Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 07:59 AM EST

PDB ID	:	4Z3S
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with antibiotic A201A, mRNA and three tRNAs in the A, P and E sites at 2.65A resolution
Authors	:	Polikanov, Y.S.; Starosta, A.L.; Juette, M.F.; Altman, R.B.; Terry, D.S.; Lu, W.; Burnett, B.J.; Dinos, G.; Reynolds, K.; Blanchard, S.C.; Steitz, T.A.; Wilson, D.N.
Deposited on	:	2015-03-31
Resolution	:	2.65 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

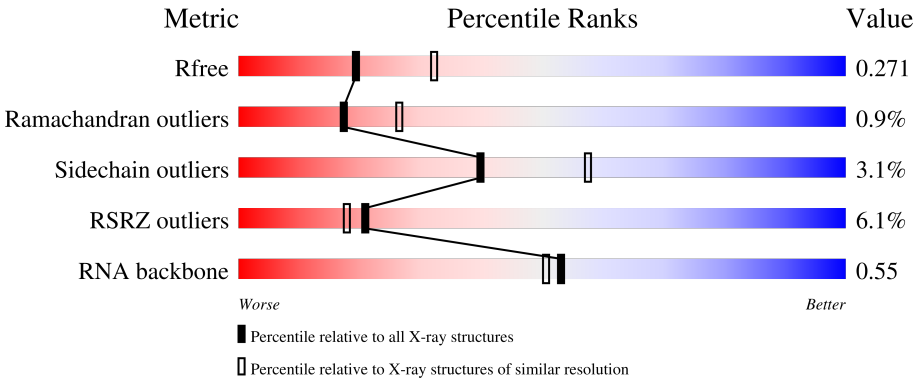
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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	1A	2915	2% 82% 16%
1	2A	2915	2% 79% 16%
2	1B	121	91% 7%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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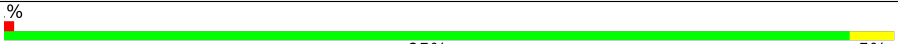
Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
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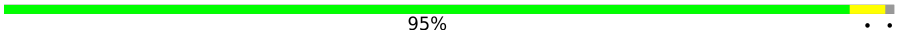
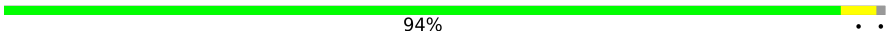
4	1E	206	
4	2E	206	
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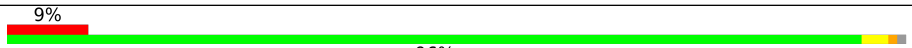
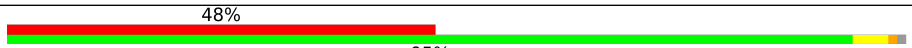
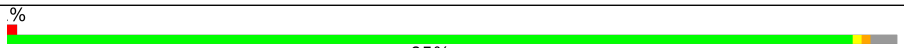
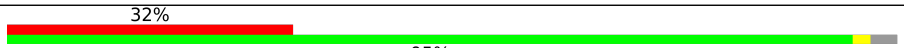
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
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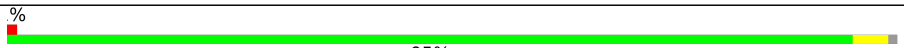
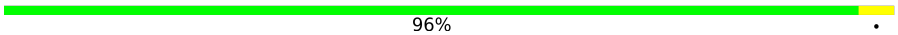
8	2I	148	
9	1N	140	
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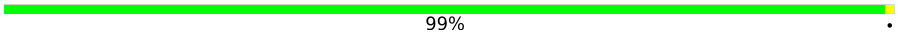
10	1O	122	
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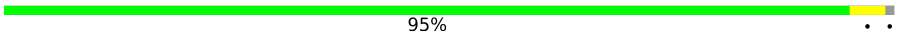
11	1P	150	
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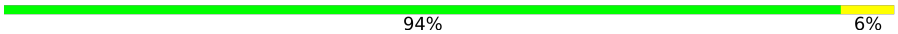
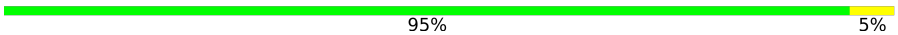
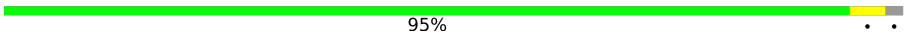
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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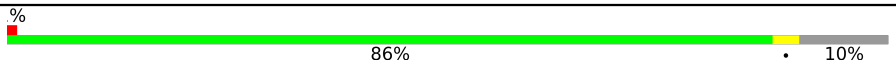
Mol	Chain	Length	Quality of chain
15	1T	146	
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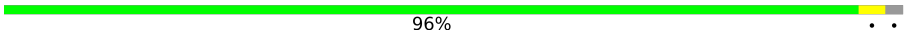
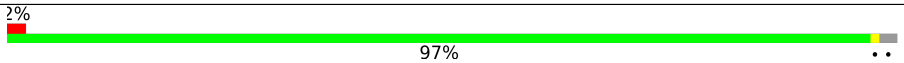
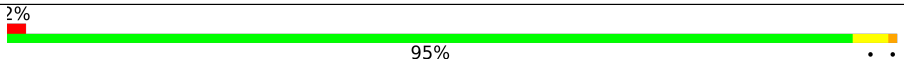
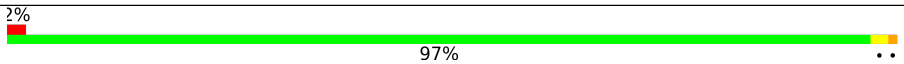
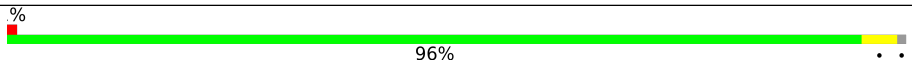
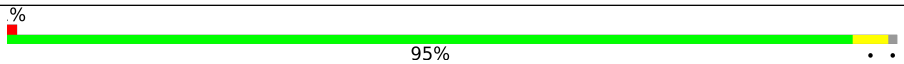
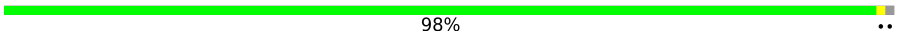
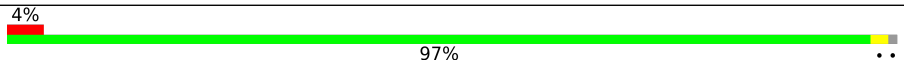
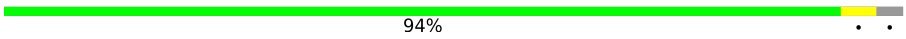
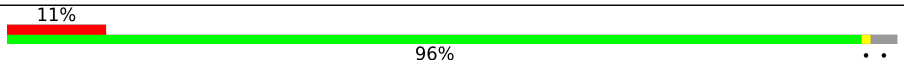
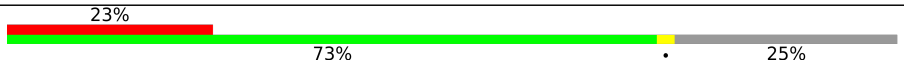
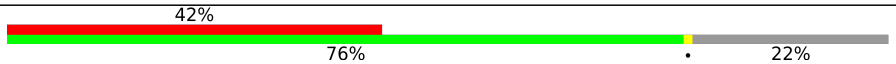
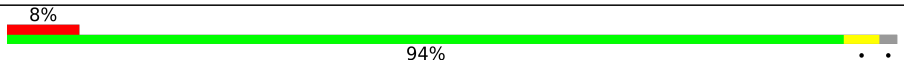
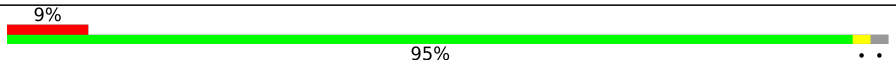
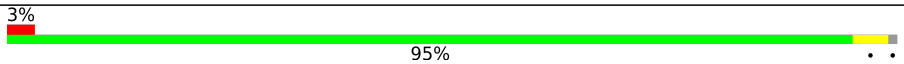
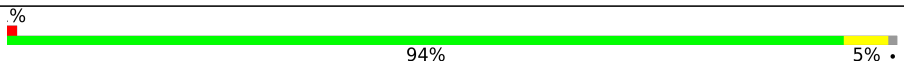
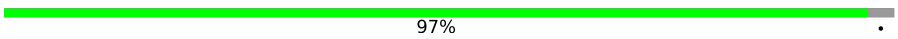
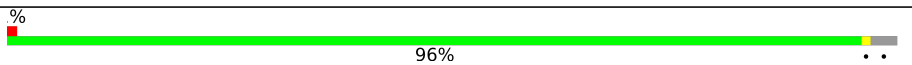
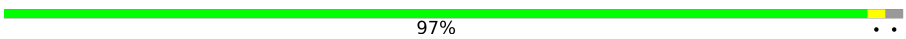
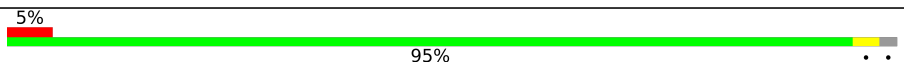
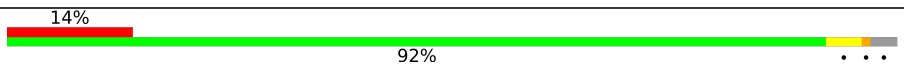
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
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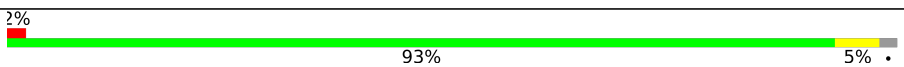
27	15	60	

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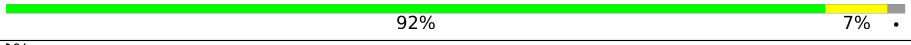
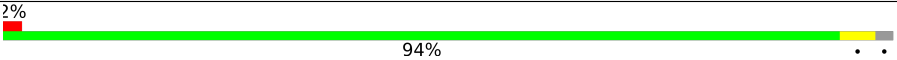
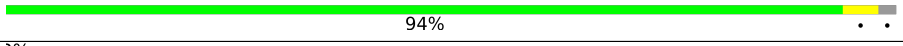
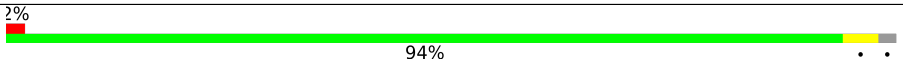
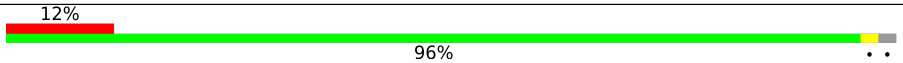
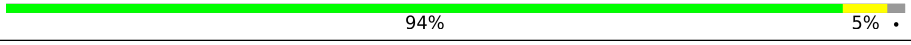
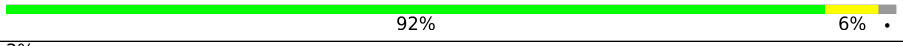
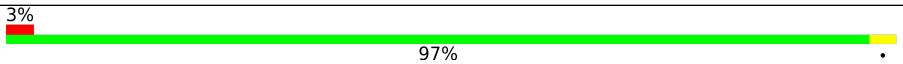
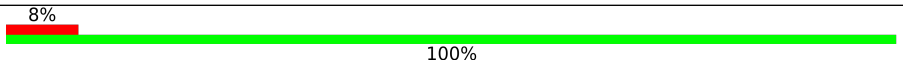
Mol	Chain	Length	Quality of chain
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
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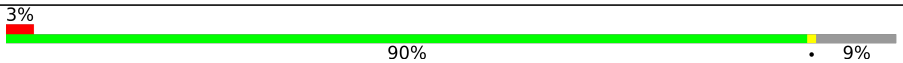
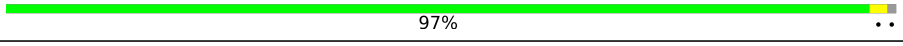
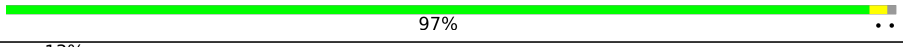
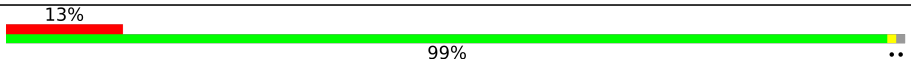
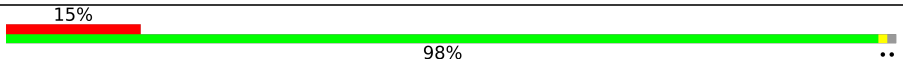
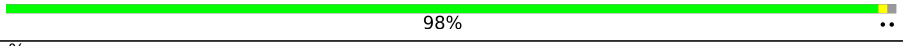
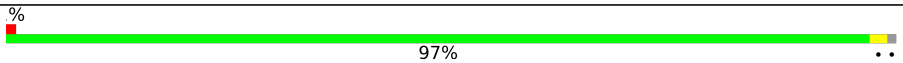
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	

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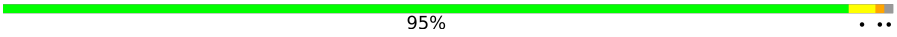
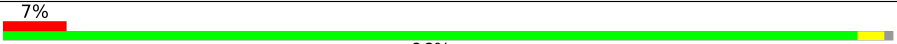
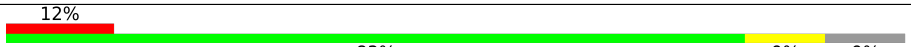
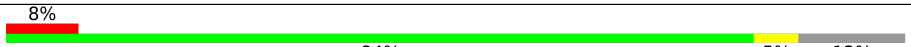
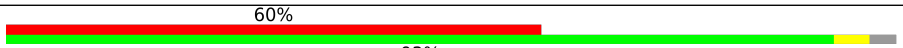
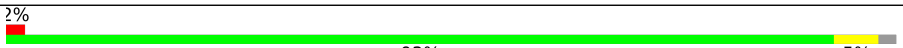
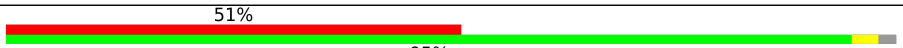
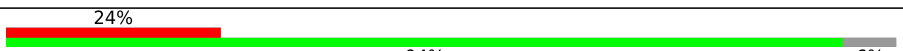
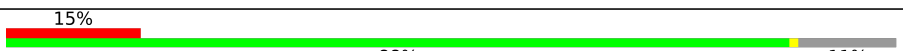
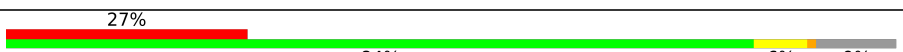
Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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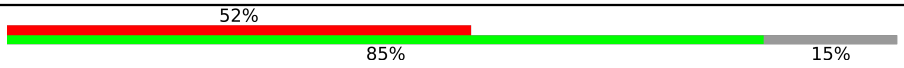
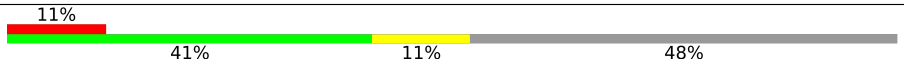
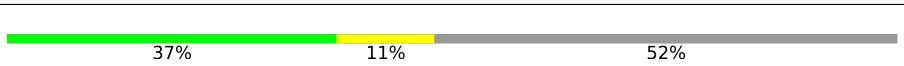
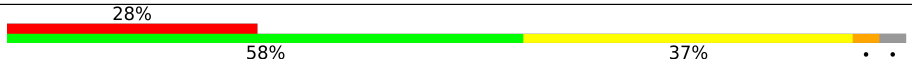
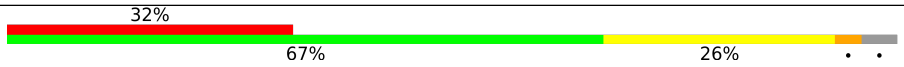
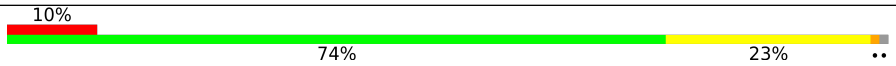
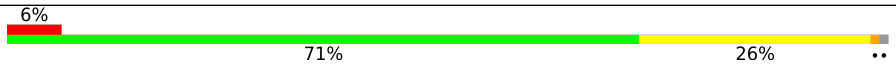
Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	27	
53	2v	27	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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
54	5MU	2y	54	-	-	-	X
56	MG	1A	3342	-	-	-	X
56	MG	1A	3640	-	-	-	X
56	MG	1P	203	-	-	-	X
56	MG	2A	3163	-	-	-	X
56	MG	2A	3466	-	-	-	X
56	MG	2A	3469	-	-	-	X
56	MG	2A	3632	-	-	-	X
56	MG	2A	3641	-	-	-	X
56	MG	2Z	8001	-	-	-	X

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 299169 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1429	916	256	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	14	Total 281	C 125	N 51	O 91	P 14	0	0	0
53	2v	13	Total 277	C 125	N 51	O 88	P 13	0	0	0

- Molecule 54 is a RNA chain called A/E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total 1588	C 713	N 285	O 515	P 73	S 2	0	0	0
54	1y	74	Total 1581	C 707	N 285	O 515	P 73	S 1	0	0	0
54	2w	73	Total 1561	C 698	N 283	O 507	P 72	S 1	0	0	0
54	2y	73	Total 1561	C 698	N 283	O 507	P 72	S 1	0	0	0

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total 1625	C 725	N 294	O 529	P 76	S 1	0	0	0
55	2x	76	Total 1625	C 725	N 294	O 529	P 76	S 1	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	935	Total 935	Mg 935	0	0
56	1B	25	Total 25	Mg 25	0	0
56	1D	9	Total 9	Mg 9	0	0
56	1E	8	Total 8	Mg 8	0	0
56	1F	8	Total 8	Mg 8	0	0
56	1G	5	Total 5	Mg 5	0	0
56	1I	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1N	6	Total Mg 6 6	0	0
56	1O	3	Total Mg 3 3	0	0
56	1P	3	Total Mg 3 3	0	0
56	1Q	5	Total Mg 5 5	0	0
56	1R	2	Total Mg 2 2	0	0
56	1S	1	Total Mg 1 1	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	4	Total Mg 4 4	0	0
56	1V	3	Total Mg 3 3	0	0
56	1W	4	Total Mg 4 4	0	0
56	1X	3	Total Mg 3 3	0	0
56	1Y	2	Total Mg 2 2	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	6	Total Mg 6 6	0	0
56	11	2	Total Mg 2 2	0	0
56	12	2	Total Mg 2 2	0	0
56	13	1	Total Mg 1 1	0	0
56	15	4	Total Mg 4 4	0	0
56	16	2	Total Mg 2 2	0	0
56	17	1	Total Mg 1 1	0	0
56	18	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	19	2	Total Mg 2 2	0	0
56	1a	234	Total Mg 234 234	0	0
56	1b	2	Total Mg 2 2	0	0
56	1c	1	Total Mg 1 1	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	1f	1	Total Mg 1 1	0	0
56	1g	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	1n	1	Total Mg 1 1	0	0
56	1r	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	5	Total Mg 5 5	0	0
56	1x	14	Total Mg 14 14	0	0
56	1y	7	Total Mg 7 7	0	0
56	2A	679	Total Mg 679 679	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	4	Total Mg 4 4	0	0
56	2E	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2F	5	Total Mg 5 5	0	0
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	2	Total Mg 2 2	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	1	Total Mg 1 1	0	0
56	2T	1	Total Mg 1 1	0	0
56	2U	2	Total Mg 2 2	0	0
56	2V	3	Total Mg 3 3	0	0
56	2X	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	3	Total Mg 3 3	0	0
56	21	2	Total Mg 2 2	0	0
56	23	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	2a	200	Total Mg 200 200	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	2	Total Mg 2 2	0	0
56	2f	2	Total Mg 2 2	0	0
56	2g	1	Total Mg 1 1	0	0

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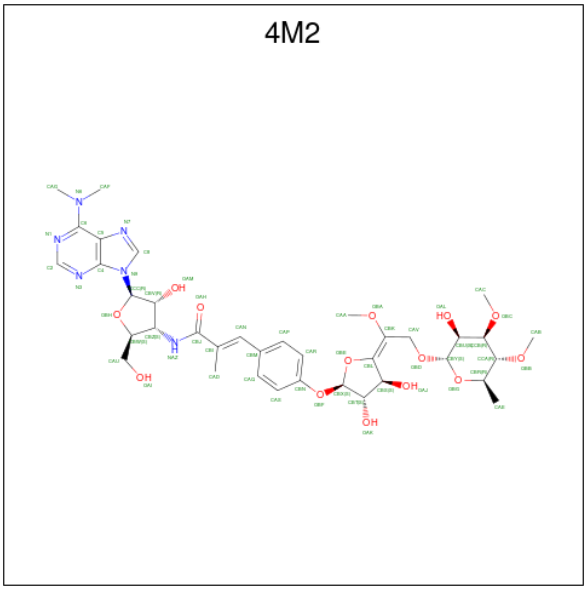
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2j	2	Total Mg 2 2	0	0
56	2l	2	Total Mg 2 2	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	2	Total Mg 2 2	0	0
56	2w	3	Total Mg 3 3	0	0
56	2x	2	Total Mg 2 2	0	0

- Molecule 57 is 3'-deoxy-3'-{[(2E)-3-(4-{[(4Z)-6-O-(6-deoxy-3,4-di-O-methyl-alpha-D-mannopyranosyl)-5-O-methyl-alpha-D-threo-hex-4-enofuranosyl]oxy}phenyl)-2-methylprop-2-enoyl]amino}-N,N-dimethyladenosine (three-letter code: 4M2) (formula: $C_{37}H_{50}N_6O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C N O 57 37 6 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2A	1	Total C N O 57 37 6 14	0	0

