.6
78	Q2	90	HIS	2.6
48	M1	40	LEU	2.6
67	o1	75	ILE	2.6
7	S5	36	ALA	2.6
8	S6	43	ASP	2.6
74	o8	2	ALA	2.6
51	m5	122	ASN	2.6
2	S0	103	THR	2.6
2	s0	4	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	s0	108	THR	2.6
4	s2	105	GLY	2.6
34	SR	156	VAL	2.6
36	5	1581	C	2.6
1	2	261	U	2.6
1	6	1798	U	2.6
78	q2	15	LYS	2.6
83	sR	107	LYS	2.6
6	S4	44	LEU	2.6
34	SR	42	LEU	2.6
2	S0	33	GLN	2.6
3	s1	146	GLN	2.6
7	s5	23	VAL	2.6
20	c8	62	THR	2.6
1	6	673	A	2.6
24	d2	65	LEU	2.6
42	L5	90	HIS	2.6
2	S0	195	TRP	2.6
46	L9	10	ILE	2.6
60	N4	48	ARG	2.6
61	N5	82	LEU	2.6
78	Q2	72	LEU	2.6
9	s7	11	GLN	2.6
34	SR	227	ALA	2.6
58	N2	107	PHE	2.6
74	O8	43	PHE	2.6
10	s8	149	SER	2.6
3	S1	53	GLY	2.6
4	S2	160	GLY	2.6
21	c9	29	GLU	2.6
20	C8	46	VAL	2.6
28	d6	38	ARG	2.6
42	L5	92	LEU	2.6
23	d1	24	ILE	2.6
23	d1	46	ILE	2.6
1	6	1698	G	2.6
1	2	708	C	2.6
1	6	1705	C	2.6
7	S5	184	PHE	2.6
34	SR	134	TRP	2.6
36	1	1605	A	2.6
42	L5	55	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
9	s7	12	ALA	2.6
5	S3	143	ARG	2.6
18	c6	55	VAL	2.6
19	C7	66	VAL	2.6
42	L5	220	SER	2.6
63	N7	26	VAL	2.6
83	sR	51	ASP	2.6
7	s5	79	ASN	2.6
10	S8	121	LEU	2.6
22	d0	65	ILE	2.6
24	d2	125	ILE	2.6
55	M9	58	HIS	2.6
11	S9	181	ALA	2.5
21	C9	110	LYS	2.5
78	Q2	76	LYS	2.5
81	c2	128	ALA	2.5
83	sR	294	TRP	2.5
33	e1	148	TYR	2.5
13	c1	142	VAL	2.5
38	8	158	U	2.5
6	S4	65	LEU	2.5
6	s4	164	LEU	2.5
24	D2	93	LEU	2.5
29	d7	7	LEU	2.5
3	S1	138	PHE	2.5
3	s1	100	PHE	2.5
9	s7	60	ILE	2.5
4	S2	52	THR	2.5
7	s5	147	THR	2.5
20	c8	11	PHE	2.5
73	O7	10	LYS	2.5
8	S6	142	ARG	2.5
18	c6	79	TYR	2.5
32	E0	2	ALA	2.5
48	M1	39	GLN	2.5
74	o8	34	ALA	2.5
16	c4	74	VAL	2.5
8	s6	216	LEU	2.5
11	S9	128	LEU	2.5
11	S9	151	ASP	2.5
21	C9	35	ASP	2.5
48	M1	119	SER	2.5

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Mol	Chain	Res	Type	RSRZ
80	c0	36	ASP	2.5
4	S2	138	PRO	2.5
21	c9	31	PRO	2.5
24	D2	34	ILE	2.5
34	SR	53	LYS	2.5
51	m5	61	ILE	2.5
65	N9	28	LYS	2.5
72	O6	58	ILE	2.5
83	sR	67	ILE	2.5
10	S8	103	GLN	2.5
20	C8	42	TYR	2.5
23	D1	12	TYR	2.5
47	m0	195	ALA	2.5
83	sR	311	ARG	2.5
44	L7	26	VAL	2.5
6	s4	245	LYS	2.5
13	c1	71	LEU	2.5
24	D2	22	LYS	2.5
67	O1	4	LEU	2.5
70	O4	51	LEU	2.5
4	s2	248	SER	2.5
17	C5	12	PHE	2.5
19	C7	58	MET	2.5
42	L5	180	PHE	2.5
48	M1	96	PHE	2.5
1	6	1082	C	2.5
1	6	1371	A	2.5
2	S0	32	HIS	2.5
2	s0	14	ALA	2.5
10	S8	144	ALA	2.5
19	C7	126	ALA	2.5
68	O2	2	ALA	2.5
83	sR	5	GLU	2.5
5	S3	161	GLY	2.5
42	L5	53	VAL	2.5
70	O4	71	THR	2.5
8	s6	167	LYS	2.5
11	s9	91	LYS	2.5
18	C6	12	LYS	2.5
19	C7	35	CYS	2.5
8	s6	215	ARG	2.5
20	c8	81	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
28	d6	92	ARG	2.5
30	d8	64	ARG	2.5
56	N0	75	PHE	2.5
2	s0	152	PRO	2.5
34	SR	246	SER	2.5
2	S0	46	HIS	2.5
5	s3	219	ALA	2.5
1	2	1151	A	2.5
1	6	1706	C	2.5
8	S6	38	GLY	2.5
10	S8	102	VAL	2.5
65	N9	57	ALA	2.5
33	E1	149	LYS	2.5
42	L5	154	THR	2.5
88	p0	28	VAL	2.5
14	C2	78	LEU	2.5
18	c6	54	LEU	2.5
9	s7	49	ILE	2.5
19	C7	11	ARG	2.5
45	L8	67	ILE	2.5
34	SR	50	ASP	2.5
42	l5	137	ASP	2.5
59	N3	2	SER	2.5
8	S6	100	ALA	2.5
9	S7	151	LYS	2.5
10	s8	117	TYR	2.5
13	c1	92	HIS	2.5
19	C7	74	GLN	2.5
30	D8	48	VAL	2.5
36	1	1765	U	2.5
63	N7	124	ALA	2.5