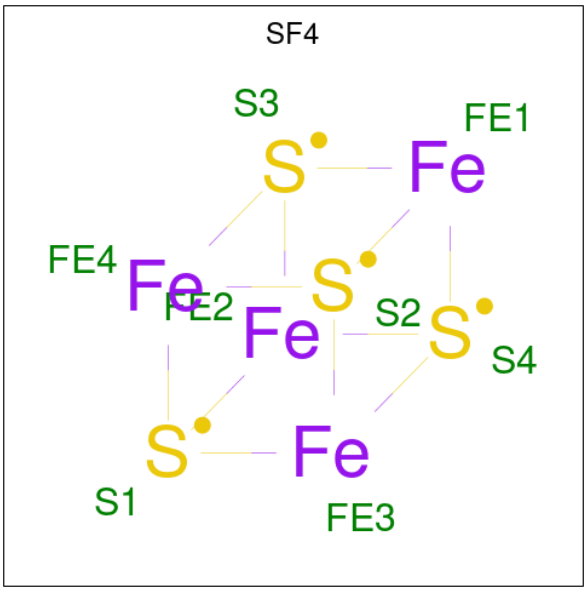
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2A	1	Total K 1 1	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

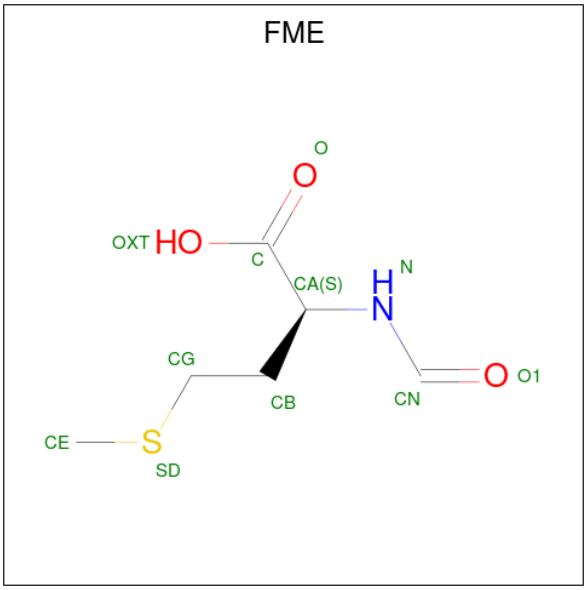
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1d	1	Total Fe S 8 4 4	0	0
60	2d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1x	1	Total C N O S 10 6 1 2 1	0	0
61	2x	1	Total C N O S 10 6 1 2 1	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	1741	Total O 1741 1741	0	0
62	1B	49	Total O 49 49	0	0
62	1D	21	Total O 21 21	0	0
62	1E	27	Total O 27 27	0	0
62	1F	22	Total O 22 22	0	0
62	1G	3	Total O 3 3	0	0
62	1I	1	Total O 1 1	0	0
62	1N	6	Total O 6 6	0	0
62	1O	4	Total O 4 4	0	0
62	1P	21	Total O 21 21	0	0
62	1Q	5	Total O 5 5	0	0
62	1R	5	Total O 5 5	0	0
62	1S	6	Total O 6 6	0	0
62	1T	13	Total O 13 13	0	0
62	1U	12	Total O 12 12	0	0
62	1V	10	Total O 10 10	0	0
62	1W	6	Total O 6 6	0	0
62	1X	4	Total O 4 4	0	0
62	1Y	4	Total O 4 4	0	0
62	1Z	1	Total O 1 1	0	0
62	10	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	11	3	Total O 3 3	0	0
62	12	4	Total O 4 4	0	0
62	13	5	Total O 5 5	0	0
62	15	1	Total O 1 1	0	0
62	17	6	Total O 6 6	0	0
62	18	10	Total O 10 10	0	0
62	19	2	Total O 2 2	0	0
62	1a	309	Total O 309 309	0	0
62	1d	1	Total O 1 1	0	0
62	1g	1	Total O 1 1	0	0
62	1j	1	Total O 1 1	0	0
62	1l	3	Total O 3 3	0	0
62	1m	1	Total O 1 1	0	0
62	1o	2	Total O 2 2	0	0
62	1p	2	Total O 2 2	0	0
62	1q	1	Total O 1 1	0	0
62	1r	1	Total O 1 1	0	0
62	1v	6	Total O 6 6	0	0
62	1w	6	Total O 6 6	0	0
62	1x	13	Total O 13 13	0	0
62	1y	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2A	1031	Total O 1031 1031	0	0
62	2B	10	Total O 10 10	0	0
62	2D	16	Total O 16 16	0	0
62	2E	10	Total O 10 10	0	0
62	2F	7	Total O 7 7	0	0
62	2I	2	Total O 2 2	0	0
62	2N	1	Total O 1 1	0	0
62	2O	1	Total O 1 1	0	0
62	2P	14	Total O 14 14	0	0
62	2Q	1	Total O 1 1	0	0
62	2R	2	Total O 2 2	0	0
62	2T	3	Total O 3 3	0	0
62	2U	1	Total O 1 1	0	0
62	2V	2	Total O 2 2	0	0
62	2W	1	Total O 1 1	0	0
62	2X	3	Total O 3 3	0	0
62	2Y	1	Total O 1 1	0	0
62	2Z	2	Total O 2 2	0	0
62	20	6	Total O 6 6	0	0
62	21	5	Total O 5 5	0	0
62	22	1	Total O 1 1	0	0

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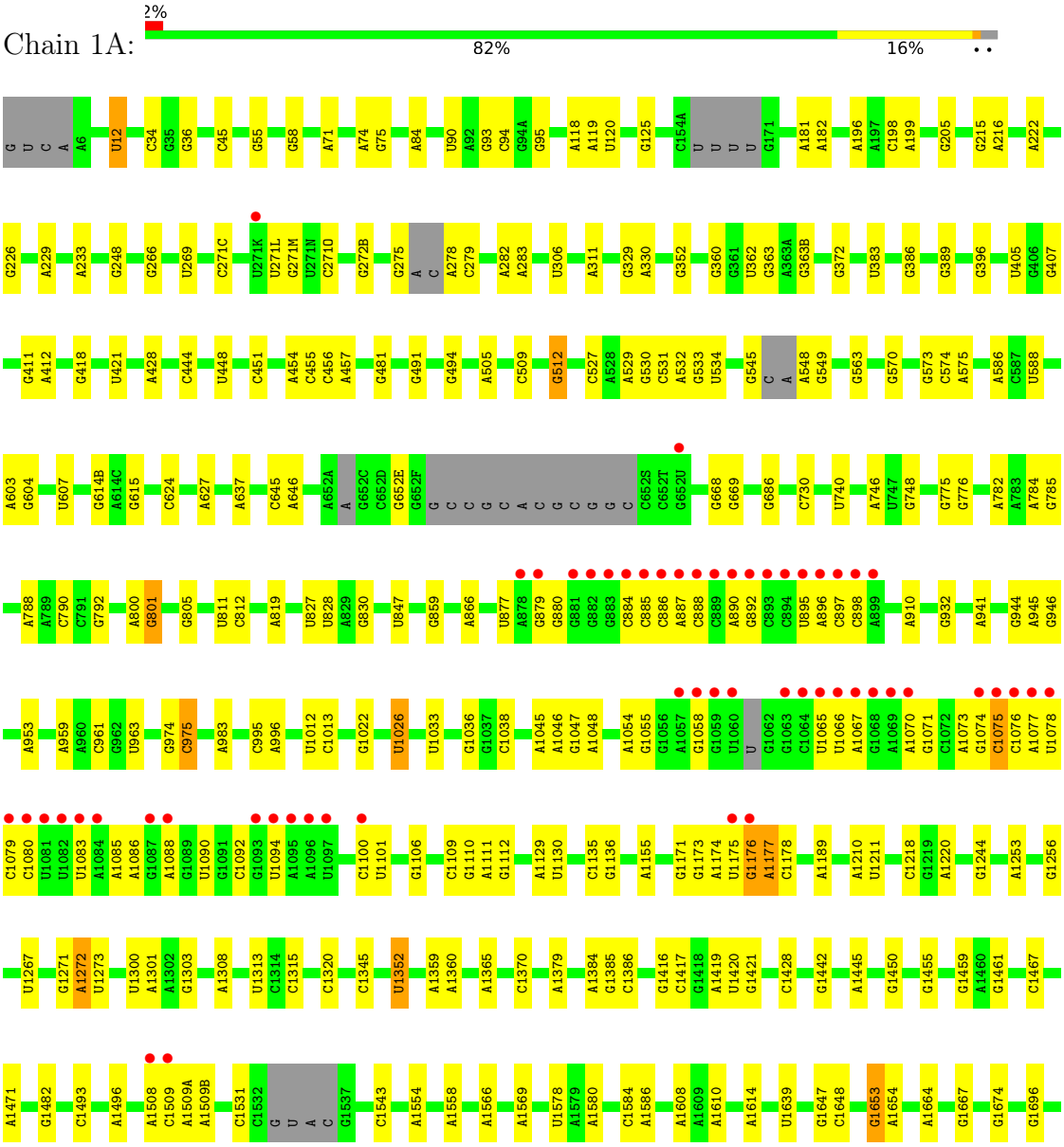
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	23	1	Total O 1 1	0	0
62	25	3	Total O 3 3	0	0
62	27	3	Total O 3 3	0	0
62	28	4	Total O 4 4	0	0
62	29	1	Total O 1 1	0	0
62	2a	203	Total O 203 203	0	0
62	2d	4	Total O 4 4	0	0
62	2g	1	Total O 1 1	0	0
62	2i	1	Total O 1 1	0	0
62	2j	4	Total O 4 4	0	0
62	2l	3	Total O 3 3	0	0
62	2o	1	Total O 1 1	0	0
62	2p	2	Total O 2 2	0	0
62	2r	1	Total O 1 1	0	0
62	2t	2	Total O 2 2	0	0
62	2v	3	Total O 3 3	0	0
62	2x	6	Total O 6 6	0	0

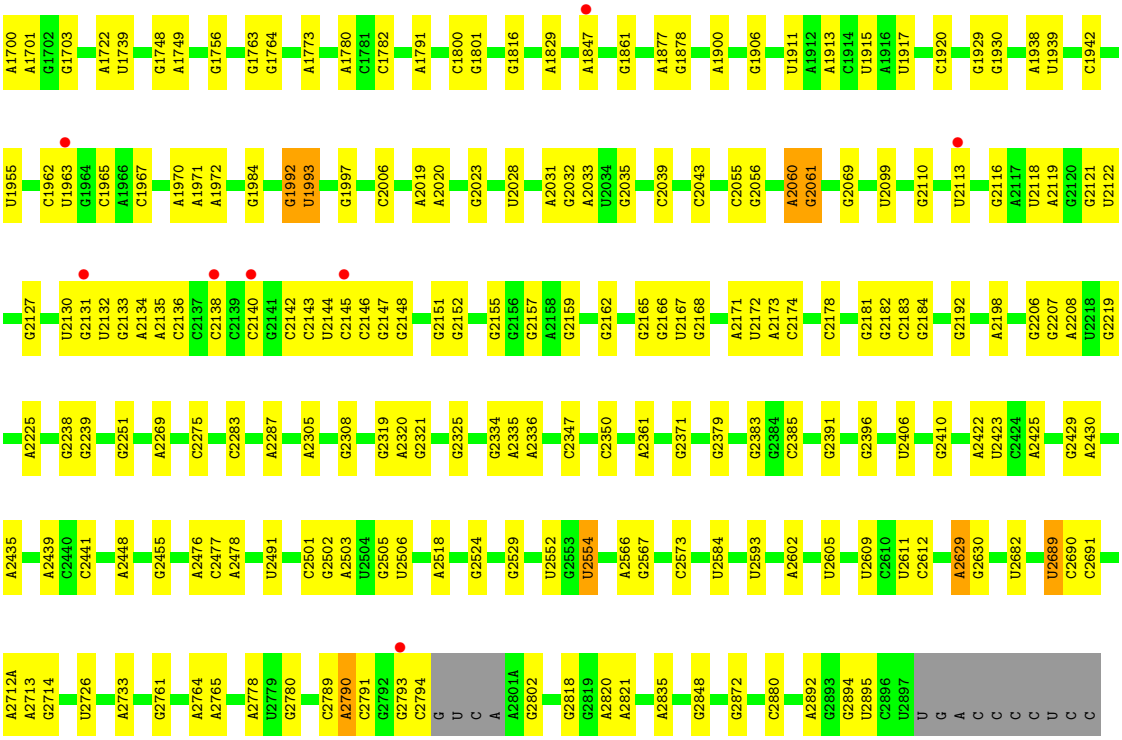
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

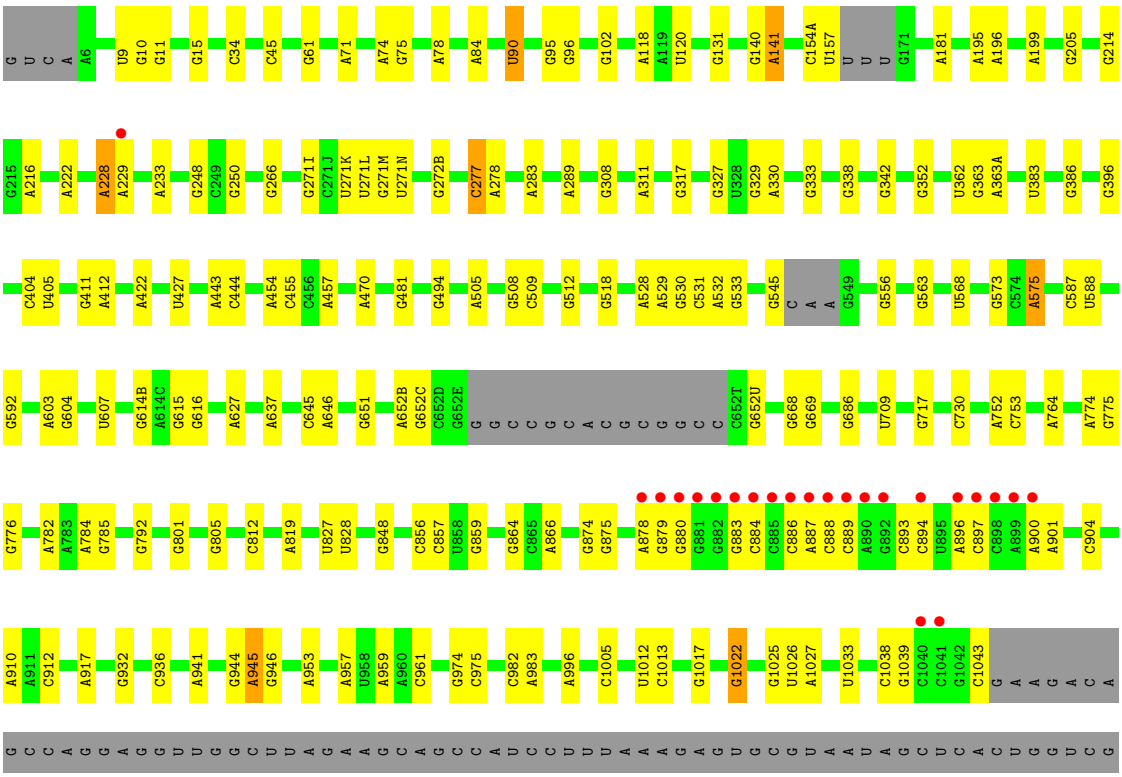
Chain 1A:

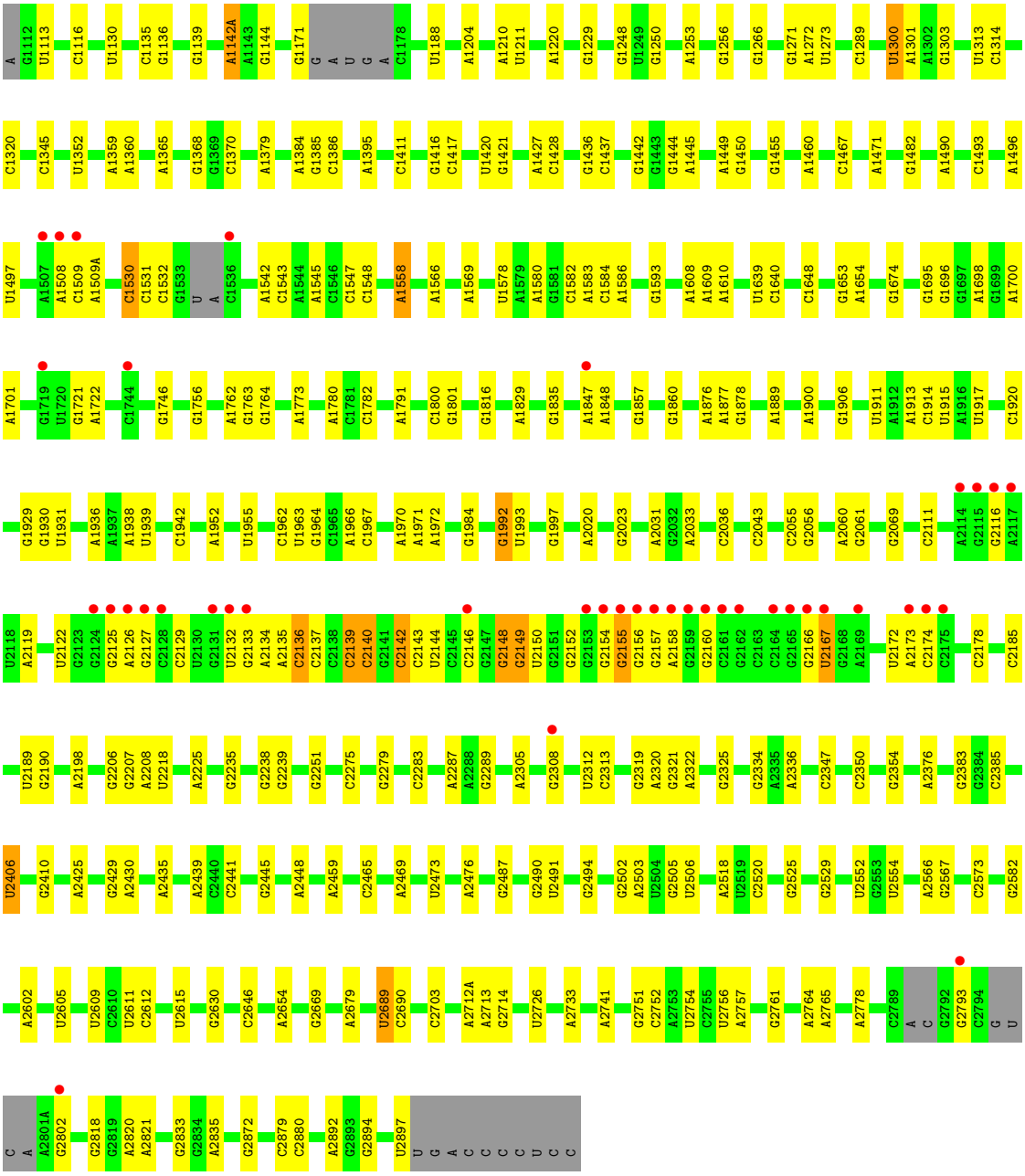




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



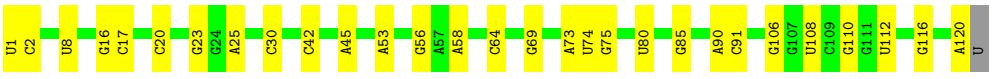


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

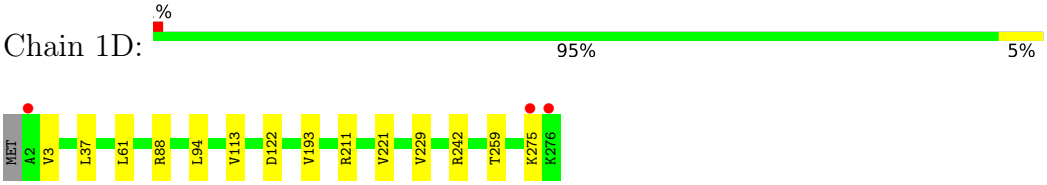
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



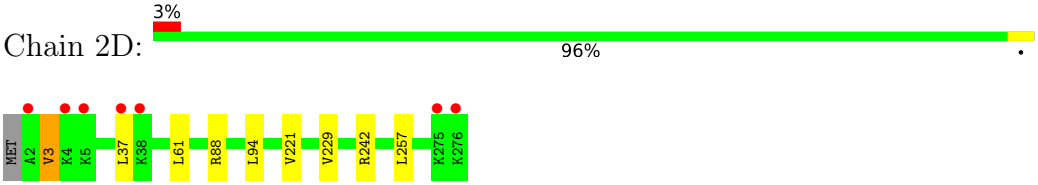
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



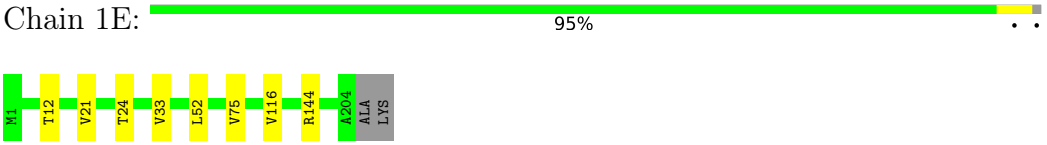
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



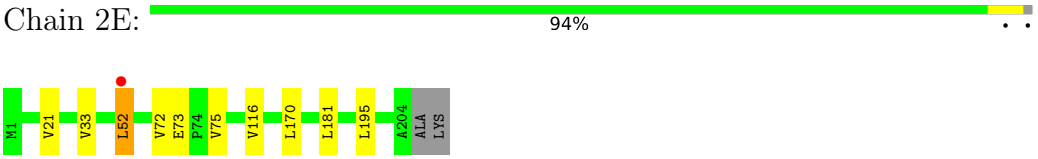
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



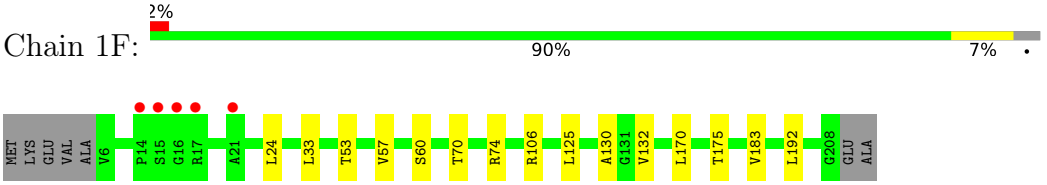
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



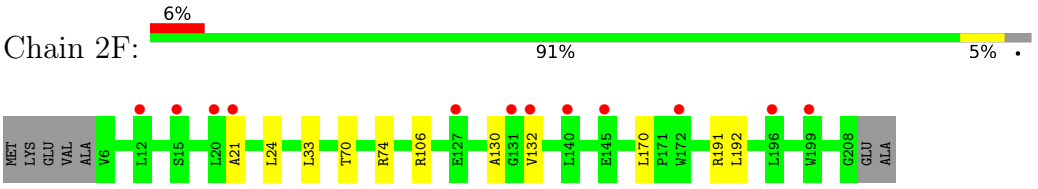
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



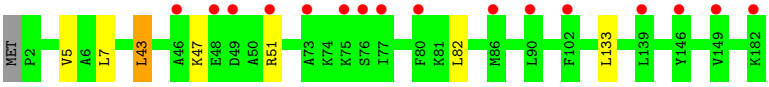
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



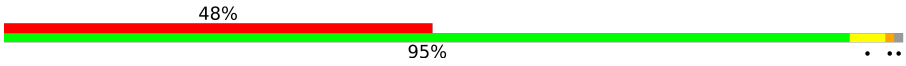
• Molecule 6: 50S ribosomal protein L5

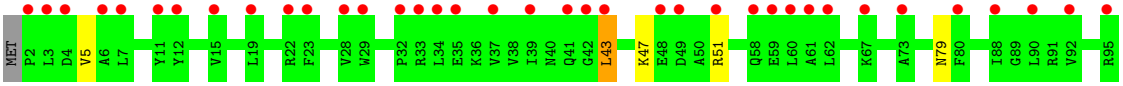
Chain 1G:

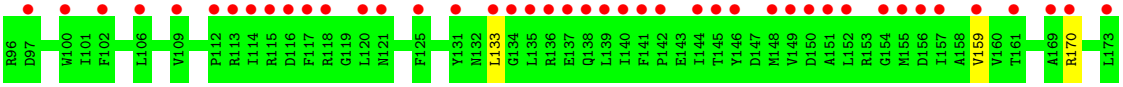


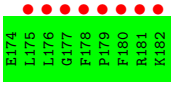
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



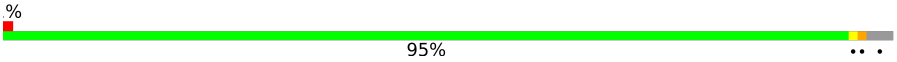






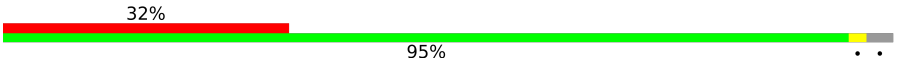
• Molecule 7: 50S ribosomal protein L6

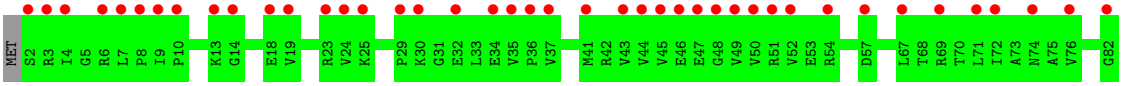
Chain 1H:

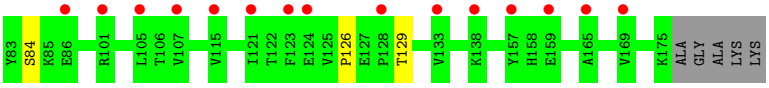


• Molecule 7: 50S ribosomal protein L6

Chain 2H:

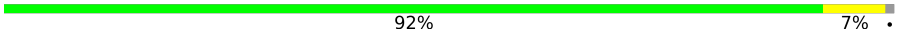






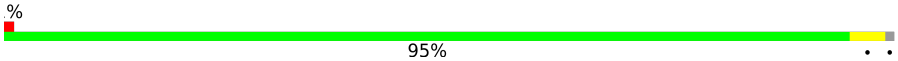
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



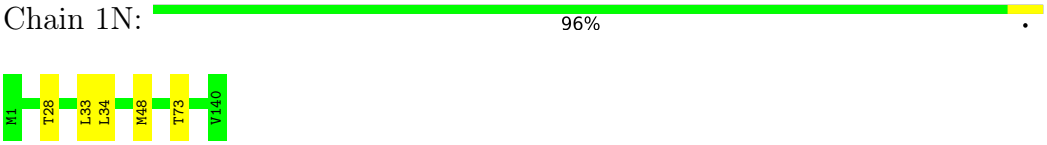
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



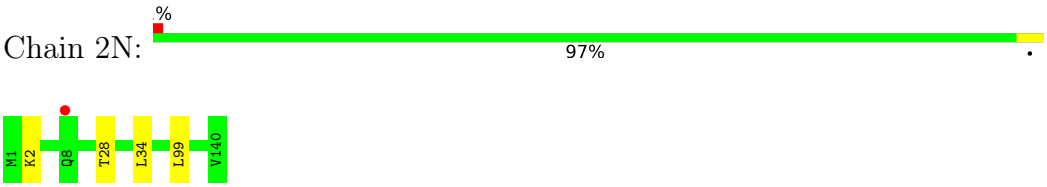
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

Chain 2N:

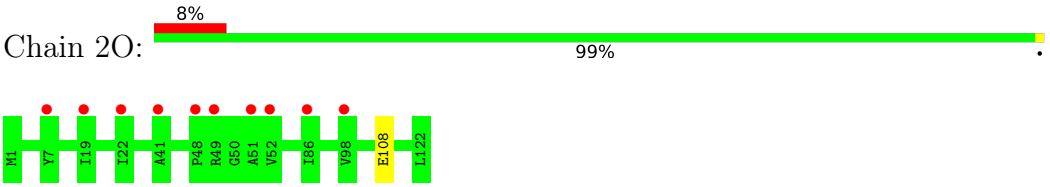


• Molecule 10: 50S ribosomal protein L14

Chain 1O:

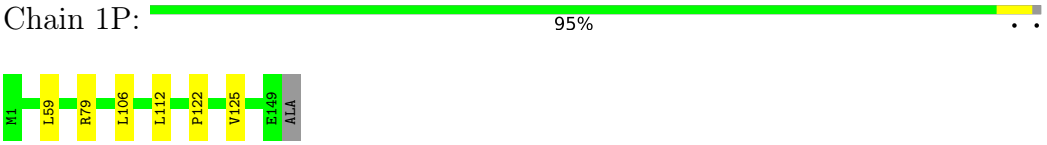
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



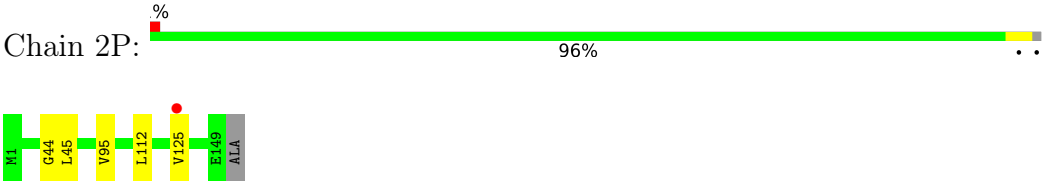
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



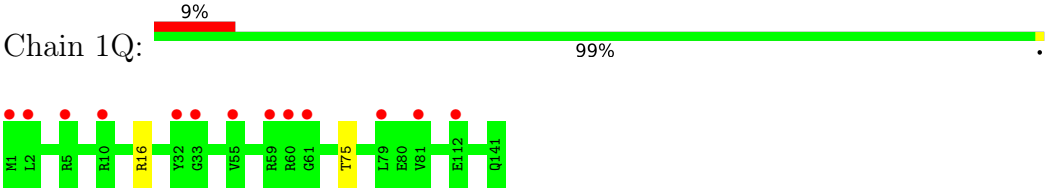
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



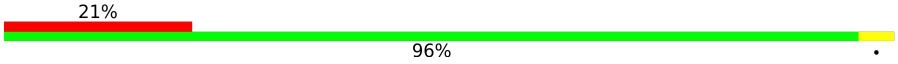
• Molecule 12: 50S ribosomal protein L16

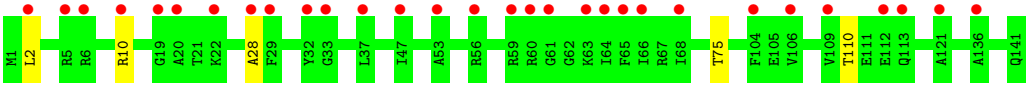
Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

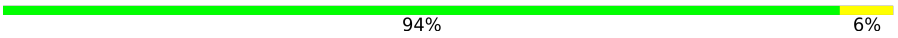
Chain 2Q:

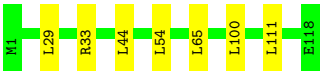




• Molecule 13: 50S ribosomal protein L17

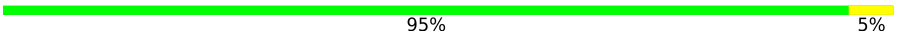
Chain 1R:





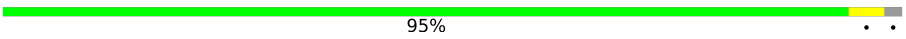
• Molecule 13: 50S ribosomal protein L17

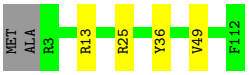
Chain 2R:



• Molecule 14: 50S ribosomal protein L18

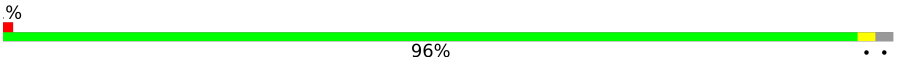
Chain 1S:





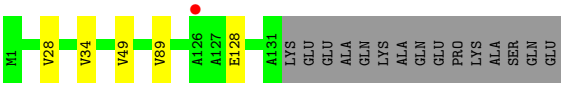
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



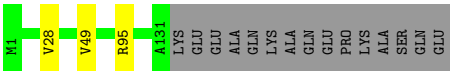
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



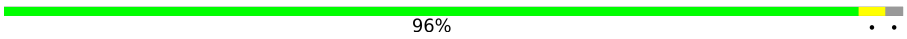
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



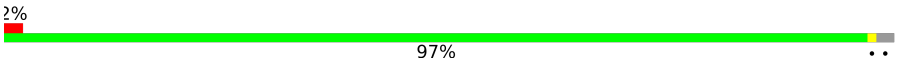
• Molecule 16: 50S ribosomal protein L20

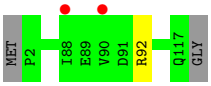
Chain 1U:



• Molecule 16: 50S ribosomal protein L20

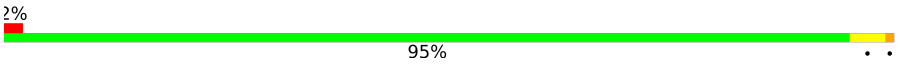
Chain 2U:





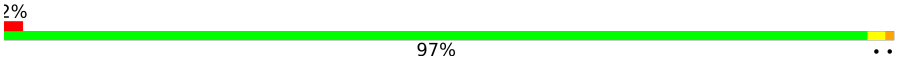
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



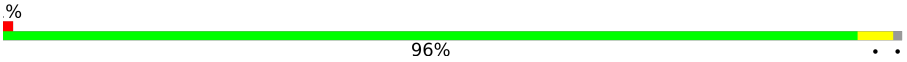
• Molecule 17: 50S ribosomal protein L21

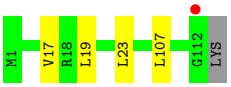
Chain 2V:



• Molecule 18: 50S ribosomal protein L22

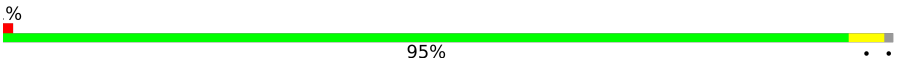
Chain 1W:

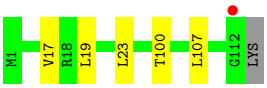




• Molecule 18: 50S ribosomal protein L22

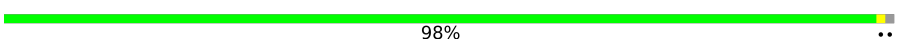
Chain 2W:

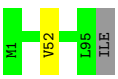




• Molecule 19: 50S ribosomal protein L23

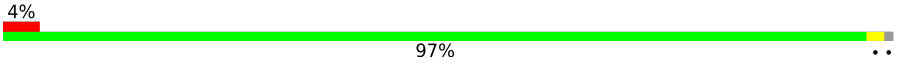
Chain 1X:

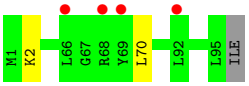




• Molecule 19: 50S ribosomal protein L23

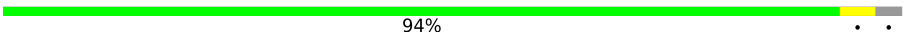
Chain 2X:

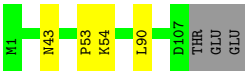




• Molecule 20: 50S ribosomal protein L24

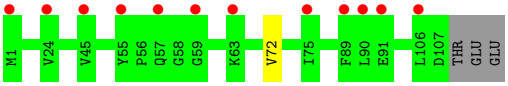
Chain 1Y:





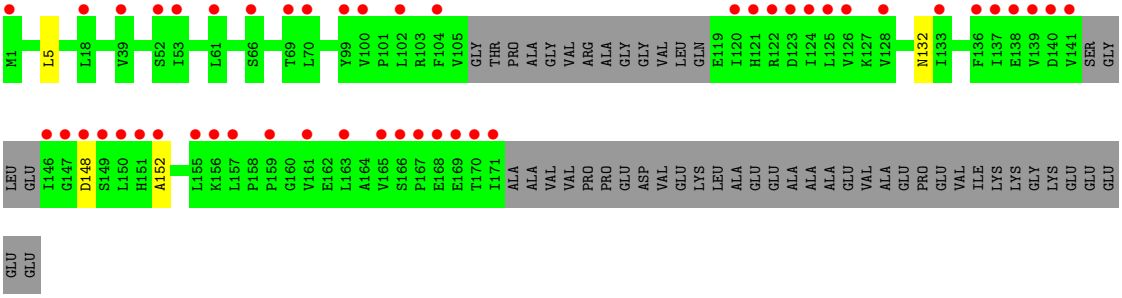
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



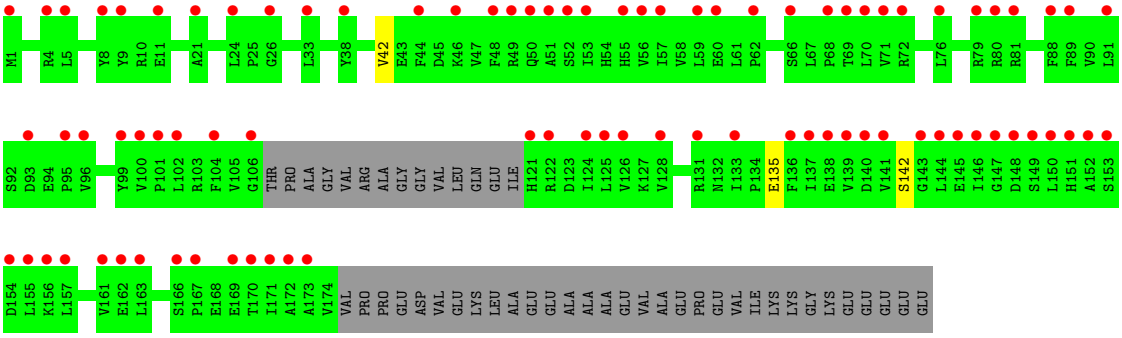
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



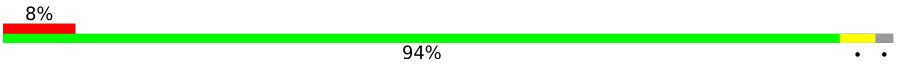
• Molecule 21: 50S ribosomal protein L25

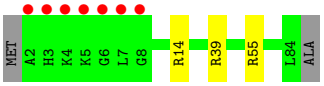
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

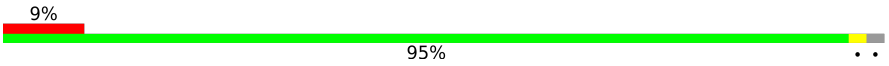
Chain 10:

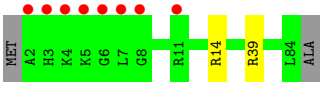




• Molecule 22: 50S ribosomal protein L27

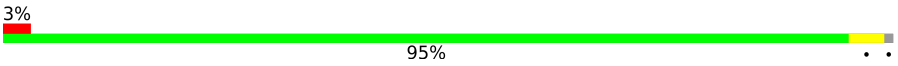
Chain 20:

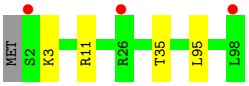




• Molecule 23: 50S ribosomal protein L28

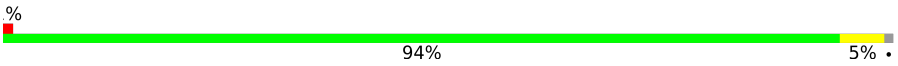
Chain 11:

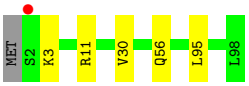




• Molecule 23: 50S ribosomal protein L28

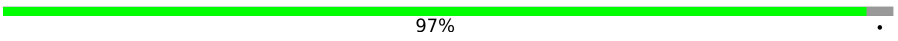
Chain 21:





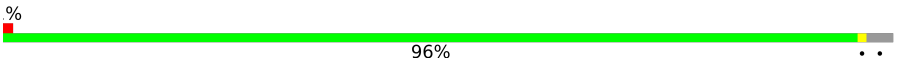
• Molecule 24: 50S ribosomal protein L29

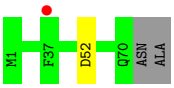
Chain 12:



• Molecule 24: 50S ribosomal protein L29

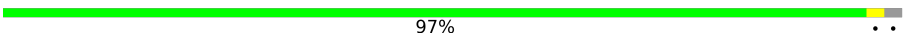
Chain 22:





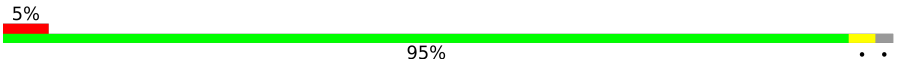
• Molecule 25: 50S ribosomal protein L30

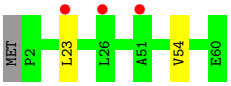
Chain 13:



• Molecule 25: 50S ribosomal protein L30

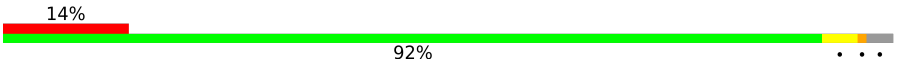
Chain 23:

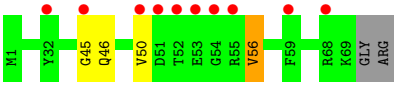




• Molecule 26: 50S ribosomal protein L31

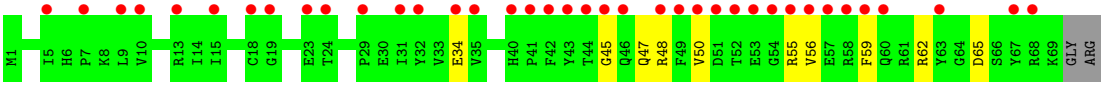
Chain 14:





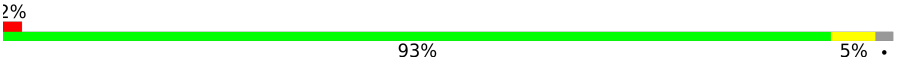
• Molecule 26: 50S ribosomal protein L31

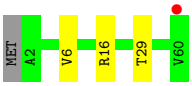
Chain 24:



• Molecule 27: 50S ribosomal protein L32

Chain 15:



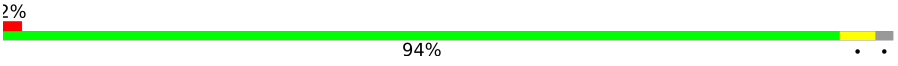


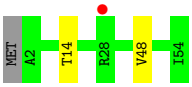
• Molecule 27: 50S ribosomal protein L32

Chain 25:

• Molecule 28: 50S ribosomal protein L33

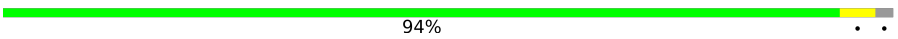
Chain 16:

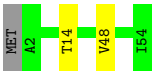




• Molecule 28: 50S ribosomal protein L33

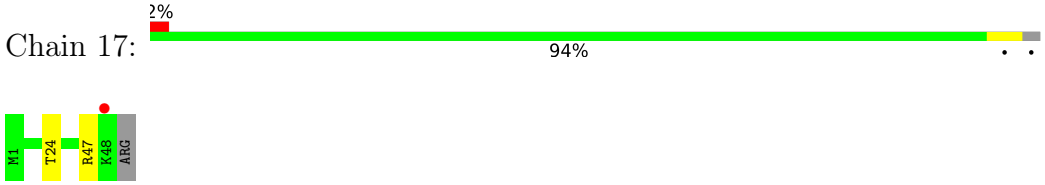
Chain 26:





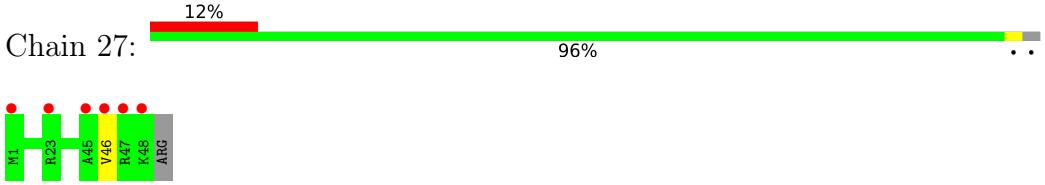
• Molecule 29: 50S ribosomal protein L34

Chain 17:



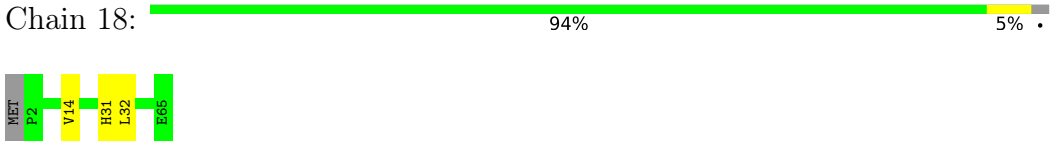
• Molecule 29: 50S ribosomal protein L34

Chain 27:



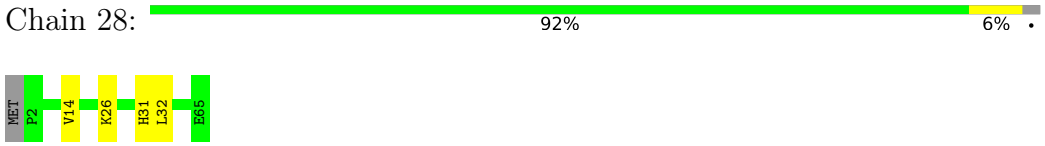
• Molecule 30: 50S ribosomal protein L35

Chain 18:



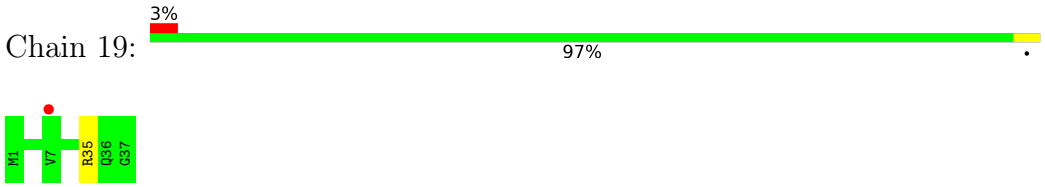
• Molecule 30: 50S ribosomal protein L35

Chain 28:



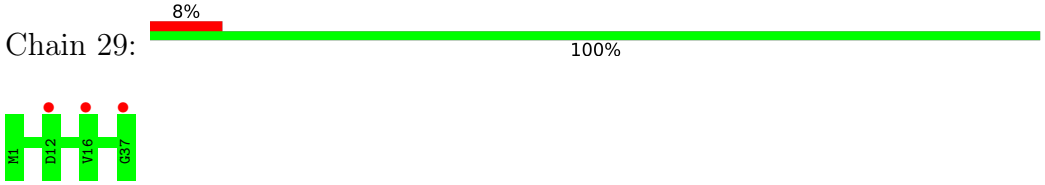
• Molecule 31: 50S ribosomal protein L36

Chain 19:



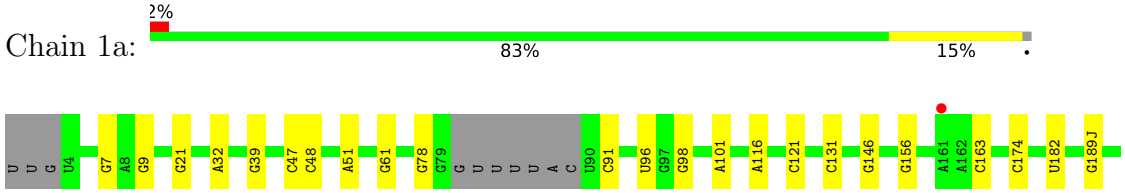
• Molecule 31: 50S ribosomal protein L36

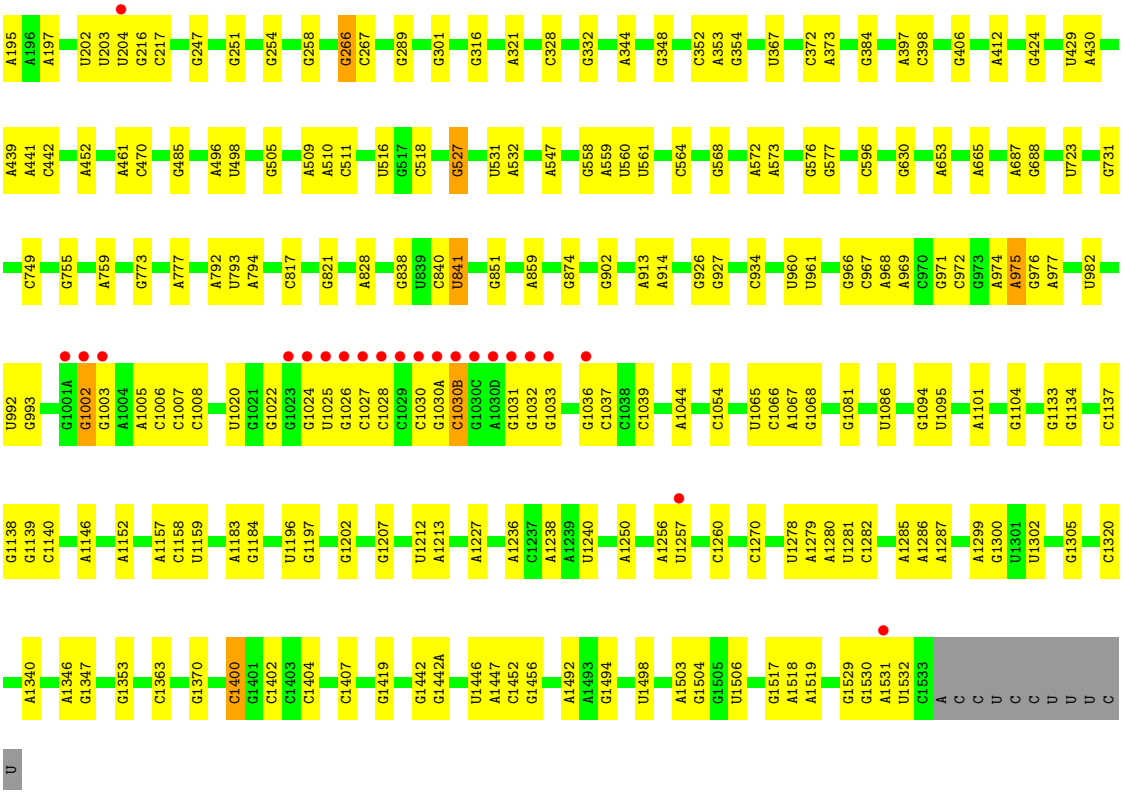
Chain 29:



• Molecule 32: 16S Ribosomal RNA

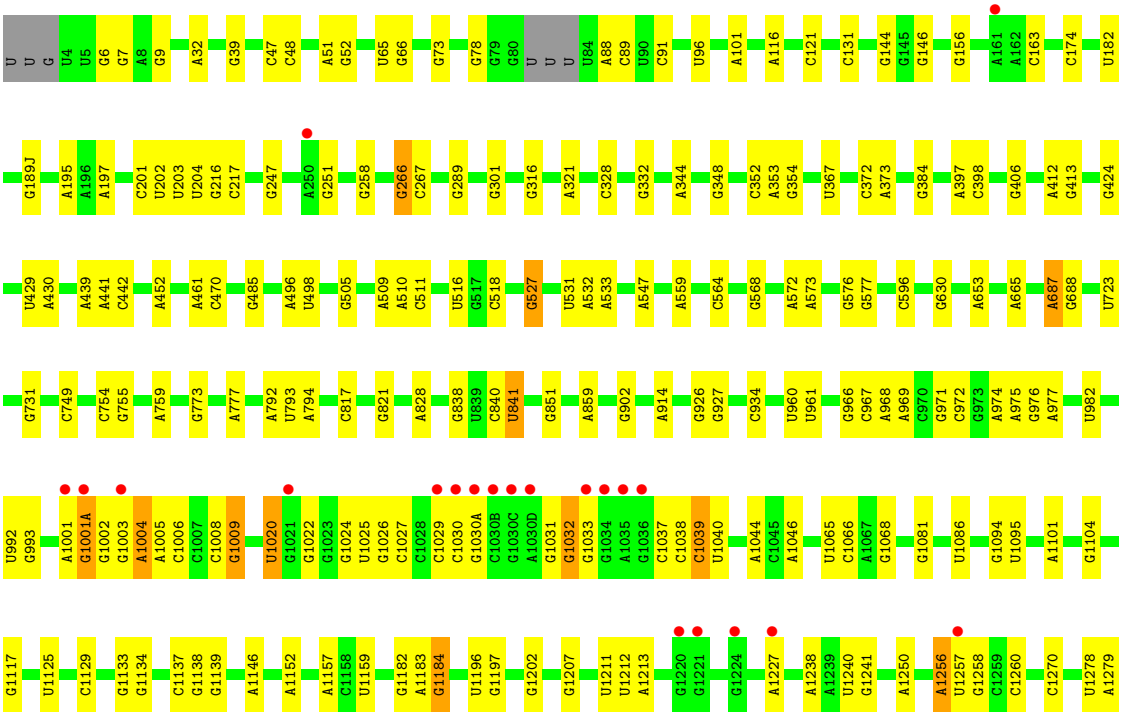
Chain 1a:





• Molecule 32: 16S Ribosomal RNA

Chain 2a:



• Molecule 33: 30S ribosomal protein S2

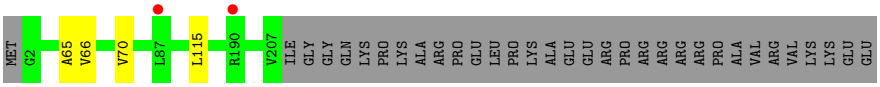
Chain 1b:

• Molecule 33: 30S ribosomal protein S2

Chain 2b:

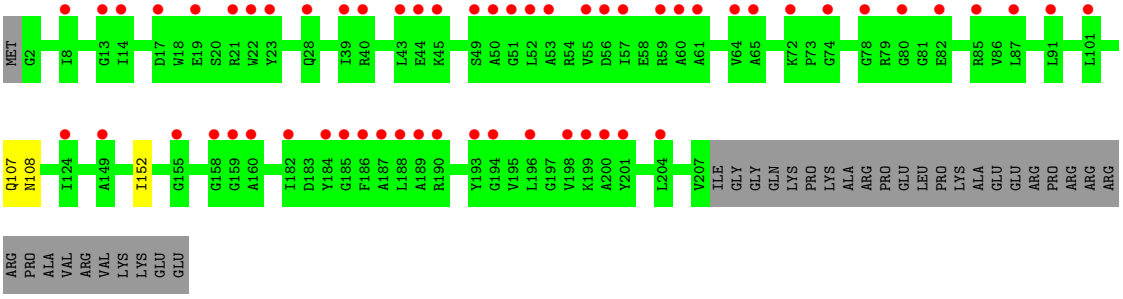
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



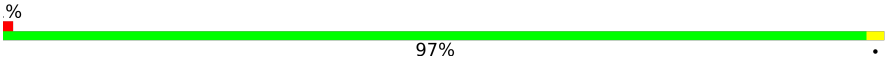
• Molecule 34: 30S ribosomal protein S3

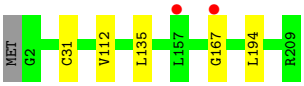
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

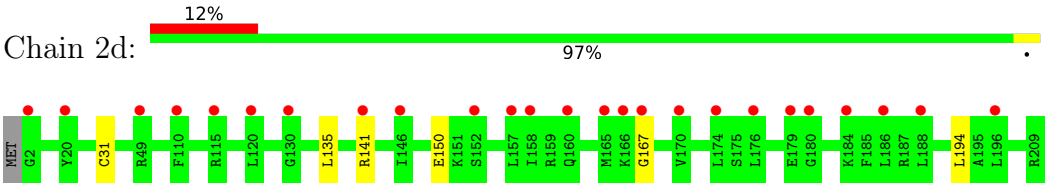
Chain 1d:





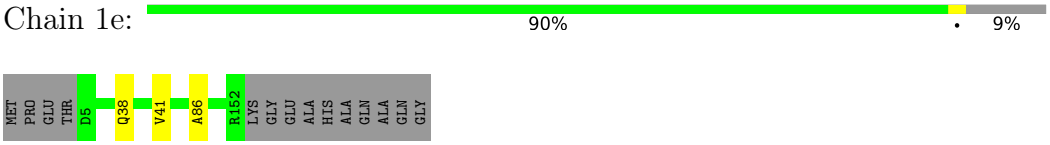
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



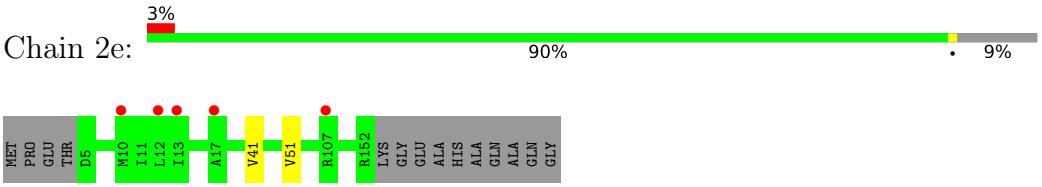
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



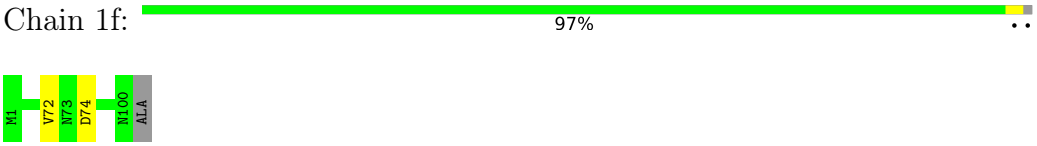
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



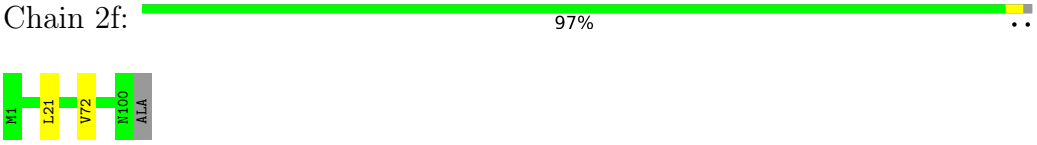
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



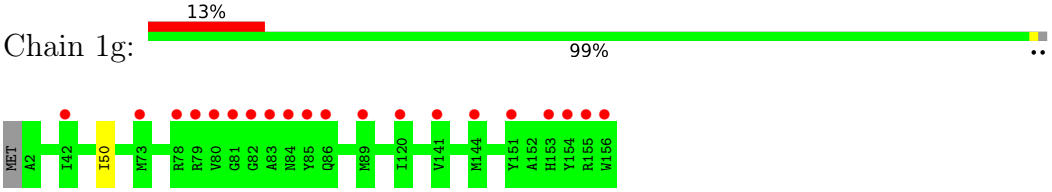
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



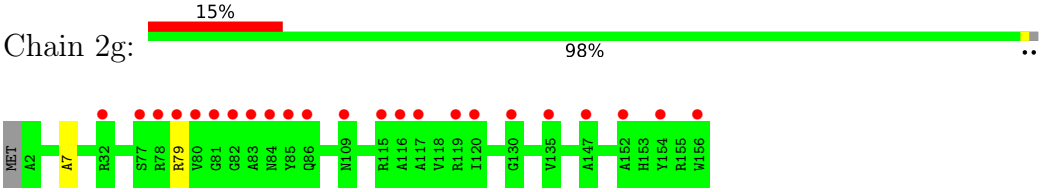
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



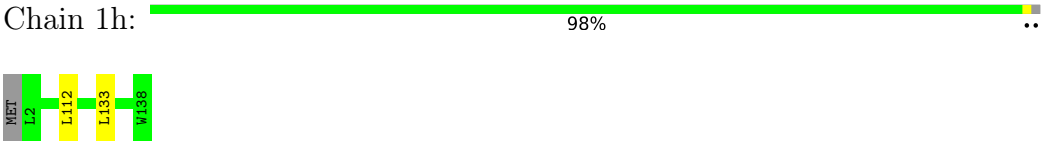
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



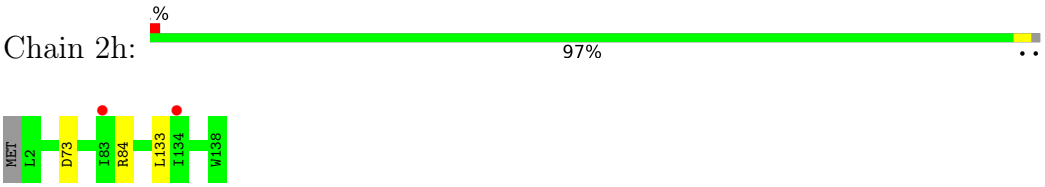
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



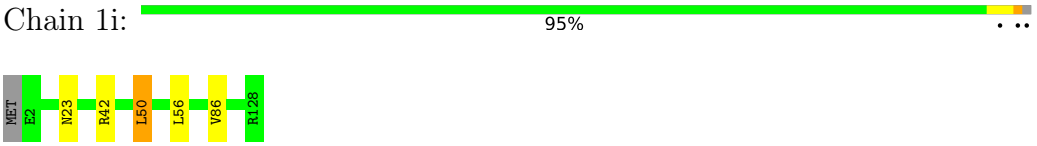
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



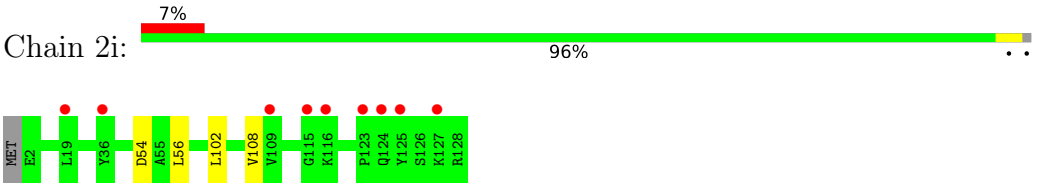
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



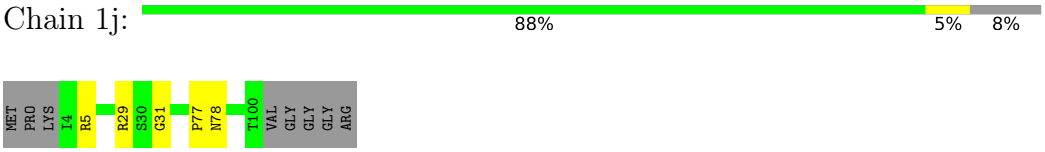
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



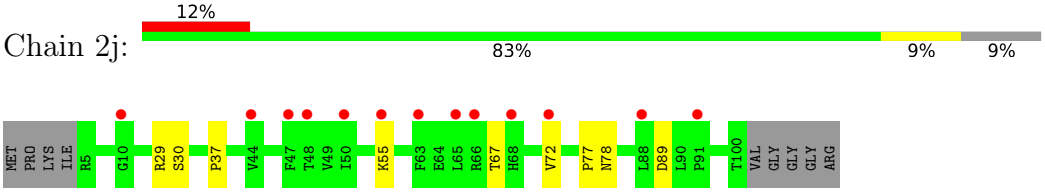
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



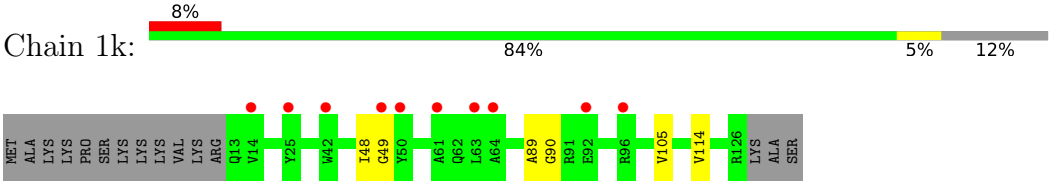
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



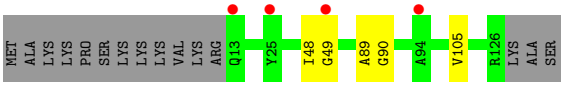
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



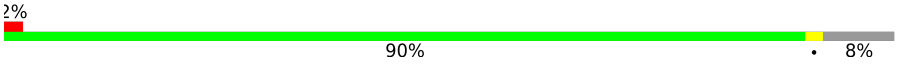
• Molecule 42: 30S ribosomal protein S11

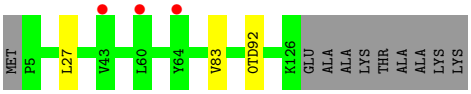
Chain 2k:



• Molecule 43: 30S ribosomal protein S12

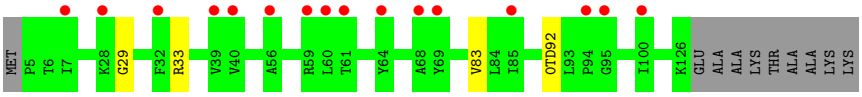
Chain 1l:





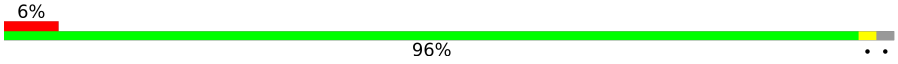
• Molecule 43: 30S ribosomal protein S12