4	S2	174	ARG	2.5
4	s2	91	ARG	2.5
30	D8	22	ARG	2.5
48	M1	159	THR	2.5
4	S2	83	ILE	2.5
40	L3	379	PHE	2.5
11	S9	138	LYS	2.5
26	d4	135	ASP	2.5
55	M9	60	LYS	2.5
2	S0	166	GLY	2.5
6	S4	182	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
13	c1	75	VAL	2.5
16	c4	59	ALA	2.5
20	c8	52	VAL	2.5
22	D0	54	GLY	2.5
33	e1	104	SER	2.5
88	p0	68	SER	2.5
88	p0	105	VAL	2.5
7	s5	167	ARG	2.5
55	m9	170	ARG	2.5
6	S4	236	ILE	2.5
10	S8	65	PHE	2.5
20	c8	72	ILE	2.5
24	d2	50	PHE	2.5
8	s6	161	GLU	2.5
62	N6	108	LYS	2.5
67	o1	83	GLU	2.5
2	S0	25	GLY	2.5
8	S6	124	LEU	2.5
16	c4	100	ALA	2.5
18	c6	27	GLY	2.5
29	d7	2	VAL	2.5
64	N8	142	GLY	2.5
73	O7	29	VAL	2.5
78	Q2	11	TYR	2.5
85	l8	142	LEU	2.5
6	S4	64	ILE	2.5
24	D2	125	ILE	2.5
4	S2	120	GLU	2.5
2	S0	165	ARG	2.5
2	s0	44	GLY	2.5
74	o8	17	ARG	2.5
2	S0	118	PRO	2.5
6	s4	149	TYR	2.5
8	S6	178	LEU	2.5
11	s9	86	LEU	2.5
28	d6	56	ALA	2.5
65	N9	56	ALA	2.5
2	S0	125	ASP	2.5
20	c8	13	HIS	2.5
67	O1	102	LYS	2.5
21	c9	36	ILE	2.5
22	d0	103	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
64	n8	79	TRP	2.5
7	s5	218	GLU	2.5
28	d6	61	GLU	2.5
11	S9	82	ARG	2.5
36	5	3351	U	2.5
53	M7	169	THR	2.5
60	N4	94	ARG	2.5
70	O4	25	THR	2.5
2	s0	57	LEU	2.5
15	c3	40	TYR	2.5
30	d8	54	LEU	2.5
61	n5	26	VAL	2.5
65	n9	34	GLY	2.5
2	S0	152	PRO	2.5
8	s6	144	PHE	2.5
19	c7	42	GLN	2.5
24	D2	79	PHE	2.5
27	d5	94	LYS	2.5
42	L5	192	PRO	2.5
83	sR	165	ASP	2.5
83	sR	185	GLN	2.5
1	2	1399	C	2.5
6	s4	192	ILE	2.5
54	M8	67	ILE	2.5
16	c4	84	ARG	2.5
2	S0	177	LEU	2.5
3	S1	21	VAL	2.5
11	S9	81	VAL	2.5
16	c4	121	VAL	2.5
55	M9	44	LEU	2.5
65	N9	26	THR	2.5
88	p0	50	VAL	2.5
9	s7	55	LYS	2.5
10	S8	142	LYS	2.5
21	C9	50	ALA	2.5
63	n7	2	ALA	2.5
7	s5	86	GLN	2.5
8	S6	13	GLN	2.5
39	L2	63	PHE	2.5
51	m5	42	PRO	2.5
8	S6	154	ARG	2.5
10	S8	101	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
34	SR	3	SER	2.5
67	O1	79	ARG	2.5
3	S1	66	VAL	2.4
3	s1	209	ASN	2.4
10	s8	39	GLY	2.4
20	C8	66	LEU	2.4
21	C9	103	LYS	2.4
31	D9	5	ASN	2.4
48	M1	36	VAL	2.4
20	c8	58	ALA	2.4
48	M1	44	THR	2.4
48	M1	70	THR	2.4
53	M7	177	ALA	2.4
61	n5	23	ALA	2.4
83	sR	204	ALA	2.4
25	D3	107	PHE	2.4
3	s1	121	ILE	2.4
16	c4	120	PRO	2.4
18	C6	65	ILE	2.4
19	c7	62	GLN	2.4
51	m5	96	ARG	2.4
28	D6	17	HIS	2.4
20	c8	25	ASN	2.4
22	d0	90	TYR	2.4
23	D1	3	ASN	2.4
28	d6	6	ALA	2.4
29	d7	59	CYS	2.4
32	e0	2	ALA	2.4
1	2	232	U	2.4
60	N4	93	ARG	2.4
78	Q2	7	THR	2.4
21	C9	100	ILE	2.4
33	e1	88	PRO	2.4
35	SM	108	GLN	2.4
42	L5	130	GLU	2.4
10	s8	46	VAL	2.4
18	C6	93	HIS	2.4
21	c9	67	MET	2.4
40	L3	80	ASP	2.4
45	L8	152	LEU	2.4
56	N0	77	VAL	2.4
2	s0	27	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
6	S4	86	PHE	2.4
2	S0	140	ASN	2.4
8	s6	214	LYS	2.4
21	c9	15	ILE	2.4
23	d1	7	GLN	2.4
34	SR	300	THR	2.4
22	D0	96	PRO	2.4
33	e1	99	LYS	2.4
36	1	1815	U	2.4
70	O4	42	PRO	2.4
71	O5	20	GLN	2.4
5	s3	150	MET	2.4
6	S4	38	LEU	2.4
11	S9	59	LEU	2.4
2	S0	205	ARG	2.4
19	C7	64	GLY	2.4
47	m0	44	ASP	2.4
51	M5	88	GLY	2.4
88	p0	33	VAL	2.4
8	s6	27	PHE	2.4
23	d1	12	TYR	2.4
70	O4	79	SER	2.4
50	M4	9	ALA	2.4
88	p0	62	ALA	2.4
10	s8	38	ILE	2.4
11	S9	92	LYS	2.4
19	C7	18	GLU	2.4
7	s5	138	THR	2.4
19	c7	69	ILE	2.4
20	C8	69	ILE	2.4