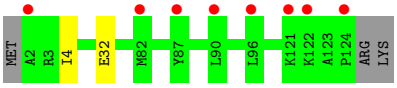
Chain 2l:



• Molecule 44: 30S ribosomal protein S13

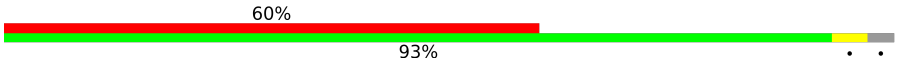
Chain 1m:

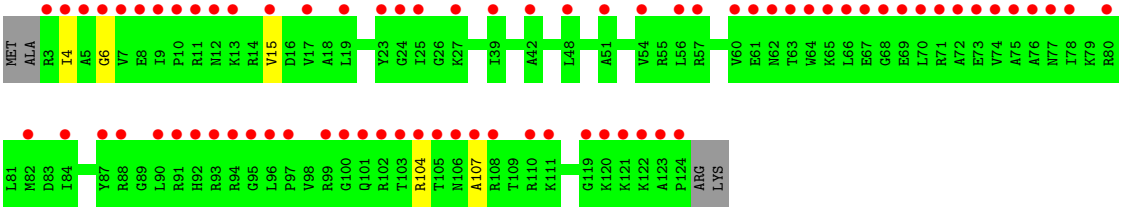




• Molecule 44: 30S ribosomal protein S13

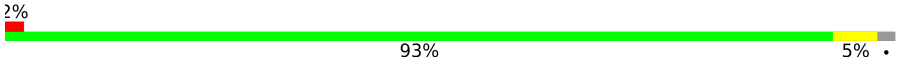
Chain 2m:

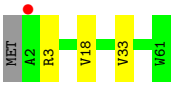




• Molecule 45: 30S ribosomal protein S14 type Z

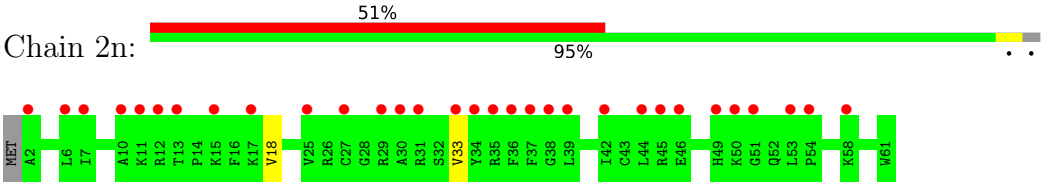
Chain 1n:





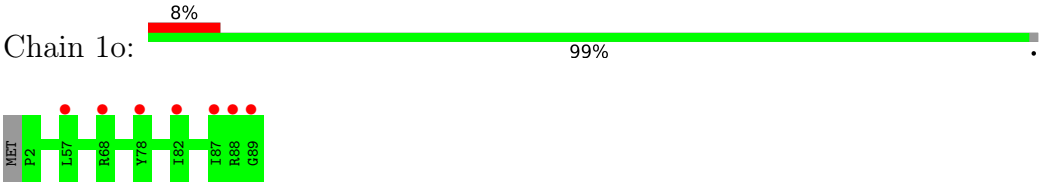
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



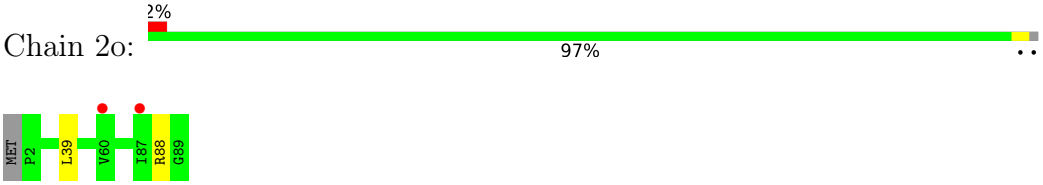
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



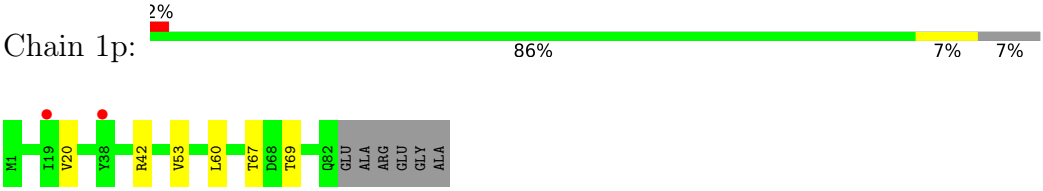
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



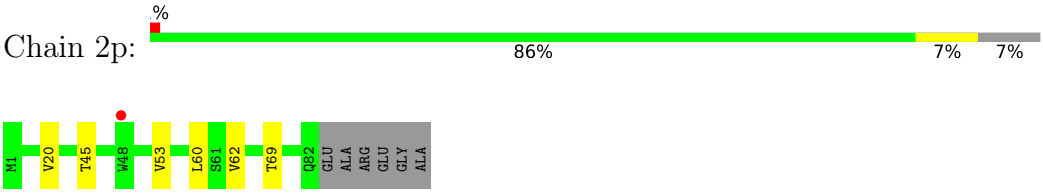
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



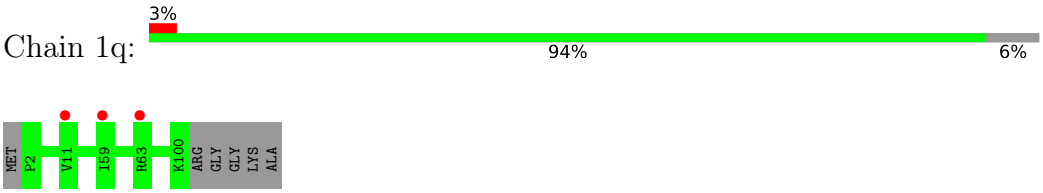
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



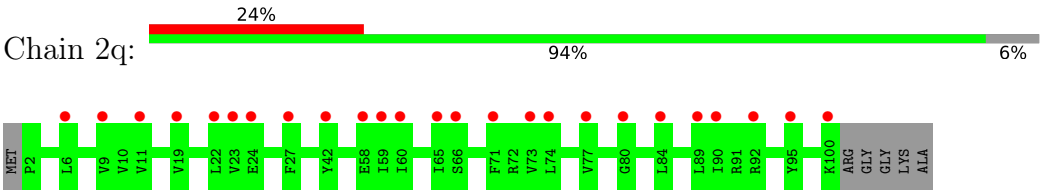
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



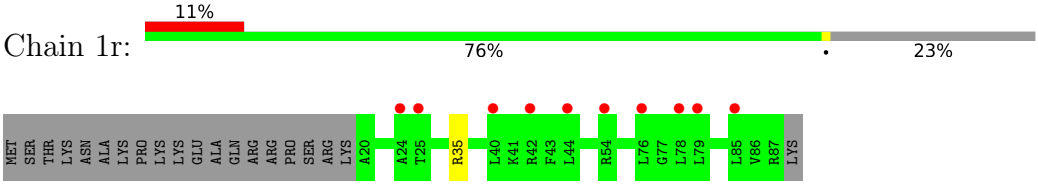
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



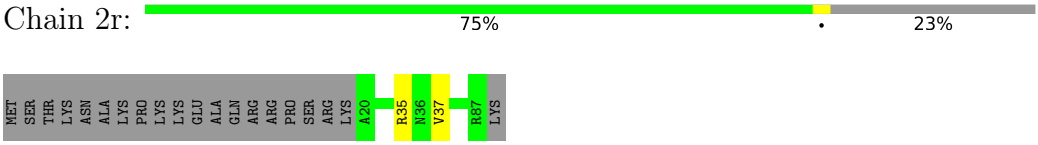
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



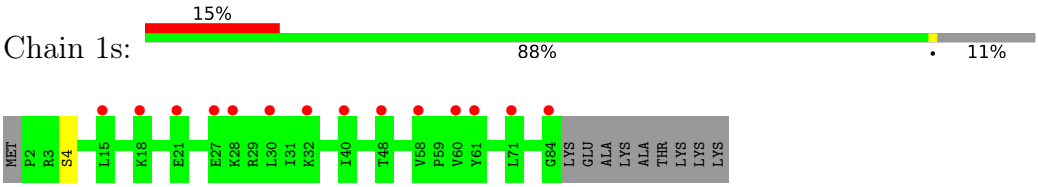
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



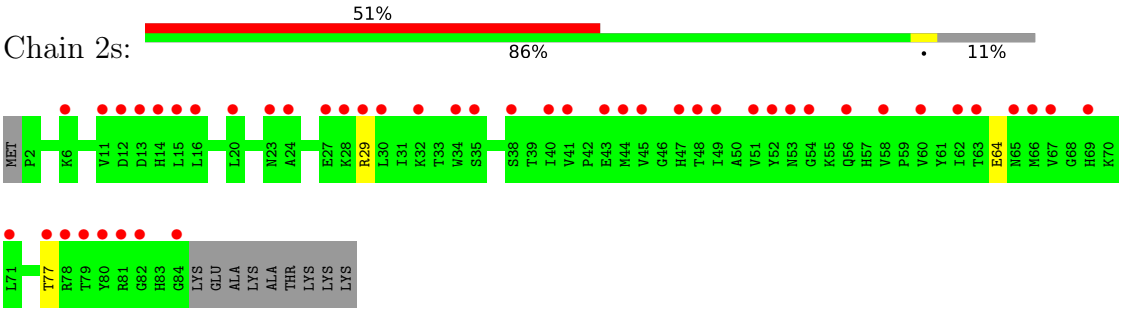
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



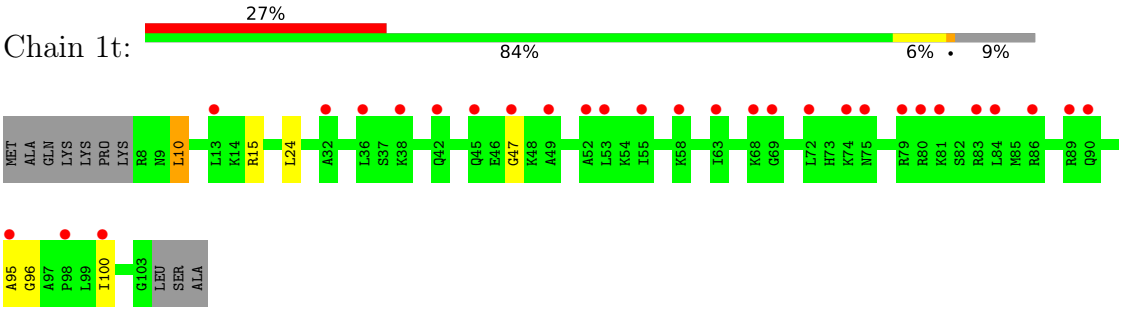
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



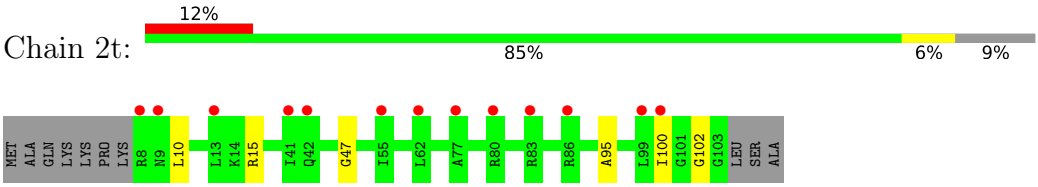
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



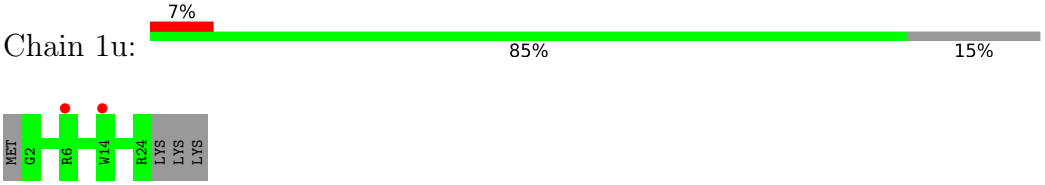
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



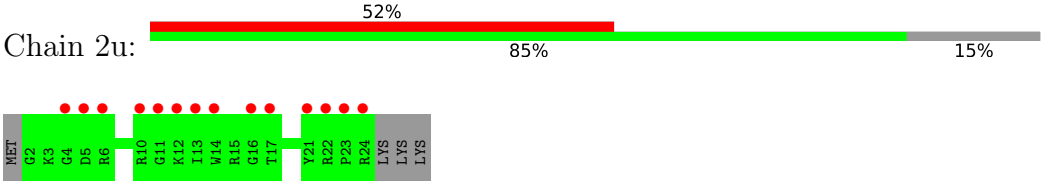
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



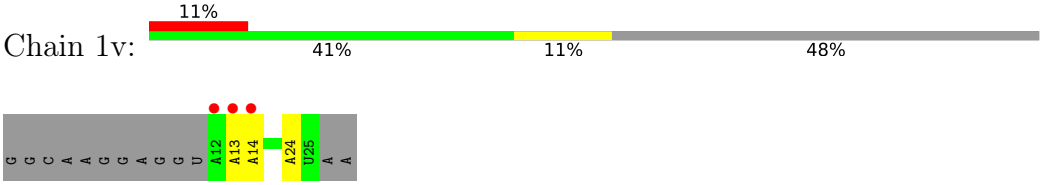
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



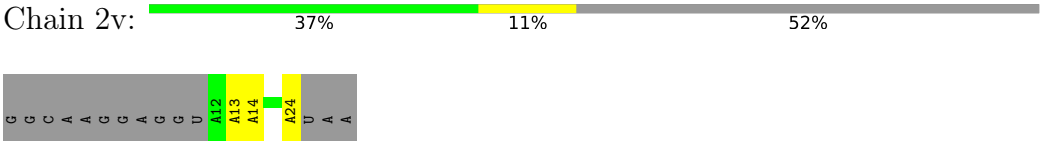
• Molecule 53: mRNA

Chain 1v:



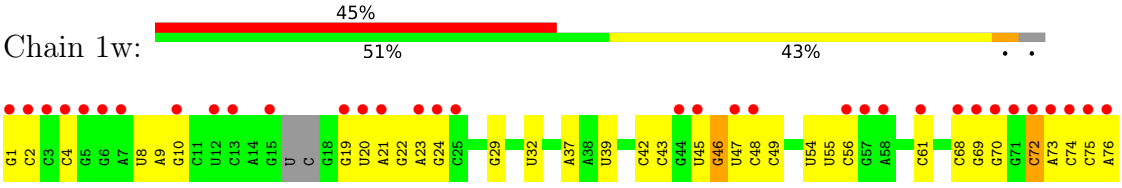
• Molecule 53: mRNA

Chain 2v:



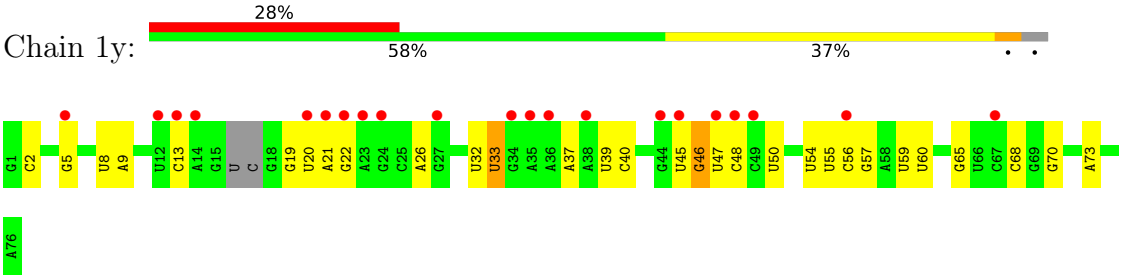
• Molecule 54: A/E-site tRNAs

Chain 1w:



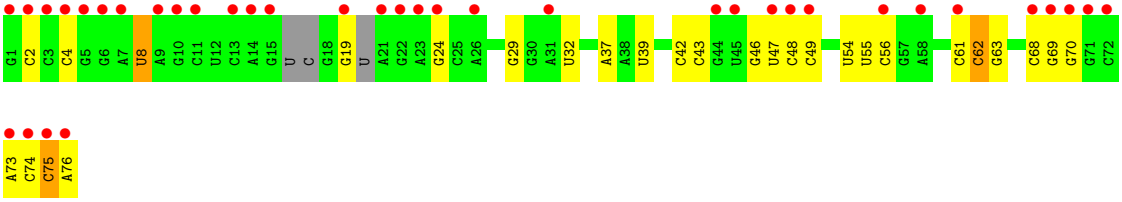
• Molecule 54: A/E-site tRNAs

Chain 1y:

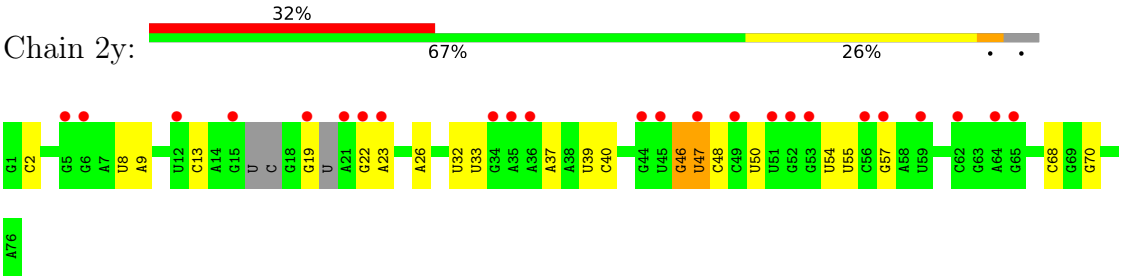


• Molecule 54: A/E-site tRNAs

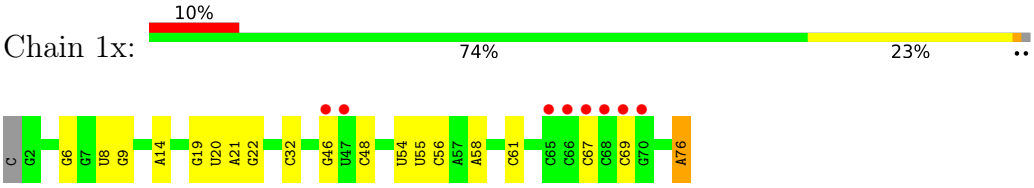
Chain 2w:



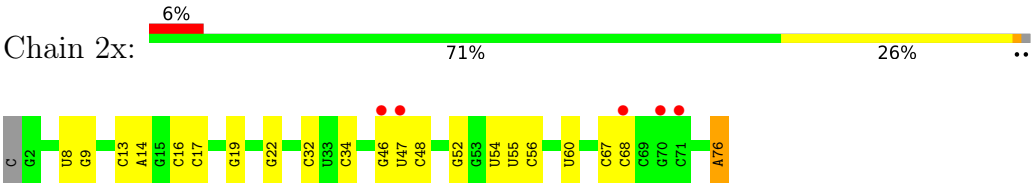
• Molecule 54: A/E-site tRNAs



• Molecule 55: P-site tRNA



• Molecule 55: P-site tRNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.89Å 446.22Å 619.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.07 – 2.65 362.07 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.5 (362.07-2.65) 98.5 (362.07-2.65)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.271 0.225 , 0.271	Depositor DCC
R_{free} test set	81734 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	299169	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, OMG, K, 2MA, FME, 2MG, 0TD, ZN, 4SU, MG, 7MG, PSU, UR3, MA6, MIA, 5MU, 5MC, 2MU, 4M2, 4OC, M2G

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	1A	0.50	0/69009	0.94	62/107712 (0.1%)
1	2A	0.42	0/67293	0.92	53/105034 (0.1%)
2	1B	0.43	1/2882 (0.0%)	0.82	0/4494
2	2B	0.48	1/2879 (0.0%)	0.92	1/4487 (0.0%)
3	1D	0.37	0/2186	0.58	0/2944
3	2D	0.34	0/2186	0.56	0/2944
4	1E	0.36	0/1592	0.55	0/2149
4	2E	0.32	0/1592	0.57	1/2149 (0.0%)
5	1F	0.35	0/1619	0.54	0/2193
5	2F	0.32	0/1615	0.55	0/2188
6	1G	0.30	0/1454	0.52	0/1964
6	2G	0.30	0/1453	0.53	0/1963
7	1H	0.31	0/1356	0.52	1/1834 (0.1%)
7	2H	0.28	0/1356	0.52	0/1834
8	1I	0.28	0/1112	0.53	0/1514
8	2I	0.26	0/1079	0.52	0/1475
9	1N	0.34	0/1144	0.52	0/1543
9	2N	0.31	0/1144	0.51	0/1543
10	1O	0.37	0/943	0.53	0/1269
10	2O	0.32	0/943	0.50	0/1269
11	1P	0.36	0/1152	0.59	0/1533
11	2P	0.31	0/1152	0.63	1/1533 (0.1%)
12	1Q	0.36	0/1143	0.53	0/1527
12	2Q	0.33	0/1143	0.54	0/1527
13	1R	0.35	0/982	0.54	0/1312
13	2R	0.31	0/982	0.52	0/1312
14	1S	0.32	0/883	0.54	0/1176
14	2S	0.31	0/880	0.56	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.31	0/1097	0.53	0/1468
16	1U	0.41	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.34	0/977	0.53	0/1301
17	1V	0.38	0/782	0.53	0/1049
17	2V	0.34	0/782	0.53	0/1049
18	1W	0.35	0/897	0.55	0/1205
18	2W	0.33	0/897	0.53	0/1205
19	1X	0.39	0/764	0.59	0/1025
19	2X	0.31	0/764	0.53	0/1025
20	1Y	0.33	0/819	0.56	0/1095
20	2Y	0.31	0/819	0.57	0/1095
21	1Z	0.30	0/1267	0.52	0/1717
21	2Z	0.31	0/1299	0.54	0/1763
22	10	0.37	0/662	0.61	0/881
22	20	0.29	0/662	0.47	0/881
23	11	0.34	0/762	0.49	0/1014
23	21	0.31	0/762	0.51	0/1014
24	12	0.32	0/590	0.50	0/781
24	22	0.30	0/590	0.47	0/781
25	13	0.34	0/474	0.56	0/635
25	23	0.29	0/469	0.52	0/630
26	14	0.33	0/565	0.65	0/761
26	24	0.33	0/545	0.66	0/737
27	15	0.35	0/469	0.59	0/635
27	25	0.32	0/469	0.55	1/635 (0.2%)
28	16	0.35	0/460	0.50	0/613
28	26	0.29	0/456	0.46	0/608
29	17	0.35	0/426	0.58	0/561
29	27	0.36	0/426	0.54	0/561
30	18	0.33	0/525	0.54	0/691
30	28	0.32	0/525	0.51	0/691
31	19	0.38	0/310	0.51	0/407
31	29	0.32	0/310	0.51	0/407
32	1a	0.37	0/35795	0.86	21/55864 (0.0%)
32	2a	0.37	0/35886	0.89	26/56005 (0.0%)
33	1b	0.29	0/1881	0.54	0/2542
33	2b	0.31	0/1860	0.59	0/2518
34	1c	0.27	0/1572	0.47	0/2126
34	2c	0.31	0/1566	0.52	0/2119
35	1d	0.29	0/1685	0.52	0/2262
35	2d	0.30	0/1704	0.51	0/2284
36	1e	0.29	0/1145	0.50	0/1543
36	2e	0.29	0/1149	0.55	0/1548
37	1f	0.29	0/823	0.50	0/1115
37	2f	0.30	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1250	0.48	0/1679
38	2g	0.28	0/1254	0.51	0/1683
39	1h	0.29	0/1108	0.51	0/1494
39	2h	0.27	0/1108	0.53	0/1494
40	1i	0.29	0/1002	0.55	1/1346 (0.1%)
40	2i	0.29	0/997	0.52	0/1343
41	1j	0.27	0/722	0.55	0/982
41	2j	0.30	0/727	0.54	0/988
42	1k	0.27	0/844	0.49	0/1145
42	2k	0.29	0/848	0.50	0/1149
43	1l	0.31	0/937	0.51	0/1260
43	2l	0.29	0/937	0.54	1/1260 (0.1%)
44	1m	0.28	0/969	0.58	0/1302
44	2m	0.29	0/961	0.57	0/1291
45	1n	0.29	0/501	0.50	0/664
45	2n	0.28	0/501	0.52	0/664
46	1o	0.28	0/739	0.49	0/985
46	2o	0.28	0/739	0.48	0/985
47	1p	0.28	0/697	0.54	0/939
47	2p	0.28	0/693	0.53	0/935
48	1q	0.28	0/836	0.50	0/1117
48	2q	0.29	0/836	0.51	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.27	0/560	0.48	0/746
50	1s	0.27	0/667	0.53	0/900
50	2s	0.33	0/661	0.61	0/893
51	1t	0.27	0/730	0.51	0/965
51	2t	0.28	0/729	0.51	0/965
52	1u	0.27	0/203	0.58	0/266
52	2u	0.29	0/203	0.49	0/266
53	1v	0.34	0/314	0.80	0/487
53	2v	0.38	0/310	0.85	0/480
54	1w	0.42	0/1602	1.08	3/2493 (0.1%)
54	1y	0.43	0/1602	1.11	4/2493 (0.2%)
54	2w	0.43	0/1579	1.02	3/2455 (0.1%)
54	2y	0.45	0/1579	1.05	2/2455 (0.1%)
55	1x	0.68	5/1725 (0.3%)	1.36	29/2689 (1.1%)
55	2x	0.65	4/1725 (0.2%)	1.43	19/2689 (0.7%)
All	All	0.41	11/316707 (0.0%)	0.84	229/474152 (0.0%)

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
38	2g	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	76	A	N7-C5	-12.92	1.31	1.39
55	2x	76	A	N7-C5	-12.80	1.31	1.39
2	1B	1	U	OP3-P	-10.26	1.48	1.61
2	2B	1	U	OP3-P	-10.14	1.49	1.61
55	2x	76	A	C5-C6	-8.69	1.33	1.41
55	1x	76	A	C5-C6	-8.52	1.33	1.41
55	2x	76	A	C5-C4	-8.06	1.33	1.38
55	1x	76	A	N9-C4	-6.19	1.34	1.37
55	2x	76	A	N9-C4	-5.92	1.34	1.37
55	1x	22	G	N7-C5	5.84	1.42	1.39
55	1x	76	A	C5-C4	-5.76	1.34	1.38

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	76	A	O4'-C1'-N9	29.13	131.50	108.20
55	1x	76	A	C2-N3-C4	19.62	120.41	110.60
55	2x	76	A	N1-C2-N3	-18.96	119.82	129.30
55	2x	76	A	C2-N3-C4	18.89	120.05	110.60
55	1x	76	A	N1-C2-N3	-18.73	119.93	129.30
55	1x	76	A	O4'-C1'-N9	14.29	119.64	108.20
55	1x	76	A	N3-C4-C5	-10.66	119.34	126.80
55	1x	46	G	C6-N1-C2	-10.46	118.82	125.10
55	2x	76	A	N3-C4-C5	-9.92	119.85	126.80
55	1x	76	A	N7-C8-N9	-9.65	108.97	113.80
55	2x	76	A	N7-C8-N9	-9.65	108.98	113.80
32	2a	1004	A	O4'-C1'-N9	9.58	115.87	108.20
55	2x	76	A	C1'-O4'-C4'	-9.35	102.42	109.90
1	1A	512	G	O4'-C1'-N9	9.34	115.67	108.20
32	1a	254	G	O5'-P-OP1	-9.15	97.46	105.70
55	1x	76	A	C5-N7-C8	8.95	108.38	103.90
1	1A	2682	U	O5'-P-OP2	-8.65	97.92	105.70
55	2x	76	A	C5-N7-C8	8.61	108.20	103.90
32	2a	1020	U	N1-C2-O2	8.48	128.74	122.80
55	1x	22	G	C5-N7-C8	-8.45	100.08	104.30
55	2x	14	A	C4-C5-C6	8.25	121.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	46	G	C6-N1-C2	-8.17	120.20	125.10
55	1x	14	A	C4-C5-C6	8.13	121.07	117.00
1	1A	2167	U	C2-N1-C1'	8.02	127.33	117.70
1	1A	975	C	N1-C2-O2	-7.97	114.12	118.90
1	2A	2149	G	N3-C4-N9	7.82	130.69	126.00
55	1x	76	A	N9-C4-C5	7.77	108.91	105.80
32	1a	1002	G	N3-C4-N9	7.72	130.63	126.00
1	1A	2554	U	O5'-P-OP1	-7.65	98.82	105.70
55	1x	22	G	C4-C5-C6	-7.64	114.21	118.80
32	2a	1001(A)	G	N3-C4-N9	7.63	130.58	126.00
55	1x	14	A	C5-N7-C8	7.60	107.70	103.90
1	1A	1075	C	N1-C2-O2	7.60	123.46	118.90
1	2A	2152	G	C5-C6-O6	-7.58	124.05	128.60
1	1A	1026	U	O5'-P-OP1	-7.53	98.92	105.70
1	1A	2167	U	N3-C2-O2	-7.44	116.99	122.20
32	1a	1002	G	C4-N9-C1'	7.37	136.07	126.50
1	1A	527	C	N1-C2-O2	-7.35	114.49	118.90
1	1A	1086	A	N1-C6-N6	-7.31	114.21	118.60
1	1A	2061	G	O5'-P-OP2	-7.31	99.12	105.70
1	1A	2167	U	N1-C2-O2	7.24	127.86	122.80
55	1x	22	G	N1-C6-O6	-7.20	115.58	119.90
2	2B	80	U	O4'-C1'-N1	7.19	113.95	108.20
32	1a	1002	G	C8-N9-C1'	-7.17	117.69	127.00
1	1A	588	U	O5'-P-OP2	-7.16	99.25	105.70
55	2x	76	A	N9-C4-C5	7.15	108.66	105.80
1	1A	12	U	C2-N1-C1'	7.04	126.15	117.70
1	2A	2140	C	N1-C2-O2	7.02	123.11	118.90
1	1A	1075	C	C2-N3-C4	6.96	123.38	119.90
55	1x	46	G	C5-C6-N1	6.93	114.97	111.50
1	1A	2028	U	N3-C4-O4	-6.92	114.56	119.40
1	2A	2473	U	C2-N1-C1'	6.90	125.98	117.70
1	1A	1639	U	O5'-P-OP2	-6.86	99.53	105.70
1	2A	1698	A	O4'-C1'-N9	6.80	113.64	108.20
1	1A	801	G	O5'-P-OP2	-6.80	99.58	105.70
1	2A	2140	C	C2-N1-C1'	6.79	126.27	118.80
55	2x	22	G	N1-C6-O6	-6.72	115.87	119.90
1	2A	2139	C	C2-N1-C1'	6.69	126.16	118.80
55	2x	14	A	C5-N7-C8	6.68	107.24	103.90
54	1y	33	U	C2-N1-C1'	6.59	125.61	117.70
1	2A	2152	G	N1-C6-O6	6.59	123.85	119.90
1	2A	2143	C	C2-N3-C4	6.56	123.18	119.90
1	1A	1992	G	P-O3'-C3'	6.52	127.52	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	22	G	N3-C4-N9	-6.51	122.10	126.00
32	2a	1001(A)	G	C8-N9-C1'	-6.50	118.54	127.00
1	1A	226	G	O4'-C1'-N9	6.45	113.36	108.20
1	2A	2136	C	N1-C2-O2	6.43	122.76	118.90
32	2a	1001(A)	G	C4-N9-C1'	6.42	134.85	126.50
54	1y	33	U	N1-C2-O2	6.40	127.28	122.80
55	1x	14	A	C5-C6-N1	-6.40	114.50	117.70
55	2x	22	G	C5-N7-C8	-6.38	101.11	104.30
55	2x	76	A	C4-C5-C6	6.38	120.19	117.00
1	1A	975	C	O5'-P-OP1	-6.36	99.97	105.70
1	2A	1266	G	C8-N9-C4	6.34	108.94	106.40
1	2A	2149	G	C8-N9-C1'	-6.31	118.80	127.00
1	1A	624	C	O5'-P-OP1	-6.27	100.06	105.70
1	1A	1614	A	O5'-P-OP1	-6.25	100.08	105.70
1	2A	2473	U	N3-C2-O2	-6.22	117.85	122.20
1	1A	1176	G	OP1-P-O3'	6.20	118.83	105.20
32	2a	1039	C	C5-C4-N4	-6.19	115.86	120.20
1	2A	2149	G	C4-N9-C1'	6.16	134.50	126.50
32	2a	841	U	C5-C6-N1	6.14	125.77	122.70
32	1a	560	U	C2-N1-C1'	6.11	125.03	117.70
1	1A	1352	U	O5'-P-OP1	-6.08	100.23	105.70
32	2a	1184	G	N3-C4-N9	6.03	129.62	126.00
1	2A	1313	U	C2-N1-C1'	6.03	124.93	117.70
1	1A	1653	G	P-O3'-C3'	6.02	126.92	119.70
32	2a	754	C	C2-N1-C1'	6.01	125.41	118.80
55	1x	22	G	N7-C8-N9	5.96	116.08	113.10
1	1A	2130	U	C5-C6-N1	5.96	125.68	122.70
1	1A	383	U	O4'-C1'-N1	5.95	112.96	108.20
40	1i	50	LEU	CA-CB-CG	5.94	128.96	115.30
1	1A	2848	G	O4'-C1'-N9	5.93	112.94	108.20
32	2a	1029	C	N1-C2-O2	5.93	122.46	118.90
54	2y	23	A	N1-C6-N6	5.91	122.15	118.60
1	1A	2629	A	P-O3'-C3'	5.88	126.75	119.70
1	1A	975	C	C2-N1-C1'	-5.87	112.34	118.80
55	1x	76	A	C4-C5-C6	5.87	119.93	117.00
32	2a	754	C	N1-C2-O2	5.84	122.41	118.90
55	2x	17	C	C2-N1-C1'	5.84	125.23	118.80
1	1A	748	G	C4-N9-C1'	-5.84	118.91	126.50
1	2A	568	U	C5-C4-O4	-5.84	122.40	125.90
1	2A	1204	A	O4'-C1'-N9	5.83	112.87	108.20
1	2A	1300	U	P-O3'-C3'	5.83	126.70	119.70
32	2a	1001(A)	G	N9-C4-C5	-5.83	103.07	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	1	G	N3-C4-N9	5.82	129.49	126.00
32	1a	1036	G	C4-N9-C1'	5.81	134.06	126.50
1	1A	12	U	N1-C2-O2	5.81	126.87	122.80
32	1a	1007	C	C2-N3-C4	5.78	122.79	119.90
55	2x	22	G	C4-C5-C6	-5.78	115.33	118.80
1	2A	2139	C	N1-C2-O2	5.78	122.36	118.90
32	1a	975	A	O4'-C1'-N9	-5.77	103.58	108.20
1	2A	1992	G	P-O3'-C3'	5.77	126.62	119.70
32	1a	1054	C	C2-N1-C1'	5.75	125.13	118.80
55	1x	76	A	C5-C6-N1	5.74	120.57	117.70
1	2A	1142(A)	A	C2-N3-C4	-5.74	107.73	110.60
55	1x	22	G	C8-N9-C1'	5.73	134.44	127.00
54	1y	56	C	N1-C2-O2	5.71	122.33	118.90
54	2y	47	U	C2-N1-C1'	5.71	124.56	117.70
1	2A	801	G	O5'-P-OP2	-5.71	100.56	105.70
32	1a	841	U	C5-C6-N1	5.70	125.55	122.70
55	1x	76	A	C4-C5-N7	-5.68	107.86	110.70
1	2A	2149	G	N9-C4-C5	-5.67	103.13	105.40
1	1A	2501	C	C2-N1-C1'	-5.67	112.56	118.80
1	1A	2006	C	O5'-P-OP1	-5.63	100.63	105.70
32	2a	1020	U	N3-C2-O2	-5.62	118.27	122.20
32	2a	65	U	P-O3'-C3'	5.61	126.44	119.70
32	1a	1002	G	N3-C4-C5	-5.61	125.79	128.60
1	1A	1100	C	C2-N1-C1'	5.59	124.95	118.80
55	1x	14	A	C8-N9-C1'	-5.59	117.64	127.70
1	2A	2689	U	P-O3'-C3'	5.58	126.40	119.70
32	2a	1020	U	C2-N1-C1'	5.58	124.39	117.70
1	2A	277	C	N1-C2-O2	5.56	122.24	118.90
1	2A	141	A	N7-C8-N9	5.55	116.58	113.80
32	1a	266	G	P-O3'-C3'	5.55	126.36	119.70
1	1A	570	G	C5-C6-O6	-5.54	125.28	128.60
1	2A	2139	C	C6-N1-C1'	-5.54	114.16	120.80
1	2A	2143	C	N1-C2-O2	5.54	122.22	118.90
1	1A	847	U	C2-N1-C1'	5.53	124.34	117.70
1	1A	1647	G	O4'-C1'-N9	-5.53	103.78	108.20
1	1A	2689	U	N3-C2-O2	-5.51	118.34	122.20
1	1A	372	G	O4'-C1'-N9	5.51	112.60	108.20
1	1A	2790	A	C2-N3-C4	5.50	113.35	110.60
43	2l	29	GLY	N-CA-C	-5.50	99.34	113.10
1	1A	12	U	N3-C2-O2	-5.50	118.35	122.20
1	2A	1639	U	O5'-P-OP2	-5.49	100.76	105.70
1	1A	2455	G	N3-C2-N2	5.45	123.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2019	A	P-O3'-C3'	5.45	126.24	119.70
32	1a	913	A	P-O3'-C3'	5.45	126.24	119.70
1	1A	1272	A	O5'-P-OP2	-5.44	100.80	105.70
55	1x	22	G	C5-C6-N1	5.43	114.21	111.50
32	2a	1256	A	O4'-C1'-N9	-5.43	103.86	108.20
54	1y	33	U	N3-C2-O2	-5.42	118.41	122.20
1	2A	2155	G	N3-C4-N9	5.42	129.25	126.00
32	1a	558	G	O5'-P-OP1	-5.42	100.83	105.70
55	1x	14	A	C4-N9-C1'	5.41	136.03	126.30
1	2A	1530	C	P-O3'-C3'	5.41	126.19	119.70
32	2a	1032	G	C6-N1-C2	5.39	128.34	125.10
11	2P	44	GLY	C-N-CA	5.39	135.17	121.70
55	1x	76	A	N3-C4-N9	5.38	131.70	127.40
1	1A	2593	U	N3-C4-O4	-5.38	115.64	119.40
32	2a	1032	G	C5-C6-O6	5.38	131.82	128.60
1	1A	1313	U	N3-C2-O2	-5.37	118.44	122.20
1	2A	575	A	O5'-P-OP1	-5.35	100.89	105.70
1	2A	2142	C	N1-C2-O2	5.35	122.11	118.90
55	1x	22	G	C6-C5-N7	5.35	133.61	130.40
32	1a	1030(B)	C	O4'-C1'-N1	5.31	112.45	108.20
1	1A	975	C	C6-N1-C1'	5.31	127.17	120.80
1	2A	228	A	P-O3'-C3'	5.28	126.04	119.70
32	2a	1001	A	N1-C6-N6	-5.28	115.43	118.60
32	2a	1001(A)	G	C6-C5-N7	-5.28	127.23	130.40
1	2A	1698	A	C4-N9-C1'	5.27	135.79	126.30
1	1A	2060	A	C8-N9-C4	5.27	107.91	105.80
32	1a	1030(B)	C	C6-N1-C2	-5.27	118.19	120.30
32	1a	1067	A	P-O3'-C3'	5.26	126.02	119.70
4	2E	72	VAL	C-N-CA	5.25	134.84	121.70
1	1A	1992	G	O4'-C1'-N9	-5.24	104.01	108.20
32	1a	1285	A	P-O3'-C3'	5.22	125.97	119.70
1	1A	1313	U	C2-N1-C1'	5.22	123.96	117.70
1	2A	2149	G	C6-C5-N7	-5.21	127.27	130.40
7	1H	88	LEU	CA-CB-CG	5.21	127.28	115.30
1	2A	2321	G	C4-N9-C1'	5.21	133.27	126.50
27	25	58	LEU	CA-CB-CG	5.21	127.28	115.30
1	2A	1698	A	C6-C5-N7	-5.21	128.66	132.30
1	2A	383	U	O4'-C1'-N1	5.20	112.36	108.20
32	2a	1040	U	C5-C4-O4	5.19	129.01	125.90
32	1a	21	G	O5'-P-OP1	-5.18	101.04	105.70
1	2A	2148	G	C5-C6-O6	5.18	131.71	128.60
1	2A	945	A	C2-N3-C4	-5.18	108.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	266	G	P-O3'-C3'	5.18	125.92	119.70
1	2A	2140	C	C6-N1-C1'	-5.17	114.59	120.80
54	1w	10	G	N3-C2-N2	-5.17	116.28	119.90
55	1x	46	G	N1-C2-N3	5.17	127.00	123.90
1	2A	2218	U	N1-C2-O2	5.17	126.42	122.80
55	1x	46	G	C5-C6-O6	-5.16	125.50	128.60
1	1A	1075	C	C5-C6-N1	5.16	123.58	121.00
1	1A	2319	G	O4'-C1'-N9	5.14	112.31	108.20
32	2a	1001(A)	G	C4-C5-N7	5.14	112.86	110.80
1	1A	2371	G	C5-C6-N1	5.13	114.07	111.50
55	2x	76	A	C4-C5-N7	-5.13	108.14	110.70
1	1A	944	G	N3-C4-N9	5.13	129.08	126.00
1	2A	1558	A	C2-N3-C4	-5.13	108.04	110.60
54	2w	62	C	C5-C6-N1	5.12	123.56	121.00
1	1A	2391	G	O4'-C1'-N9	5.12	112.29	108.20
1	1A	2689	U	P-O3'-C3'	5.12	125.84	119.70
1	2A	2473	U	N1-C2-O2	5.12	126.38	122.80
1	1A	1993	U	O5'-P-OP1	-5.11	101.10	105.70
1	2A	2167	U	N1-C2-O2	5.10	126.37	122.80
1	1A	1177	A	O5'-P-OP1	-5.10	101.11	105.70
55	1x	46	G	N9-C4-C5	5.09	107.44	105.40
32	2a	1039	C	N3-C4-N4	5.08	121.56	118.00
55	2x	76	A	N3-C4-N9	5.06	131.45	127.40
32	2a	1009	G	C6-N1-C2	-5.06	122.06	125.10
32	2a	687	A	P-O3'-C3'	5.05	125.77	119.70
54	2w	75	C	P-O3'-C3'	5.05	125.76	119.70
1	2A	2689	U	N3-C2-O2	-5.04	118.67	122.20
32	1a	1036	G	C8-N9-C1'	-5.04	120.45	127.00
1	2A	1022	G	O4'-C1'-N9	5.03	112.22	108.20
1	2A	512	G	O4'-C1'-N9	5.03	112.22	108.20
1	2A	2149	G	N3-C2-N2	5.03	123.42	119.90
32	1a	1158	C	C2-N1-C1'	5.03	124.33	118.80
1	2A	2140	C	N3-C2-O2	-5.02	118.39	121.90
1	2A	2406	U	O4'-C1'-N1	-5.02	104.19	108.20
1	1A	36	G	O5'-P-OP2	-5.01	101.19	105.70
1	1A	788	A	C8-N9-C4	5.01	107.80	105.80
54	1w	72	C	C2-N1-C1'	5.01	124.31	118.80
54	2w	63	G	C5-C6-O6	5.01	131.60	128.60
55	2x	17	C	C6-N1-C2	-5.00	118.30	120.30
1	2A	90	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	2g	79	ARG	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
3	1D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	34 48
3	2D	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	34 48
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29 43
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15 23
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29 43
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	15 23
6	1G	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	9 13
6	2G	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	9 13
7	1H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	25 37
7	2H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	25 37
8	1I	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	7 10
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22 33
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22 33
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	22 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22 33
12	1Q	139/141 (99%)	136 (98%)	3 (2%)	0	100 100
12	2Q	139/141 (99%)	135 (97%)	3 (2%)	1 (1%)	22 33
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100 100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100 100
15	1T	129/146 (88%)	119 (92%)	10 (8%)	0	100 100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	114 (100%)	0	0	100 100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15 23
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15 23
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	92 (99%)	1 (1%)	0	100 100
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14 21
20	1Y	105/110 (96%)	100 (95%)	3 (3%)	2 (2%)	8 11
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100 100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	22 33
21	2Z	156/206 (76%)	133 (85%)	23 (15%)	0	100 100
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14 21
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14 21
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	54 (81%)	10 (15%)	3 (4%)	2 2
26	24	67/71 (94%)	51 (76%)	10 (15%)	6 (9%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	9
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	3
33	2b	229/256 (90%)	201 (88%)	20 (9%)	8 (4%)	3	4
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	15	23
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	23
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	43
35	2d	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	43
36	1e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	22	33
36	2e	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
38	2g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	22	33
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	22	33
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	19	29
40	2i	125/128 (98%)	108 (86%)	15 (12%)	2 (2%)	9	14
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	3
41	2j	94/105 (90%)	81 (86%)	8 (8%)	5 (5%)	2	1
42	1k	112/129 (87%)	103 (92%)	5 (4%)	4 (4%)	3	4
42	2k	112/129 (87%)	104 (93%)	4 (4%)	4 (4%)	3	4
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100 100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100 100
44	2m	120/126 (95%)	110 (92%)	7 (6%)	3 (2%)	5 7
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
46	2o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13 19
47	1p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	12 18
47	2p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	12 18
48	1q	97/105 (92%)	94 (97%)	3 (3%)	0	100 100
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100 100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100 100
50	2s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	13 19
51	1t	94/106 (89%)	86 (92%)	3 (3%)	5 (5%)	2 1
51	2t	94/106 (89%)	86 (92%)	3 (3%)	5 (5%)	2 1
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
All	All	11370/12128 (94%)	10690 (94%)	575 (5%)	105 (1%)	17 26