25	D3	30	LYS	2.4
26	D4	127	LYS	2.4
28	d6	43	ASN	2.4
33	E1	90	LYS	2.4
67	o1	111	GLU	2.4
81	c2	136	ILE	2.4
2	S0	17	LEU	2.4
2	s0	24	LEU	2.4
22	d0	118	VAL	2.4
36	1	2539	C	2.4
48	M1	86	VAL	2.4
36	1	1025	A	2.4

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Mol	Chain	Res	Type	RSRZ
55	m9	151	ARG	2.4
1	6	652	G	2.4
64	N8	76	ASP	2.4
3	S1	55	LYS	2.4
9	s7	168	SER	2.4
11	S9	154	LYS	2.4
16	C4	40	ALA	2.4
23	D1	19	ALA	2.4
34	SR	283	LYS	2.4
57	N1	60	LYS	2.4
11	S9	182	GLU	2.4
30	d8	58	GLU	2.4
2	S0	113	ARG	2.4
9	s7	150	GLN	2.4
9	S7	16	LEU	2.4
10	S8	62	THR	2.4
34	SR	4	ASN	2.4
20	c8	45	LEU	2.4
34	SR	206	PRO	2.4
34	SR	222	LEU	2.4
42	L5	163	LEU	2.4
66	O0	104	LEU	2.4
14	C2	26	ASP	2.4
15	c3	129	TYR	2.4
2	S0	154	GLU	2.4
6	S4	199	GLU	2.4
36	1	1260	A	2.4
39	L2	70	ARG	2.4
56	N0	138	GLN	2.4
8	S6	114	VAL	2.4
47	M0	140	THR	2.4
58	N2	80	THR	2.4
70	O4	6	THR	2.4
70	O4	22	VAL	2.4
81	c2	30	VAL	2.4
7	S5	213	LYS	2.4
21	c9	92	LYS	2.4
83	sR	74	THR	2.4
1	2	193	U	2.4
23	d1	53	TYR	2.4
28	D6	76	SER	2.4
39	l2	72	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
7	S5	162	VAL	2.4
17	C5	13	LYS	2.4
4	s2	166	THR	2.4
13	c1	115	PHE	2.4
78	Q2	5	PRO	2.4
7	S5	144	GLU	2.4
21	C9	33	TYR	2.4
24	d2	130	TYR	2.4
29	d7	19	HIS	2.4
1	2	1397	U	2.4
8	s6	158	ILE	2.4
33	e1	109	ASP	2.4
51	m5	151	ILE	2.4
81	c2	26	ASP	2.4
87	n4	63	ILE	2.4
4	S2	101	VAL	2.4
12	C0	24	LYS	2.4
13	C1	123	VAL	2.4
23	d1	5	LYS	2.4
24	D2	76	SER	2.4
48	M1	138	VAL	2.4
63	N7	52	LYS	2.4
70	o4	57	LEU	2.4
18	c6	83	GLN	2.4
83	sR	53	LYS	2.4
8	S6	31	ARG	2.4
11	S9	186	GLU	2.4
28	d6	82	ARG	2.4
42	l5	134	ALA	2.4
85	l8	107	GLU	2.4
4	s2	178	ILE	2.4
6	s4	248	ILE	2.4
13	C1	141	LYS	2.4
83	sR	188	ILE	2.4
70	O4	30	LEU	2.4
88	p0	19	LEU	2.4
2	S0	196	SER	2.4
10	S8	176	SER	2.4
18	c6	121	SER	2.4
23	D1	63	GLY	2.4
63	n7	75	VAL	2.4
79	Q3	71	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
22	d0	102	ARG	2.4
42	L5	141	PRO	2.4
8	s6	143	LYS	2.4
65	N9	32	LEU	2.4
7	s5	168	VAL	2.4
1	2	725	U	2.4
1	2	1308	G	2.4
39	L2	76	PHE	2.4
73	O7	2	GLY	2.4
1	2	1332	C	2.4
1	6	1703	C	2.4
2	s0	20	ALA	2.4
18	c6	20	ALA	2.4
24	d2	119	LYS	2.4
45	L8	46	LEU	2.4
1	2	1296	A	2.3
2	s0	157	ASP	2.3
8	S6	29	ASP	2.3
10	s8	143	TRP	2.3
35	SM	93	ARG	2.3
45	L8	40	VAL	2.3
83	sR	133	VAL	2.3
16	c4	47	LYS	2.3
26	d4	2	SER	2.3
41	l4	61	SER	2.3
85	l8	231	LYS	2.3
87	n4	92	GLU	2.3
1	2	234	G	2.3
7	s5	30	PRO	2.3
35	SM	135	ALA	2.3
57	N1	121	ALA	2.3
59	n3	4	ASN	2.3
87	n4	96	LEU	2.3
18	C6	17	THR	2.3
64	N8	144	VAL	2.3
83	sR	88	THR	2.3
34	SR	294	TRP	2.3
10	S8	159	GLN	2.3
29	d7	22	LYS	2.3
78	q2	76	LYS	2.3
88	p0	43	LYS	2.3
1	6	670	U	2.3

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Mol	Chain	Res	Type	RSRZ
54	m8	146	SER	2.3
63	N7	132	SER	2.3
11	S9	134	ILE	2.3
46	L9	187	ILE	2.3
30	D8	29	ARG	2.3
53	m7	112	LEU	2.3
87	n4	93	ARG	2.3
16	C4	79	VAL	2.3
6	S4	220	THR	2.3
11	S9	29	LYS	2.3
22	D0	44	ASN	2.3
29	d7	47	PHE	2.3
39	L2	28	LYS	2.3
42	L5	160	PHE	2.3
42	L5	161	GLY	2.3
47	m0	188	GLY	2.3
54	M8	100	THR	2.3
81	c2	38	HIS	2.3
1	6	1399	C	2.3
4	S2	68	ILE	2.3
8	s6	212	LEU	2.3
20	C8	145	ARG	2.3
24	D2	97	ARG	2.3
24	D2	108	ALA	2.3