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1D	275	LYS
5	1F	130	ALA
6	1G	47	LYS
6	1G	51	ARG
7	1H	126	PRO
21	1Z	152	ALA
33	1b	17	PHE
33	1b	22	LYS
34	1c	65	ALA
42	1k	89	ALA
47	1p	53	VAL

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Mol	Chain	Res	Type
5	2F	130	ALA
6	2G	47	LYS
6	2G	51	ARG
7	2H	126	PRO
11	2P	45	LEU
23	21	3	LYS
26	24	48	ARG
26	24	55	ARG
26	24	62	ARG
29	27	46	VAL
33	2b	16	HIS
33	2b	123	ALA
34	2c	107	GLN
34	2c	108	ASN
42	2k	89	ALA
42	2k	90	GLY
44	2m	107	ALA
47	2p	53	VAL
51	2t	10	LEU
8	1I	105	HIS
8	1I	106	GLY
23	11	3	LYS
26	14	45	GLY
41	1j	31	GLY
41	1j	77	PRO
42	1k	49	GLY
51	1t	10	LEU
51	1t	47	GLY
51	1t	96	GLY
51	1t	100	ILE
3	2D	3	VAL
4	2E	52	LEU
12	2Q	28	ALA
17	2V	79	VAL
26	24	45	GLY
33	2b	17	PHE
33	2b	21	ARG
33	2b	128	GLU
41	2j	29	ARG
44	2m	4	ILE
51	2t	47	GLY
6	1G	43	LEU

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Mol	Chain	Res	Type
17	1V	79	VAL
20	1Y	53	PRO
26	14	56	VAL
33	1b	9	GLU
33	1b	20	GLU
33	1b	231	GLU
36	1e	86	ALA
41	1j	29	ARG
41	1j	78	ASN
6	2G	43	LEU
19	2X	2	LYS
26	24	47	GLN
26	24	65	ASP
33	2b	20	GLU
33	2b	231	GLU
38	2g	7	ALA
41	2j	30	SER
41	2j	78	ASN
44	2m	6	GLY
50	2s	29	ARG
51	2t	102	GLY
4	1E	52	LEU
34	1c	66	VAL
40	1i	56	LEU
51	1t	95	ALA
4	2E	73	GLU
5	2F	21	ALA
8	2I	10	GLU
42	2k	49	GLY
46	2o	88	ARG
51	2t	95	ALA
51	2t	100	ILE
20	1Y	54	LYS
33	1b	16	HIS
33	1b	125	PRO
33	1b	126	GLU
35	1d	167	GLY
42	1k	90	GLY
35	2d	167	GLY
40	2i	54	ASP
40	2i	56	LEU
42	2k	105	VAL

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Mol	Chain	Res	Type
8	1I	107	VAL
26	14	46	GLN
33	1b	10	LEU
9	2N	2	LYS
39	2h	73	ASP
41	2j	77	PRO
42	1k	105	VAL
41	2j	37	PRO
11	1P	122	PRO
33	2b	125	PRO

5.3.2 Protein sidechains (i)

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	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	19	30
3	2D	215/218 (99%)	206 (96%)	9 (4%)	30	45
4	1E	164/166 (99%)	157 (96%)	7 (4%)	29	44
4	2E	164/166 (99%)	156 (95%)	8 (5%)	25	38
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10	14
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20	31
6	1G	144/156 (92%)	139 (96%)	5 (4%)	36	52
6	2G	143/156 (92%)	137 (96%)	6 (4%)	30	45
7	1H	144/148 (97%)	142 (99%)	2 (1%)	67	81
7	2H	144/148 (97%)	142 (99%)	2 (1%)	67	81
8	1I	113/124 (91%)	106 (94%)	7 (6%)	18	29
8	2I	105/124 (85%)	100 (95%)	5 (5%)	25	39
9	1N	118/119 (99%)	113 (96%)	5 (4%)	30	45
9	2N	118/119 (99%)	115 (98%)	3 (2%)	47	66
10	1O	100/100 (100%)	99 (99%)	1 (1%)	76	86
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	44
11	2P	115/116 (99%)	112 (97%)	3 (3%)	46	64
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	75
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	51
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15	24
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	30
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	40
14	2S	85/88 (97%)	83 (98%)	2 (2%)	49	67
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	44
15	2T	113/127 (89%)	110 (97%)	3 (3%)	44	63
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	56
16	2U	93/94 (99%)	92 (99%)	1 (1%)	73	85
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	28
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	49
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28	43
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	33
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	82
19	2X	77/78 (99%)	76 (99%)	1 (1%)	69	82
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	49	67
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	71	84
21	1Z	135/179 (75%)	132 (98%)	3 (2%)	52	70
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	70
22	10	65/67 (97%)	62 (95%)	3 (5%)	27	41
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	57
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	49
23	21	80/83 (96%)	76 (95%)	4 (5%)	24	38
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	80
25	13	51/52 (98%)	50 (98%)	1 (2%)	55	73
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	47
26	14	59/63 (94%)	57 (97%)	2 (3%)	37	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	24	53/63 (84%)	49 (92%)	4 (8%)	13 21
27	15	50/52 (96%)	47 (94%)	3 (6%)	19 30
27	25	50/52 (96%)	47 (94%)	3 (6%)	19 30
28	16	51/52 (98%)	49 (96%)	2 (4%)	32 48
28	26	50/52 (96%)	48 (96%)	2 (4%)	31 47
29	17	41/42 (98%)	39 (95%)	2 (5%)	25 38
29	27	41/42 (98%)	41 (100%)	0	100 100
30	18	54/55 (98%)	51 (94%)	3 (6%)	21 33
30	28	54/55 (98%)	50 (93%)	4 (7%)	13 21
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 60
31	29	34/34 (100%)	34 (100%)	0	100 100
33	1b	192/220 (87%)	189 (98%)	3 (2%)	62 78
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53 72
34	1c	142/188 (76%)	140 (99%)	2 (1%)	67 81
34	2c	140/188 (74%)	139 (99%)	1 (1%)	84 91
35	1d	169/181 (93%)	165 (98%)	4 (2%)	49 67
35	2d	173/181 (96%)	168 (97%)	5 (3%)	42 60
36	1e	113/123 (92%)	111 (98%)	2 (2%)	59 75
36	2e	114/123 (93%)	112 (98%)	2 (2%)	59 75
37	1f	84/90 (93%)	82 (98%)	2 (2%)	49 67
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49 67
38	1g	119/127 (94%)	118 (99%)	1 (1%)	81 89
38	2g	120/127 (94%)	120 (100%)	0	100 100
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59 75
39	2h	114/119 (96%)	112 (98%)	2 (2%)	59 75
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28 43
40	2i	89/99 (90%)	87 (98%)	2 (2%)	52 70
41	1j	66/92 (72%)	65 (98%)	1 (2%)	65 80
41	2j	69/92 (75%)	65 (94%)	4 (6%)	20 31
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49 67
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	1l	96/108 (89%)	94 (98%)	2 (2%)	53 72
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53 72
44	1m	93/101 (92%)	91 (98%)	2 (2%)	52 70
44	2m	92/101 (91%)	90 (98%)	2 (2%)	52 70
45	1n	49/50 (98%)	46 (94%)	3 (6%)	18 29
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30 46
46	1o	78/80 (98%)	78 (100%)	0	100 100
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69 82
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14 22
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 21
48	1q	94/97 (97%)	94 (100%)	0	100 100
48	2q	94/97 (97%)	94 (100%)	0	100 100
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60 77
49	2r	59/77 (77%)	57 (97%)	2 (3%)	37 53
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67 81
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41 59
51	1t	70/82 (85%)	67 (96%)	3 (4%)	29 44
51	2t	70/82 (85%)	69 (99%)	1 (1%)	67 81
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9304/10064 (92%)	9012 (97%)	292 (3%)	40 57

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	61	LEU
3	1D	88	ARG
3	1D	94	LEU
3	1D	113	VAL
3	1D	122	ASP
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL

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Mol	Chain	Res	Type
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	33	VAL
4	1E	75	VAL
4	1E	116	VAL
4	1E	144	ARG
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	125	LEU
5	1F	132	VAL
5	1F	170	LEU
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	43	LEU
6	1G	82	LEU
6	1G	133	LEU
7	1H	88	LEU
7	1H	98	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	108	THR
8	1I	109	ILE
8	1I	123	LEU
8	1I	142	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	73	THR
10	1O	10	VAL
11	1P	59	LEU
11	1P	79	ARG
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	16	ARG
12	1Q	75	THR
13	1R	29	LEU
13	1R	33	ARG
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	13	ARG
14	1S	25	ARG
14	1S	36	TYR
14	1S	49	VAL
15	1T	28	VAL
15	1T	34	VAL
15	1T	49	VAL
15	1T	89	VAL
15	1T	128	GLU
16	1U	8	VAL
16	1U	74	LEU
16	1U	108	GLU
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	72	VAL
17	1V	79	VAL
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	107	LEU
19	1X	52	VAL
20	1Y	43	ASN
20	1Y	90	LEU
21	1Z	5	LEU
21	1Z	132	ASN

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Mol	Chain	Res	Type
21	1Z	148	ASP
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
23	11	11	ARG
23	11	35	THR
23	11	95	LEU
25	13	23	LEU
26	14	50	VAL
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	14	THR
28	16	48	VAL
29	17	24	THR
29	17	47	ARG
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU
31	19	35	ARG
33	1b	7	VAL
33	1b	8	LYS
33	1b	158	LEU
34	1c	70	VAL
34	1c	115	LEU
35	1d	31	CYS
35	1d	112	VAL
35	1d	135	LEU
35	1d	194	LEU
36	1e	38	GLN
36	1e	41	VAL
37	1f	72	VAL
37	1f	74	ASP
38	1g	50	ILE
39	1h	112	LEU
39	1h	133	LEU
40	1i	23	ASN
40	1i	42	ARG
40	1i	50	LEU
40	1i	86	VAL
41	1j	5	ARG

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Mol	Chain	Res	Type
42	1k	48	ILE
42	1k	114	VAL
43	1l	27	LEU
43	1l	83	VAL
44	1m	4	ILE
44	1m	32	GLU
45	1n	3	ARG
45	1n	18	VAL
45	1n	33	VAL
47	1p	20	VAL
47	1p	42	ARG
47	1p	60	LEU
47	1p	67	THR
47	1p	69	THR
49	1r	35	ARG
50	1s	4	SER
51	1t	10	LEU
51	1t	15	ARG
51	1t	24	LEU
3	2D	3	VAL
3	2D	37	LEU
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
4	2E	21	VAL
4	2E	33	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	116	VAL
4	2E	170	LEU
4	2E	181	LEU
4	2E	195	LEU
5	2F	24	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	74	ARG
5	2F	106	ARG
5	2F	132	VAL

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Mol	Chain	Res	Type
5	2F	170	LEU
5	2F	191	ARG
5	2F	192	LEU
6	2G	5	VAL
6	2G	43	LEU
6	2G	79	ASN
6	2G	133	LEU
6	2G	159	VAL
6	2G	170	ARG
7	2H	84	SER
7	2H	129	THR
8	2I	47	LEU
8	2I	50	ARG
8	2I	92	VAL
8	2I	123	LEU
8	2I	140	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	99	LEU
10	2O	108	GLU
11	2P	95	VAL
11	2P	112	LEU
11	2P	125	VAL
12	2Q	2	LEU
12	2Q	10	ARG
12	2Q	75	THR
12	2Q	110	THR
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	13	ARG
14	2S	110	LEU
15	2T	28	VAL
15	2T	49	VAL
15	2T	95	ARG
16	2U	92	ARG
17	2V	21	ARG
17	2V	46	VAL
17	2V	79	VAL

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Mol	Chain	Res	Type
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	100	THR
18	2W	107	LEU
19	2X	70	LEU
20	2Y	72	VAL
21	2Z	42	VAL
21	2Z	135	GLU
21	2Z	142	SER
22	20	14	ARG
22	20	39	ARG
23	21	11	ARG
23	21	30	VAL
23	21	56	GLN
23	21	95	LEU
24	22	52	ASP
25	23	23	LEU
25	23	54	VAL
26	24	34	GLU
26	24	50	VAL
26	24	56	VAL
26	24	59	PHE
27	25	16	ARG
27	25	29	THR
27	25	35	GLU
28	26	14	THR
28	26	48	VAL
30	28	14	VAL
30	28	26	LYS
30	28	31	HIS
30	28	32	LEU
33	2b	7	VAL
33	2b	94	ASN
33	2b	185	ILE
33	2b	235	SER
34	2c	152	ILE
35	2d	31	CYS
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	194	LEU

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Mol	Chain	Res	Type
36	2e	41	VAL
36	2e	51	VAL
37	2f	21	LEU
37	2f	72	VAL
39	2h	84	ARG
39	2h	133	LEU
40	2i	102	LEU
40	2i	108	VAL
41	2j	55	LYS
41	2j	67	THR
41	2j	72	VAL
41	2j	89	ASP
42	2k	48	ILE
43	2l	33	ARG
43	2l	83	VAL
44	2m	15	VAL
44	2m	104	ARG
45	2n	18	VAL
45	2n	33	VAL
46	2o	39	LEU
47	2p	20	VAL
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	69	THR
49	2r	35	ARG
49	2r	37	VAL
50	2s	64	GLU
50	2s	77	THR
51	2t	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	69	HIS
6	1G	132	ASN
8	1I	104	GLN
12	1Q	57	HIS
14	1S	95	HIS
16	1U	94	ASN
18	1W	60	ASN

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Mol	Chain	Res	Type
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
21	1Z	55	HIS
21	1Z	132	ASN
24	12	9	GLN
24	12	65	ASN
33	1b	40	HIS
34	1c	6	HIS
34	1c	102	ASN
34	1c	176	HIS
35	1d	77	ASN
35	1d	123	HIS
35	1d	161	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
39	1h	82	HIS
40	1i	23	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
42	1k	99	GLN
43	1l	99	HIS
44	1m	92	HIS
48	1q	26	GLN
50	1s	23	ASN
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	116	GLN
5	2F	69	HIS
8	2I	104	GLN
9	2N	38	HIS
9	2N	131	GLN
10	2O	3	GLN
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	91	GLN

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Mol	Chain	Res	Type
14	2S	38	GLN
14	2S	84	GLN
14	2S	95	HIS
16	2U	94	ASN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	55	HIS
21	2Z	73	GLN
24	22	65	ASN
33	2b	40	HIS
33	2b	78	GLN
33	2b	94	ASN
34	2c	6	HIS
34	2c	162	GLN
35	2d	77	ASN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
37	2f	13	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	64	GLN
38	2g	86	GLN
38	2g	97	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	117	HIS
40	2i	124	GLN
42	2k	93	GLN
43	2l	99	HIS
44	2m	77	ASN
46	2o	28	GLN
46	2o	62	GLN
50	2s	65	ASN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	439 (15%)	28 (0%)
1	2A	2788/2915 (95%)	462 (16%)	26 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1494/1521 (98%)	217 (14%)	0
32	2a	1498/1521 (98%)	225 (15%)	0
53	1v	12/27 (44%)	3 (25%)	0
53	2v	12/27 (44%)	3 (25%)	0
54	1w	71/76 (93%)	27 (38%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	69/76 (90%)	21 (30%)	0
54	2y	69/76 (90%)	15 (21%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	13 (17%)	0
All	All	9333/9626 (96%)	1496 (16%)	55 (0%)

All (1496) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	93	G
1	1A	94	C
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	198	C
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A

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Mol	Chain	Res	Type
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	282	A
1	1A	283	A
1	1A	306	U
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	360	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	491	G

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Mol	Chain	Res	Type
1	1A	494	G
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	529	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	534	U
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	801	G
1	1A	805	G
1	1A	811	U

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Mol	Chain	Res	Type
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	892	G
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	910	A
1	1A	932	G
1	1A	941	A
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	995	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1045	A

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Mol	Chain	Res	Type
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1066	U
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1085	A
1	1A	1088	A
1	1A	1090	U
1	1A	1092	C
1	1A	1094	U
1	1A	1101	U
1	1A	1106	G
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1189	A

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Mol	Chain	Res	Type
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1267	U
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1315	C
1	1A	1320	C
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1379	A
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1419	A
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1461	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C

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Mol	Chain	Res	Type
1	1A	1496	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1509(B)	A
1	1A	1531	C
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1653	G
1	1A	1654	A
1	1A	1664	A
1	1A	1667	G
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1748	G
1	1A	1749	A
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A

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Mol	Chain	Res	Type
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2035	G
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2099	U
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2122	U

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Mol	Chain	Res	Type
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2138	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2151	G
1	1A	2152	G
1	1A	2155	G
1	1A	2157	G
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G

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Mol	Chain	Res	Type
1	1A	2269	A
1	1A	2275	C
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2476	A
1	1A	2477	C
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2524	G
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A

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Mol	Chain	Res	Type
1	1A	2567	G
1	1A	2573	C
1	1A	2584	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2780	G
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	52	A
2	1B	56	G

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Mol	Chain	Res	Type
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	146	G
32	1a	156	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	316	G
32	1a	321	A

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Mol	Chain	Res	Type
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A

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Mol	Chain	Res	Type
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	773	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A

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Mol	Chain	Res	Type
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A

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Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1281	U
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C

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Mol	Chain	Res	Type
32	1a	1456	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
32	1a	1532	U
53	1v	13	A
53	1v	14	A
53	1v	24	A
54	1w	2	C
54	1w	4	C
54	1w	9	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	22	G
54	1w	23	A
54	1w	24	G
54	1w	29	G
54	1w	42	C
54	1w	43	C
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	49	C
54	1w	56	C
54	1w	61	C
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
54	1w	75	C
54	1w	76	A
55	1x	6	G

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Mol	Chain	Res	Type
55	1x	9	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	48	C
55	1x	56	C
55	1x	58	A
55	1x	61	C
55	1x	67	C
55	1x	69	C
55	1x	76	A
54	1y	2	C
54	1y	5	G
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	26	A
54	1y	33	U
54	1y	40	C
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	50	U
54	1y	57	G
54	1y	59	U
54	1y	60	U
54	1y	65	G
54	1y	68	C
54	1y	70	G
54	1y	73	A
1	2A	9	U
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A

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Mol	Chain	Res	Type
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	96	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	140	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	271(I)	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	289	A
1	2A	308	G
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G

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Mol	Chain	Res	Type
1	2A	330	A
1	2A	333	G
1	2A	338	G
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(A)	A
1	2A	386	G
1	2A	396	G
1	2A	404	C
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	427	U
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	518	G
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	587	C
1	2A	588	U
1	2A	592	G
1	2A	603	A

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Mol	Chain	Res	Type
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	864	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G

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Mol	Chain	Res	Type
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	912	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	982	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G

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Mol	Chain	Res	Type
1	2A	1043	C
1	2A	1113	U
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1171	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1248	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1289	C
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1320	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1411	C
1	2A	1416	G

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Mol	Chain	Res	Type
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1436	G
1	2A	1437	C
1	2A	1444	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1542	A
1	2A	1543	C
1	2A	1545	A
1	2A	1547	C
1	2A	1548	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1593	G
1	2A	1608	A
1	2A	1609	A

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Mol	Chain	Res	Type
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1695	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1860	G
1	2A	1876	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A

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Mol	Chain	Res	Type
1	2A	1952	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2111	C
1	2A	2116	G
1	2A	2119	A
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2144	U

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Mol	Chain	Res	Type
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2160	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2190	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2313	C
1	2A	2319	G
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A

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Mol	Chain	Res	Type
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2459	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G