28	d6	22	ARG	2.3
70	O4	29	ILE	2.3
88	p0	48	ARG	2.3
63	n7	82	PRO	2.3
6	S4	175	PHE	2.3
3	s1	103	MET	2.3
17	C5	28	MET	2.3
34	SR	191	ASP	2.3
40	l3	139	GLN	2.3
78	q2	10	THR	2.3
1	6	1697	G	2.3
30	D8	18	ARG	2.3
2	S0	197	ILE	2.3
8	s6	18	ILE	2.3
16	c4	19	ILE	2.3
23	d1	8	LEU	2.3
28	D6	35	ALA	2.3
36	5	2539	C	2.3

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Mol	Chain	Res	Type	RSRZ
41	l4	235	LEU	2.3
83	sR	47	LEU	2.3
6	S4	219	VAL	2.3
6	S4	225	VAL	2.3
10	s8	109	PHE	2.3
13	C1	117	VAL	2.3
65	n9	23	LYS	2.3
13	c1	106	ASN	2.3
82	c5	128	HIS	2.3
30	d8	5	THR	2.3
42	L5	153	THR	2.3
53	M7	179	GLN	2.3
33	E1	137	ASP	2.3
4	S2	172	ALA	2.3
5	S3	171	ALA	2.3
33	E1	143	LYS	2.3
45	L8	113	ALA	2.3
83	sR	62	LYS	2.3
83	sR	142	ALA	2.3
1	2	1078	C	2.3
4	S2	104	VAL	2.3
8	S6	27	PHE	2.3
51	m5	59	PHE	2.3
51	m5	137	PRO	2.3
83	sR	312	VAL	2.3
16	c4	109	GLY	2.3
21	c9	3	GLY	2.3
34	SR	197	SER	2.3
54	M8	167	SER	2.3
1	6	493	U	2.3
14	C2	83	GLU	2.3
28	d6	87	ARG	2.3
30	D8	42	ARG	2.3
4	s2	210	THR	2.3
13	C1	15	LYS	2.3
13	C1	22	ASN	2.3
61	n5	36	LYS	2.3
64	N8	89	GLN	2.3
2	S0	202	TYR	2.3
3	S1	59	ASP	2.3
10	S8	139	ALA	2.3
23	d1	23	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
61	n5	90	ALA	2.3
3	S1	30	PHE	2.3
21	c9	14	PHE	2.3
51	m5	60	VAL	2.3
24	D2	73	GLY	2.3
5	S3	40	ARG	2.3
1	2	1426	C	2.3
13	c1	141	LYS	2.3
51	m5	14	LYS	2.3
2	S0	111	ILE	2.3
3	s1	97	LEU	2.3
16	C4	83	ILE	2.3
22	D0	34	LEU	2.3
26	D4	125	LEU	2.3
29	d7	5	GLN	2.3
67	o1	60	TRP	2.3
4	S2	243	TYR	2.3
42	L5	213	ASP	2.3
45	L8	49	TYR	2.3
64	n8	85	ASP	2.3
84	sM	66	ALA	2.3
13	C1	68	GLY	2.3
47	m0	45	GLU	2.3
55	M9	52	LYS	2.3
58	n2	70	LYS	2.3
64	n8	119	PRO	2.3
32	E0	7	SER	2.3
2	s0	149	LEU	2.3
15	C3	5	HIS	2.3
22	d0	34	LEU	2.3
36	5	1574	C	2.3
48	M1	84	LEU	2.3
67	O1	51	LEU	2.3
1	2	493	U	2.3
1	6	795	U	2.3
2	S0	86	VAL	2.3
2	S0	129	ASP	2.3
2	s0	43	ASP	2.3
8	S6	140	ASN	2.3
16	c4	52	ARG	2.3
34	SR	293	ALA	2.3
81	c2	94	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
78	Q2	95	GLY	2.3
65	n9	22	LYS	2.3
80	c0	3	MET	2.3
3	s1	228	LEU	2.3
9	s7	176	LEU	2.3
4	s2	139	ILE	2.3
21	C9	94	ILE	2.3
26	d4	13	ILE	2.3
24	d2	6	VAL	2.3
28	d6	84	VAL	2.3
34	SR	284	ALA	2.3
42	L5	134	ALA	2.3
45	L8	52	TRP	2.3
51	M5	37	HIS	2.3
70	O4	34	HIS	2.3
17	C5	11	VAL	2.3
61	n5	123	TYR	2.3
1	2	1798	U	2.3
2	S0	124	THR	2.3
3	s1	52	THR	2.3
33	e1	96	LYS	2.3
34	SR	96	THR	2.3
41	l4	60	THR	2.3
61	N5	22	LYS	2.3
83	sR	46	LYS	2.3
4	S2	208	GLU	2.3
21	c9	35	ASP	2.3
42	L5	133	GLU	2.3
58	n2	44	GLU	2.3
4	s2	234	PRO	2.3
9	S7	32	PRO	2.3
10	S8	193	LEU	2.3
83	sR	141	LEU	2.3
7	S5	223	SER	2.3
7	s5	68	ILE	2.3
10	S8	195	ARG	2.3
10	s8	66	SER	2.3
13	c1	90	TYR	2.3
18	C6	8	GLN	2.3
24	d2	64	GLN	2.3
48	M1	59	ILE	2.3
56	N0	94	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
70	o4	58	ARG	2.3
2	S0	40	ALA	2.3
5	S3	119	ALA	2.3
23	d1	54	ALA	2.3
51	m5	62	TYR	2.3
78	q2	59	HIS	2.3
83	sR	118	LYS	2.3
4	s2	163	GLY	2.3
15	c3	83	GLU	2.3
1	2	189	C	2.3
1	6	903	U	2.3
3	S1	98	THR	2.3
16	c4	24	ASN	2.3
4	S2	187	LEU	2.3
6	S4	52	LEU	2.3
11	S9	147	MET	2.3
30	d8	49	ARG	2.3
61	N5	27	ARG	2.3
4	S2	203	LYS	2.3
13	C1	122	ILE	2.3
22	d0	19	ILE	2.3
55	M9	186	LYS	2.3
83	sR	310	ILE	2.3
2	s0	23	HIS	2.3
4	s2	233	GLN	2.3
14	C2	42	ALA	2.3
16	C4	29	HIS	2.3
18	C6	19	VAL	2.3
36	1	1270	A	2.3
51	m5	30	TYR	2.3
57	N1	125	ALA	2.3
73	O7	15	SER	2.3
81	c2	118	ALA	2.3
5	S3	157	LEU	2.2
13	c1	91	LEU	2.2
19	C7	40	THR	2.2
32	E0	46	ASN	2.2
51	m5	22	LEU	2.2
72	o6	36	ARG	2.2
14	C2	136	ILE	2.2
27	d5	71	ILE	2.2
64	N8	82	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
4	S2	102	VAL	2.2
39	l2	250	GLN	2.2
42	L5	151	GLN	2.2
51	m5	35	VAL	2.2
11	S9	20	GLU	2.2
21	C9	109	GLU	2.2
25	D3	145	SER	2.2
70	O4	32	ALA	2.2
76	Q0	81	SER	2.2
83	sR	172	ALA	2.2
28	d6	95	ARG	2.2
3	s1	214	LYS	2.2
4	S2	235	LEU	2.2
9	s7	154	LEU	2.2
11	S9	49	LEU	2.2
22	D0	63	LEU	2.2
11	S9	74	ASN	2.2
33	E1	89	LYS	2.2
51	m5	34	ASN	2.2
8	S6	144	PHE	2.2
16	c4	115	ILE	2.2
24	d2	86	ILE	2.2
23	d1	36	VAL	2.2
24	d2	33	VAL	2.2
35	SM	76	VAL	2.2
51	m5	135	VAL	2.2
74	o8	25	VAL	2.2
2	s0	33	GLN	2.2
24	d2	123	GLY	2.2
30	D8	20	GLY	2.2
36	5	3154	C	2.2
45	L8	115	ALA	2.2
78	Q2	14	GLY	2.2
2	S0	151	SER	2.2
60	N4	47	ARG	2.2
11	S9	68	LYS	2.2
13	c1	69	LYS	2.2
32	E0	49	LEU	2.2
46	L9	161	LEU	2.2
47	m0	206	LEU	2.2
65	N9	59	LYS	2.2
81	c2	36	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	S4	159	THR	2.2
13	c1	66	ILE	2.2
18	c6	46	PHE	2.2
23	d1	75	ASN	2.2
42	L5	214	ASP	2.2
19	c7	66	VAL	2.2
28	d6	97	PRO	2.2
46	L9	83	THR	2.2
1	6	231	U	2.2
19	C7	76	GLU	2.2
36	1	3351	U	2.2
36	5	766	U	2.2
42	L5	210	GLU	2.2
62	N6	88	GLU	2.2
70	O4	62	TYR	2.2
70	O4	76	TYR	2.2
71	o5	120	ALA	2.2
81	c2	40	GLY	2.2
21	C9	92	LYS	2.2
48	M1	87	LYS	2.2
5	s3	142	LEU	2.2
20	c8	129	TRP	2.2
26	D4	69	SER	2.2
54	m8	167	SER	2.2
78	Q2	83	LEU	2.2
31	d9	52	PHE	2.2
42	L5	64	ILE	2.2
42	L5	142	PHE	2.2
61	N5	63	ILE	2.2
74	o8	11	PHE	2.2
18	c6	31	VAL	2.2
6	S4	134	LYS	2.2
7	S5	181	GLU	2.2
9	s7	54	GLY	2.2
10	S8	34	ALA	2.2
10	s8	162	ALA	2.2
13	C1	78	THR	2.2
30	d8	24	GLY	2.2
84	sM	50	ASN	2.2
20	C8	8	GLN	2.2
51	m5	111	ALA	2.2
78	q2	24	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
83	sR	132	LYS	2.2
87	n4	99	GLU	2.2
5	S3	182	LEU	2.2
5	s3	182	LEU	2.2
11	S9	105	LEU	2.2
23	d1	55	LEU	2.2
48	M1	80	LEU	2.2
74	o8	31	LEU	2.2
18	C6	101	SER	2.2
10	S8	60	ILE	2.2
21	C9	21	PHE	2.2
6	S4	111	VAL	2.2
21	c9	68	ARG	2.2
3	s1	104	ASP	2.2
4	S2	79	GLU	2.2
19	C7	7	LYS	2.2
4	S2	100	ALA	2.2
10	S8	68	ALA	2.2
11	s9	95	TYR	2.2
23	d1	38	LYS	2.2
59	N3	3	GLY	2.2
65	N9	27	TYR	2.2
83	sR	229	LYS	2.2
36	5	1022	U	2.2
51	m5	152	CYS	2.2
47	m0	171	TRP	2.2
3	S1	219	LYS	2.2
5	S3	137	VAL	2.2
6	s4	174	LYS	2.2
19	C7	67	ARG	2.2
24	d2	62	VAL	2.2
85	l8	183	LYS	2.2
1	2	1297	G	2.2
6	S4	231	GLN	2.2
14	C2	82	PRO	2.2
48	M1	111	ASP	2.2
51	m5	53	TYR	2.2
78	q2	103	ALA	2.2
16	c4	62	LEU	2.2
30	d8	39	THR	2.2
81	c2	52	LEU	2.2
81	c2	67	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	s1	151	LYS	2.2
10	S8	151	LYS	2.2
51	m5	37	HIS	2.2
75	O9	49	MET	2.2
78	Q2	91	PHE	2.2
17	C5	84	ILE	2.2
28	d6	76	SER	2.2
32	E0	45	VAL	2.2
33	e1	108	VAL	2.2
42	L5	122	VAL	2.2
67	O1	76	SER	2.2
2	s0	36	TYR	2.2
2	S0	148	ASP	2.2
9	S7	58	LEU	2.2
22	d0	15	GLN	2.2
36	1	1272	C	2.2
39	L2	179	LEU	2.2
49	M3	160	GLN	2.2
78	q2	83	LEU	2.2
1	6	1713	G	2.2
2	S0	108	THR	2.2
4	S2	49	LYS	2.2
20	C8	44	ASN	2.2
67	O1	10	ARG	2.2
80	c0	25	LYS	2.2
83	sR	143	THR	2.2
7	s5	29	ILE	2.2
19	C7	9	VAL	2.2
48	M1	148	VAL	2.2
56	N0	79	VAL	2.2
1	2	260	U	2.2
1	6	229	U	2.2
83	sR	286	GLU	2.2
5	s3	160	SER	2.2
28	D6	73	TYR	2.2
70	O4	73	SER	2.2
73	O7	87	SER	2.2
45	L8	117	ALA	2.2
2	S0	88	LYS	2.2
2	s0	83	GLN	2.2
63	n7	80	LEU	2.2
87	n4	87	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
34	SR	93	ASP	2.2
3	S1	143	THR	2.2
5	S3	207	THR	2.2
2	S0	168	HIS	2.2
6	S4	87	MET	2.2
75	o9	34	THR	2.2
24	d2	51	GLU	2.2
70	o4	34	HIS	2.2
80	c0	78	GLU	2.2
1	2	1150	G	2.2
3	S1	93	GLY	2.2
41	l4	66	GLY	2.2
11	S9	69	ARG	2.2
16	C4	78	ALA	2.2
20	C8	41	ARG	2.2
21	C9	123	ARG	2.2
22	d0	52	LYS	2.2
23	D1	45	ALA	2.2
25	D3	123	LYS	2.2
28	D6	62	TYR	2.2
83	sR	183	LEU	2.2
24	d2	72	CYS	2.2
6	S4	176	ASP	2.2
2	S0	121	VAL	2.2
13	C1	111	VAL	2.2
13	c1	98	ASN	2.2
18	C6	85	ILE	2.2
18	c6	85	ILE	2.2
22	d0	83	GLU	2.2
24	D2	111	MET	2.2
34	SR	316	MET	2.2
57	n1	118	GLU	2.2
15	c3	8	GLY	2.2
4	S2	76	LEU	2.2
7	S5	214	LYS	2.2
22	D0	21	LYS	2.2
23	d1	22	ARG	2.2
24	D2	71	LYS	2.2
28	d6	53	LEU	2.2
70	O4	19	LYS	2.2
5	S3	205	ALA	2.2
75	o9	23	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
88	p0	11	TYR	2.2
85	l8	73	PRO	2.2
8	s6	39	GLU	2.2
21	C9	104	VAL	2.2
34	SR	20	VAL	2.2
54	M8	93	ILE	2.2
64	n8	46	ASP	2.2
6	s4	159	THR	2.2
16	c4	91	THR	2.2
18	C6	115	THR	2.2
20	C8	55	HIS	2.2
33	e1	136	LYS	2.2
58	n2	52	ASN	2.2
61	N5	31	THR	2.2
2	s0	17	LEU	2.1
10	S8	165	LEU	2.1
13	c1	53	TYR	2.1
16	c4	110	LEU	2.1
22	D0	82	TYR	2.1
58	N2	84	LEU	2.1
83	sR	225	LEU	2.1
88	p0	15	LEU	2.1
2	S0	169	SER	2.1
10	S8	141	ARG	2.1
24	D2	103	ILE	2.1
46	L9	31	ARG	2.1
57	n1	124	VAL	2.1
10	s8	179	CYS	2.1
11	S9	73	GLY	2.1
18	c6	13	LYS	2.1
63	N7	65	ARG	2.1
1	2	651	G	2.1
2	s0	184	LEU	2.1
14	C2	32	LEU	2.1
61	n5	37	THR	2.1
66	O0	105	ALA	2.1
66	o0	23	TYR	2.1
7	s5	69	PHE	2.1
13	C1	20	PHE	2.1
22	D0	98	GLN	2.1
40	L3	139	GLN	2.1
1	2	491	C	2.1

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Mol	Chain	Res	Type	RSRZ
11	S9	122	VAL	2.1
11	s9	2	PRO	2.1
21	c9	34	VAL	2.1
34	SR	90	ARG	2.1
34	SR	110	VAL	2.1
36	1	3154	C	2.1
57	N1	93	VAL	2.1
82	c5	5	VAL	2.1
85	l8	195	SER	2.1
60	N4	1	MET	2.1
64	N8	119	PRO	2.1
6	s4	253	ASP	2.1
62	N6	92	GLY	2.1
70	O4	27	GLY	2.1
40	l3	178	LEU	2.1
2	S0	96	THR	2.1
15	C3	133	ALA	2.1
24	D2	72	CYS	2.1
41	l4	58	HIS	2.1
36	1	1234	G	2.1
54	M8	94	PHE	2.1
2	s0	144	ILE	2.1
4	S2	54	GLU	2.1
4	s2	232	GLU	2.1
10	S8	74	LYS	2.1
25	D3	124	VAL	2.1
27	d5	86	GLU	2.1
34	SR	185	GLN	2.1
48	M1	43	GLN	2.1
48	M1	90	GLN	2.1
87	n4	129	LYS	2.1
20	C8	76	PRO	2.1
28	D6	97	PRO	2.1
1	2	794	U	2.1
1	6	1619	C	2.1
42	L5	191	ASP	2.1
58	N2	105	LEU	2.1
10	S8	160	PHE	2.1
28	D6	11	ASN	2.1
28	d6	25	ASN	2.1
49	m3	183	ARG	2.1
2	S0	15	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	S1	197	ILE	2.1
19	C7	77	GLU	2.1
28	D6	41	ILE	2.1
61	N5	142	ILE	2.1
1	2	1635	A	2.1
11	S9	99	LEU	2.1
16	c4	95	GLY	2.1
19	C7	22	PRO	2.1
34	SR	13	LEU	2.1
36	5	2401	A	2.1
43	l6	66	SER	2.1
60	N4	96	LEU	2.1
10	S8	8	ARG	2.1
10	S8	21	PHE	2.1
15	c3	15	ALA	2.1
16	c4	70	LYS	2.1
23	D1	38	LYS	2.1
36	1	3156	U	2.1
47	M0	181	TYR	2.1
54	m8	159	LYS	2.1
65	N9	23	LYS	2.1
2	s0	124	THR	2.1
3	s1	106	THR	2.1
5	S3	101	GLN	2.1
6	s4	227	VAL	2.1
10	s8	95	THR	2.1
19	c7	4	VAL	2.1
39	L2	73	GLU	2.1
3	s1	73	LEU	2.1
7	s5	198	LEU	2.1
8	S6	54	GLY	2.1
20	C8	3	LEU	2.1
27	D5	73	GLY	2.1
23	d1	86	SER	2.1
24	d2	29	PRO	2.1
24	d2	30	SER	2.1
24	d2	107	SER	2.1
46	L9	13	PRO	2.1
87	n4	109	LEU	2.1
11	S9	146	PHE	2.1
11	s9	62	ARG	2.1
18	C6	68	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	S0	132	ALA	2.1
5	S3	88	ALA	2.1
19	C7	82	ASP	2.1
39	l2	59	ALA	2.1
57	N1	34	TYR	2.1
80	c0	79	TYR	2.1
22	D0	48	HIS	2.1
35	SM	94	HIS	2.1
36	5	1564	U	2.1
45	L8	107	GLU	2.1
54	M8	74	GLU	2.1
48	M1	65	ILE	2.1
54	m8	84	VAL	2.1
57	n1	80	VAL	2.1
87	n4	76	VAL	2.1
7	S5	94	THR	2.1
27	D5	102	THR	2.1
9	s7	53	GLY	2.1
19	C7	72	LYS	2.1
27	d5	104	ALA	2.1
41	l4	89	ALA	2.1
51	m5	148	TYR	2.1
56	n0	2	ALA	2.1
2	s0	50	VAL	2.1
9	s7	51	VAL	2.1
13	C1	75	VAL	2.1
64	N8	135	GLU	2.1
74	o8	55	VAL	2.1
81	c2	115	VAL	2.1
1	2	1153	G	2.1
6	S4	9	LEU	2.1
6	S4	153	ASN	2.1
7	s5	175	LEU	2.1
9	s7	147	ASN	2.1
11	s9	185	GLY	2.1
13	c1	78	THR	2.1
17	C5	10	ARG	2.1
21	c9	132	LEU	2.1
25	d3	7	ARG	2.1
36	1	1236	G	2.1
36	1	1242	G	2.1
36	1	2095	G	2.1

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Mol	Chain	Res	Type	RSRZ
54	m8	168	THR	2.1
6	S4	47	PHE	2.1
28	D6	20	PRO	2.1
42	L5	207	TYR	2.1
51	m5	3	ALA	2.1
51	m5	131	GLU	2.1
57	n1	121	ALA	2.1
4	S2	157	LYS	2.1
18	C6	22	VAL	2.1
9	s7	47	ARG	2.1
10	s8	60	ILE	2.1
48	M1	122	ILE	2.1
55	m9	22	VAL	2.1
11	S9	150	LEU	2.1
20	C8	129	TRP	2.1
23	D1	29	HIS	2.1
49	m3	180	ARG	2.1
63	N7	60	LYS	2.1
25	D3	57	LEU	2.1
81	c2	62	LEU	2.1
83	sR	28	GLY	2.1
1	6	1687	U	2.1
85	l8	77	GLN	2.1
4	s2	224	PHE	2.1
22	d0	107	THR	2.1
34	SR	203	THR	2.1
79	q3	63	THR	2.1
1	2	1625	C	2.1
10	s8	137	LYS	2.1
16	c4	63	ALA	2.1
24	d2	49	GLU	2.1
24	d2	96	ALA	2.1
28	d6	59	TYR	2.1
34	SR	279	ALA	2.1
51	m5	40	ALA	2.1
51	m5	119	TYR	2.1
78	q2	81	ALA	2.1
7	S5	157	ARG	2.1
21	C9	57	ARG	2.1
24	D2	74	VAL	2.1
33	E1	150	VAL	2.1
34	SR	6	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
46	l9	18	VAL	2.1
61	n5	39	LYS	2.1
48	M1	120	ILE	2.1
81	c2	31	VAL	2.1
61	n5	106	ASP	2.1
64	N8	46	ASP	2.1
70	O4	31	ARG	2.1
4	S2	35	TRP	2.1
4	S2	190	LEU	2.1
24	D2	11	LEU	2.1
27	D5	65	LEU	2.1
39	L2	32	LEU	2.1
4	s2	250	GLN	2.1
10	s8	103	GLN	2.1
13	c1	42	PHE	2.1
23	D1	21	ASN	2.1
31	d9	55	PHE	2.1
36	1	1241	U	2.1
3	S1	60	ALA	2.1
4	s2	222	TYR	2.1
10	s8	114	GLU	2.1
4	S2	167	VAL	2.1
10	s8	150	ALA	2.1
28	d6	12	LYS	2.1
30	d8	60	GLU	2.1
35	SM	27	LYS	2.1
85	l8	130	TYR	2.1
13	c1	123	VAL	2.1
16	C4	111	ARG	2.1
18	C6	114	ARG	2.1
18	c6	7	VAL	2.1
41	l4	76	ARG	2.1
18	c6	63	ILE	2.1
18	c6	81	ILE	2.1
24	D2	122	SER	2.1
29	d7	21	LEU	2.1
33	e1	146	SER	2.1
48	M1	21	ILE	2.1
3	s1	184	LEU	2.1
15	C3	139	TRP	2.1
2	S0	204	TYR	2.1
9	s7	88	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
7	S5	221	ALA	2.1
24	D2	96	ALA	2.1
42	L5	129	TYR	2.1
55	M9	11	ALA	2.1
1	2	1766	A	2.1
22	d0	63	LEU	2.1
24	d2	53	ILE	2.1
33	e1	139	LEU	2.1
83	sR	260	ILE	2.1
88	p0	184	GLY	2.1
5	S3	166	ASP	2.1
83	sR	191	ASP	2.1
64	n8	27	LYS	2.0
75	o9	46	ARG	2.0
83	sR	129	LYS	2.0
4	S2	47	ALA	2.0
22	D0	45	ALA	2.0
67	O1	93	VAL	2.0
4	S2	229	LEU	2.0
22	D0	91	ILE	2.0
25	D3	117	ILE	2.0
46	L9	52	LEU	2.0
57	n1	160	ILE	2.0
63	N7	21	LYS	2.0
83	sR	137	LYS	2.0
9	S7	97	ARG	2.0
10	S8	119	GLN	2.0
20	c8	23	ASP	2.0
64	N8	117	ARG	2.0
73	o7	11	ARG	2.0
42	L5	209	GLU	2.0
5	S3	87	TYR	2.0
11	S9	135	ALA	2.0
13	C1	93	TYR	2.0
14	C2	20	ALA	2.0
19	C7	85	VAL	2.0
30	d8	30	VAL	2.0
42	L5	100	ALA	2.0
42	L5	144	VAL	2.0
83	sR	83	ALA	2.0
88	p0	84	VAL	2.0
4	S2	71	THR	2.0

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Mol	Chain	Res	Type	RSRZ
13	C1	31	THR	2.0
15	C3	23	PRO	2.0
17	C5	14	THR	2.0
24	d2	12	ASN	2.0
26	d4	18	LEU	2.0
48	M1	112	LEU	2.0
55	M9	142	ILE	2.0
61	N5	108	LEU	2.0
1	6	718	U	2.0
51	m5	72	LYS	2.0
23	d1	44	ARG	2.0
55	M9	85	ARG	2.0
83	sR	147	HIS	2.0
3	S1	114	VAL	2.0
8	S6	169	TYR	2.0
16	c4	21	ALA	2.0
28	d6	24	VAL	2.0
46	L9	180	TYR	2.0
5	S3	106	LYS	2.0
6	S4	198	LYS	2.0
22	d0	86	ILE	2.0
29	D7	7	LEU	2.0
65	N9	53	ALA	2.0
67	o1	61	LYS	2.0
70	o4	29	ILE	2.0
4	s2	57	PHE	2.0
6	s4	221	ARG	2.0
10	S8	174	GLY	2.0
16	c4	15	GLY	2.0
79	q3	3	LYS	2.0
35	SM	96	ARG	2.0
88	p0	71	PRO	2.0
11	S9	164	PHE	2.0
36	1	2209	U	2.0
3	s1	122	GLU	2.0
11	s9	182	GLU	2.0
13	C1	50	GLU	2.0
2	S0	77	SER	2.0
6	S4	209	HIS	2.0
6	S4	247	SER	2.0
63	N7	122	HIS	2.0
72	O6	100	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
7	S5	212	LYS	2.0
7	s5	162	VAL	2.0
10	s8	192	TYR	2.0
16	C4	42	VAL	2.0
22	D0	116	VAL	2.0
9	S7	149	ILE	2.0
23	D1	16	LYS	2.0
23	D1	36	VAL	2.0
51	M5	127	TYR	2.0
51	m5	132	VAL	2.0
58	n2	33	TYR	2.0
6	s4	124	GLY	2.0
16	C4	98	GLY	2.0
16	c4	41	ARG	2.0
16	c4	90	ARG	2.0
24	D2	38	LEU	2.0
40	L3	47	LEU	2.0
85	l8	200	LEU	2.0
43	l6	67	GLY	2.0
13	C1	60	PHE	2.0
54	M8	97	PRO	2.0
88	p0	197	PHE	2.0
73	O7	5	THR	2.0
88	p0	83	ASN	2.0
1	6	1795	U	2.0
13	C1	127	GLN	2.0
34	SR	187	GLN	2.0
2	S0	92	HIS	2.0
5	S3	164	VAL	2.0
6	S4	89	VAL	2.0
8	S6	12	SER	2.0
8	s6	36	VAL	2.0
21	c9	9	VAL	2.0
5	S3	149	ALA	2.0
1	2	1100	G	2.0
5	S3	95	GLY	2.0
5	s3	208	ILE	2.0
6	s4	13	ALA	2.0
7	S5	143	ARG	2.0
7	S5	159	ALA	2.0
10	s8	79	ALA	2.0
11	S9	63	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
23	D1	61	SER	2.0
34	SR	150	TRP	2.0
19	C7	38	ILE	2.0
34	SR	2	ALA	2.0
55	M9	151	ARG	2.0
56	N0	129	ILE	2.0
67	O1	36	ILE	2.0
5	s3	220	PRO	2.0
34	SR	158	PRO	2.0
1	2	1081	A	2.0
2	s0	28	ASN	2.0
11	S9	111	THR	2.0
12	C0	34	GLU	2.0
26	D4	81	GLU	2.0
29	D7	42	ASN	2.0
69	o3	3	GLU	2.0
6	s4	22	LYS	2.0
35	SM	103	LYS	2.0
61	n5	25	LYS	2.0
78	Q2	24	LYS	2.0
87	n4	79	GLN	2.0
4	s2	41	LEU	2.0
5	S3	54	ARG	2.0
6	S4	102	VAL	2.0
18	C6	117	LEU	2.0
18	c6	116	LEU	2.0
24	d2	101	TYR	2.0
28	d6	51	ARG	2.0
48	M1	60	ARG	2.0
68	O2	128	LEU	2.0
70	O4	16	ARG	2.0
88	p0	51	VAL	2.0

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

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
90	PPU	A	76	37/38	0.83	0.33	47,88,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
90	PPU	a	76	37/38	0.85	0.37	44,80,139,139	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

LIGAND-RSR INFOmissingINFO

6.5 Other polymers ⓘ

There are no such residues in this entry.