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Mol	Chain	Res	Type
1	2A	2646	C
1	2A	2654	A
1	2A	2669	G
1	2A	2679	A
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2741	A
1	2A	2751	G
1	2A	2752	C
1	2A	2754	U
1	2A	2757	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2793	G
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	16	G
2	2B	17	C
2	2B	20	C
2	2B	23	G
2	2B	25	A
2	2B	30	C

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Mol	Chain	Res	Type
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	64	C
2	2B	69	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	90	A
2	2B	91	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	112	U
2	2B	116	G
2	2B	120	A
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	78	G
32	2a	88	A
32	2a	89	C
32	2a	91	C
32	2a	96	U
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	146	G
32	2a	156	G

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Mol	Chain	Res	Type
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	348	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	441	A

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Mol	Chain	Res	Type
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	759	A
32	2a	773	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G

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Mol	Chain	Res	Type
32	2a	828	A
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1020	U
32	2a	1022	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G

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Mol	Chain	Res	Type
32	2a	1033	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1044	A
32	2a	1046	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1117	G
32	2a	1125	U
32	2a	1129	C
32	2a	1133	G
32	2a	1134	G
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1250	A
32	2a	1256	A

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Mol	Chain	Res	Type
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1282	C
32	2a	1287	A
32	2a	1299	A
32	2a	1305	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1498	UR3
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	24	A
54	2w	2	C
54	2w	4	C
54	2w	8	4SU
54	2w	19	G
54	2w	24	G

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Mol	Chain	Res	Type
54	2w	29	G
54	2w	42	C
54	2w	43	C
54	2w	47	U
54	2w	48	C
54	2w	49	C
54	2w	56	C
54	2w	61	C
54	2w	62	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
54	2w	75	C
54	2w	76	A
55	2x	9	G
55	2x	13	C
55	2x	16	C
55	2x	19	G
55	2x	34	C
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	56	C
55	2x	60	U
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	2	C
54	2y	9	A
54	2y	13	C
54	2y	19	G
54	2y	22	G
54	2y	26	A
54	2y	33	U
54	2y	40	C
54	2y	46	7MG
54	2y	47	U
54	2y	48	C
54	2y	50	U
54	2y	57	G

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Mol	Chain	Res	Type
54	2y	68	C
54	2y	70	G

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	800	A
1	1A	827	U
1	1A	1036	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2238	G
1	1A	2406	U
1	1A	2422	A
1	1A	2629	A
1	1A	2689	U
2	1B	1	U
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A

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Mol	Chain	Res	Type
1	2A	587	C
1	2A	752	A
1	2A	774	A
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1300	U
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

84 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	$\#\|Z\| > 2$
1	5MC	2A	1942	1	18,22,23	1.01	2 (11%)	26,32,35	1.25	3 (11%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
32	PSU	2a	516	32	18,21,22	1.30	2 (11%)	22,30,33	1.89	4 (18%)
54	PSU	1w	32	56,54	18,21,22	1.33	2 (11%)	22,30,33	1.90	4 (18%)
1	2MA	1A	2503	1,56	17,25,26	0.94	0	17,37,40	1.17	2 (11%)
54	MIA	2y	37	54	18,24,32	1.13	2 (11%)	18,35,47	1.31	2 (11%)
54	MIA	1w	37	54	24,31,32	2.31	3 (12%)	26,44,47	2.58	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	1a	1404	32	18,22,23	1.02	1 (5%)	26,32,35	1.09	2 (7%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	26,32,35	1.03	1 (3%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
54	7MG	2w	46	54	22,26,27	1.31	2 (9%)	29,39,42	2.54	7 (24%)
1	OMG	1A	2251	1,56,55	18,26,27	0.96	1 (5%)	19,38,41	1.10	2 (10%)
1	5MC	2A	1962	1,56	18,22,23	1.01	2 (11%)	26,32,35	1.22	3 (11%)
32	5MC	2a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.15	3 (11%)
32	7MG	2a	527	32,56	22,26,27	1.38	4 (18%)	29,39,42	2.46	6 (20%)
54	5MU	1w	54	54	19,22,23	1.37	4 (21%)	28,32,35	1.91	5 (17%)
54	MIA	2w	37	54	18,24,32	1.15	2 (11%)	18,35,47	1.28	2 (11%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	28,32,35	2.17	6 (21%)
32	5MC	2a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.16	3 (11%)
1	OMG	2A	2251	1,56,55	18,26,27	0.97	1 (5%)	19,38,41	1.13	2 (10%)
32	M2G	1a	966	32	20,27,28	1.33	3 (15%)	22,40,43	1.03	2 (9%)
54	PSU	2w	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.81	3 (13%)
54	5MU	2y	54	54	19,22,23	1.47	4 (21%)	28,32,35	2.02	8 (28%)
54	PSU	1w	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.98	4 (18%)
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.24	4 (15%)
54	PSU	2y	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.95	3 (13%)
1	2MA	2A	2503	1,56	17,25,26	1.02	1 (5%)	17,37,40	1.01	2 (11%)
54	PSU	2y	32	54	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	22,30,33	1.90	4 (18%)
54	7MG	1y	46	54	22,26,27	1.33	4 (18%)	29,39,42	2.59	7 (24%)
54	4SU	2w	8	54	18,21,22	1.66	5 (27%)	26,30,33	1.83	4 (15%)
1	PSU	1A	2605	1	18,21,22	1.39	3 (16%)	22,30,33	1.91	4 (18%)
1	4OC	2A	1920	1	19,22,24	0.78	0	26,31,35	0.89	1 (3%)
43	0TD	1l	92	43	7,9,10	5.00	1 (14%)	6,11,13	7.26	2 (33%)
32	PSU	1a	516	32,56	18,21,22	1.38	2 (11%)	22,30,33	1.96	4 (18%)
32	2MG	2a	1207	32	18,26,27	0.89	1 (5%)	16,38,41	1.16	3 (18%)
32	MA6	2a	1519	32	19,26,27	1.06	1 (5%)	18,38,41	1.63	4 (22%)
32	M2G	2a	966	32	20,27,28	1.48	3 (15%)	22,40,43	0.94	2 (9%)
32	MA6	2a	1518	32	19,26,27	1.01	1 (5%)	18,38,41	1.65	4 (22%)
32	5MC	1a	1400	32	18,22,23	1.00	2 (11%)	26,32,35	1.10	3 (11%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.07	2 (7%)
43	0TD	2l	92	43	7,9,10	4.71	1 (14%)	6,11,13	2.43	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	UR3	2a	1498	32	19,22,23	1.14	1 (5%)	26,32,35	1.48	2 (7%)
55	PSU	1x	55	55	18,21,22	1.28	2 (11%)	22,30,33	1.96	4 (18%)
1	PSU	2A	1911	1	18,21,22	1.31	2 (11%)	22,30,33	1.80	3 (13%)
54	PSU	2w	39	54	18,21,22	1.35	2 (11%)	22,30,33	1.56	3 (13%)
1	5MU	1A	1939	1	19,22,23	1.47	5 (26%)	28,32,35	2.21	5 (17%)
1	PSU	2A	2605	1	18,21,22	1.29	2 (11%)	22,30,33	1.96	4 (18%)
32	MA6	1a	1519	32	19,26,27	1.03	1 (5%)	18,38,41	1.63	4 (22%)
1	5MC	1A	1962	1,56	18,22,23	0.94	2 (11%)	26,32,35	1.17	2 (7%)
32	5MC	1a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.10	2 (7%)
32	7MG	1a	527	32,56	22,26,27	1.43	4 (18%)	29,39,42	2.47	7 (24%)
1	5MU	2A	1939	1,56	19,22,23	1.42	5 (26%)	28,32,35	2.08	6 (21%)
1	PSU	1A	1917	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
54	4SU	2y	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.20	5 (19%)
54	MIA	1y	37	54	18,24,32	1.15	2 (11%)	18,35,47	1.21	2 (11%)
1	4OC	1A	1920	1	19,22,24	0.81	0	26,31,35	0.96	1 (3%)
55	5MU	2x	54	55	19,22,23	1.39	4 (21%)	28,32,35	1.91	7 (25%)
54	PSU	1y	32	54	18,21,22	1.31	2 (11%)	22,30,33	1.84	4 (18%)
55	4SU	2x	8	55	18,21,22	1.98	6 (33%)	26,30,33	1.59	4 (15%)
55	5MC	1x	32	55	18,22,23	1.05	2 (11%)	26,32,35	1.19	2 (7%)
54	5MU	1y	54	54	19,22,23	1.43	5 (26%)	28,32,35	1.94	5 (17%)
54	PSU	2y	39	54	18,21,22	1.37	3 (16%)	22,30,33	1.95	3 (13%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.92	3 (13%)
54	7MG	2y	46	54	22,26,27	1.36	4 (18%)	29,39,42	2.58	7 (24%)
54	PSU	1y	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.19	2 (12%)
32	5MC	2a	1407	32	18,22,23	1.03	2 (11%)	26,32,35	1.12	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.93	1 (3%)
32	MA6	1a	1518	32	19,26,27	1.02	1 (5%)	18,38,41	1.66	5 (27%)
54	7MG	1w	46	54	22,26,27	1.35	3 (13%)	29,39,42	2.55	7 (24%)
32	UR3	1a	1498	32	19,22,23	0.99	0	26,32,35	1.36	2 (7%)
1	2MU	1A	2552	1,56	19,22,24	1.25	2 (10%)	26,31,36	1.96	6 (23%)
1	5MU	1A	1915	1	19,22,23	1.32	5 (26%)	28,32,35	2.18	6 (21%)
1	5MC	1A	1942	1,56	18,22,23	0.95	2 (11%)	26,32,35	1.15	2 (7%)
1	2MU	2A	2552	1,56	19,22,24	1.25	3 (15%)	26,31,36	1.65	6 (23%)
55	5MU	1x	54	56,55	19,22,23	1.39	5 (26%)	28,32,35	1.81	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	4SU	1y	8	54	18,21,22	1.73	5 (27%)	26,30,33	1.87	5 (19%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
55	4SU	1x	8	55	18,21,22	1.93	5 (27%)	26,30,33	1.27	4 (15%)
54	4SU	1w	8	54	18,21,22	1.71	5 (27%)	26,30,33	2.02	4 (15%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.18	3 (11%)
54	5MU	2w	54	54	19,22,23	1.42	5 (26%)	28,32,35	1.78	6 (21%)

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
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	1/3/25/26	0/3/3/3
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
1	OMG	1A	2251	1,56,55	-	0/5/27/28	0/3/3/3
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/3/25/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	1/5/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	UR3	2a	1498	32	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	1A	1962	1,56	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	2/3/25/34	0/3/3/3
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	4/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1y	55	54	-	3/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	1/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.81	1.69	1.82
43	2l	92	0TD	CB-SB	-12.17	1.69	1.82
54	1w	37	MIA	C2-S10	-7.38	1.69	1.75
54	1w	37	MIA	C13-C14	7.26	1.53	1.32
32	2a	966	M2G	C2-N3	4.89	1.36	1.30
55	2x	8	4SU	C4-S4	-4.53	1.59	1.68
55	1x	8	4SU	C4-N3	-4.51	1.32	1.37
55	2x	8	4SU	C4-N3	-4.47	1.32	1.37
54	1w	8	4SU	C4-S4	-4.40	1.60	1.68
54	2y	8	4SU	C4-S4	-4.32	1.60	1.68
54	1y	8	4SU	C4-S4	-4.29	1.60	1.68
54	2w	8	4SU	C4-S4	-4.01	1.60	1.68
32	1a	966	M2G	C2-N3	3.97	1.35	1.30
54	2y	55	PSU	C6-C5	3.83	1.39	1.35
54	1y	55	PSU	C6-C5	3.81	1.39	1.35
54	2y	32	PSU	C6-C5	3.72	1.39	1.35
54	2w	39	PSU	C6-C5	3.67	1.39	1.35
54	1w	55	PSU	C6-C5	3.65	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1917	PSU	C6-C5	3.64	1.39	1.35
54	1y	39	PSU	C6-C5	3.64	1.39	1.35
55	1x	8	4SU	C4-S4	-3.56	1.61	1.68
55	2x	55	PSU	C6-C5	3.53	1.39	1.35
55	1x	8	4SU	C2-N3	-3.50	1.31	1.38
54	2y	39	PSU	C6-C5	3.48	1.39	1.35
54	2w	32	PSU	C6-C5	3.47	1.39	1.35
54	2w	55	PSU	C6-C5	3.47	1.39	1.35
54	2w	46	7MG	C4-N9	-3.47	1.33	1.37
32	1a	1404	5MC	C6-C5	3.42	1.40	1.34
32	2a	527	7MG	C4-N9	-3.32	1.33	1.37
54	1y	8	4SU	C4-N3	-3.30	1.34	1.37
54	1w	46	7MG	C4-N9	-3.27	1.33	1.37
54	1y	32	PSU	C6-C5	3.25	1.39	1.35
1	1A	1911	PSU	C6-C5	3.23	1.39	1.35
54	2w	8	4SU	C4-N3	-3.21	1.34	1.37
32	1a	516	PSU	C6-C5	3.21	1.39	1.35
54	2y	46	7MG	C5-C4	3.20	1.48	1.38
54	1w	32	PSU	C6-C5	3.18	1.39	1.35
54	1y	46	7MG	C5-C4	3.17	1.48	1.38
55	1x	55	PSU	C6-C5	3.14	1.39	1.35
1	2A	2605	PSU	C6-C5	3.13	1.39	1.35
32	1a	1400	5MC	C6-C5	3.09	1.39	1.34
54	1w	46	7MG	C5-C4	3.09	1.48	1.38
55	2x	8	4SU	C5-C4	-3.09	1.38	1.42
32	2a	516	PSU	C6-C5	3.08	1.38	1.35
32	1a	527	7MG	C4-N9	-3.08	1.34	1.37
1	2A	1917	PSU	C6-C5	3.07	1.38	1.35
54	2y	54	5MU	C2-N1	3.07	1.43	1.38
1	1A	1939	5MU	C6-C5	3.07	1.39	1.34
1	1A	1939	5MU	C4-N3	-3.06	1.33	1.38
54	1w	39	PSU	C6-C5	3.05	1.38	1.35
54	1w	8	4SU	C4-N3	-3.05	1.34	1.37
32	2a	1407	5MC	C6-C5	3.03	1.39	1.34
1	1A	2605	PSU	C4-N3	-3.02	1.33	1.38
32	1a	527	7MG	C5-C4	3.01	1.47	1.38
1	2A	1942	5MC	C6-C5	3.00	1.39	1.34
55	1x	32	5MC	C6-C5	2.99	1.39	1.34
1	2A	1917	PSU	C4-N3	-2.98	1.33	1.38
55	1x	8	4SU	C5-C4	-2.95	1.38	1.42
32	2a	527	7MG	C5-C4	2.94	1.47	1.38
32	2a	1404	5MC	C6-C5	2.94	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	8	4SU	C4-N3	-2.92	1.34	1.37
1	1A	2605	PSU	C6-C5	2.92	1.38	1.35
32	1a	967	5MC	C6-C5	2.91	1.39	1.34
1	2A	1911	PSU	C6-C5	2.90	1.38	1.35
54	1y	37	MIA	C2-N3	2.88	1.36	1.32
32	2a	1400	5MC	C6-C5	2.88	1.39	1.34
32	1a	1407	5MC	C6-C5	2.83	1.39	1.34
55	2x	54	5MU	C6-C5	2.82	1.39	1.34
54	2y	54	5MU	C6-C5	2.82	1.39	1.34
1	2A	1915	5MU	C4-N3	-2.81	1.33	1.38
54	1y	54	5MU	C6-C5	2.81	1.39	1.34
54	2w	46	7MG	C5-C4	2.80	1.47	1.38
1	1A	1942	5MC	C6-C5	2.80	1.39	1.34
54	2w	54	5MU	C6-C5	2.79	1.39	1.34
32	1a	516	PSU	C4-N3	-2.77	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.77	1.33	1.37
54	1w	32	PSU	C4-N3	-2.77	1.33	1.38
54	2w	37	MIA	C2-N3	2.77	1.36	1.32
54	1w	39	PSU	C4-N3	-2.75	1.33	1.38
54	2w	37	MIA	C5-C4	2.75	1.48	1.40
1	1A	1911	PSU	C4-N3	-2.74	1.33	1.38
55	1x	54	5MU	C4-N3	-2.73	1.33	1.38
54	2y	8	4SU	C2-N1	2.73	1.42	1.38
54	1w	54	5MU	C6-C5	2.72	1.39	1.34
1	2A	1939	5MU	C6-C5	2.72	1.39	1.34
54	2y	37	MIA	C5-C4	2.70	1.48	1.40
54	2y	37	MIA	C2-N3	2.70	1.36	1.32
32	2a	966	M2G	C2-N2	2.69	1.40	1.35
1	1A	2552	2MU	C4-N3	-2.68	1.33	1.38
1	2A	1915	5MU	C6-C5	2.68	1.39	1.34
54	1y	54	5MU	C4-N3	-2.67	1.33	1.38
55	2x	32	5MC	C6-C5	2.66	1.39	1.34
54	1y	37	MIA	C5-C4	2.66	1.48	1.40
55	1x	54	5MU	C6-C5	2.63	1.38	1.34
32	2a	967	5MC	C6-C5	2.62	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.61	1.34	1.38
1	2A	1962	5MC	C6-C5	2.61	1.38	1.34
1	1A	1962	5MC	C6-C5	2.60	1.38	1.34
55	2x	55	PSU	C4-N3	-2.59	1.34	1.38
54	1w	54	5MU	C4-N3	-2.58	1.34	1.38
54	2w	54	5MU	C4-N3	-2.58	1.34	1.38
32	2a	1519	MA6	C5-C4	2.57	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	54	5MU	C4-C5	2.57	1.49	1.44
1	1A	1915	5MU	C6-C5	2.57	1.38	1.34
54	1w	37	MIA	C5-C4	2.56	1.47	1.40
1	2A	1962	5MC	C6-N1	-2.56	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.55	1.34	1.38
32	2a	1518	MA6	C5-C4	2.55	1.47	1.40
55	1x	32	5MC	C6-N1	-2.53	1.33	1.38
54	1y	32	PSU	C4-N3	-2.52	1.34	1.38
54	2y	46	7MG	C8-N9	2.52	1.47	1.46
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40
54	1y	54	5MU	C2-N3	-2.51	1.33	1.38
32	1a	966	M2G	C6-N1	-2.51	1.34	1.37
1	2A	2552	2MU	C4-N3	-2.50	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.50	1.33	1.38
1	1A	2251	OMG	C6-N1	-2.48	1.34	1.37
54	2w	39	PSU	C4-N3	-2.47	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.47	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.47	1.34	1.37
32	1a	527	7MG	C8-N9	2.45	1.47	1.46
32	1a	1519	MA6	C5-C4	2.45	1.47	1.40
54	2y	55	PSU	C4-N3	-2.45	1.34	1.38
54	1y	55	PSU	C4-N3	-2.43	1.34	1.38
55	2x	54	5MU	C4-N3	-2.42	1.34	1.38
55	2x	54	5MU	C4-C5	2.42	1.48	1.44
1	2A	1939	5MU	C6-N1	-2.42	1.33	1.38
32	2a	516	PSU	C4-N3	-2.42	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.42	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.41	1.34	1.38
32	1a	527	7MG	C6-N1	-2.40	1.34	1.38
1	2A	1915	5MU	C2-N1	2.40	1.42	1.38
1	1A	1915	5MU	C2-N1	2.39	1.42	1.38
1	2A	1939	5MU	C2-N1	2.38	1.42	1.38
54	2y	46	7MG	C6-N1	-2.38	1.34	1.38
54	1w	8	4SU	C5-C4	-2.38	1.39	1.42
54	1y	8	4SU	C5-C4	-2.38	1.39	1.42
1	1A	2552	2MU	C5-C4	2.37	1.48	1.43
54	1y	54	5MU	C2-N1	2.37	1.42	1.38
54	2y	32	PSU	C4-N3	-2.37	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.36	1.33	1.37
32	2a	1498	UR3	C2-N1	2.36	1.41	1.38
32	2a	527	7MG	C6-N1	-2.36	1.34	1.38
32	2a	527	7MG	C8-N9	2.36	1.47	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	46	7MG	C8-N9	2.35	1.47	1.46
54	2y	54	5MU	C4-N3	-2.35	1.34	1.38
55	2x	32	5MC	C6-N1	-2.35	1.34	1.38
54	2w	54	5MU	C2-N1	2.35	1.42	1.38
54	2w	55	PSU	C4-N3	-2.34	1.34	1.38
54	2w	32	PSU	C4-N3	-2.33	1.34	1.38
54	2y	8	4SU	C5-C4	-2.33	1.39	1.42
54	1w	55	PSU	C4-N3	-2.32	1.34	1.38
54	2w	54	5MU	C4-C5	2.32	1.48	1.44
54	1y	8	4SU	C2-N1	2.31	1.42	1.38
55	2x	8	4SU	C2-N3	-2.31	1.33	1.38
55	1x	55	PSU	C4-N3	-2.31	1.34	1.38
32	1a	966	M2G	C2-N2	2.31	1.39	1.35
55	2x	54	5MU	C2-N1	2.30	1.42	1.38
32	2a	966	M2G	C6-N1	-2.29	1.34	1.37
54	2w	8	4SU	C2-N3	-2.28	1.33	1.38
1	2A	1915	5MU	C4-C5	2.28	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.26	1.34	1.38
54	1w	46	7MG	C6-N1	-2.25	1.34	1.38
1	1A	1939	5MU	C2-N1	2.25	1.42	1.38
54	2y	46	7MG	C4-N9	-2.25	1.35	1.37
32	2a	1400	5MC	C6-N1	-2.24	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.23	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.23	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.22	1.34	1.38
1	2A	1939	5MU	C4-C5	2.22	1.48	1.44
1	1A	1942	5MC	C6-N1	-2.22	1.34	1.38
54	1y	39	PSU	C4-N3	-2.21	1.34	1.38
54	2y	39	PSU	C4-N3	-2.21	1.34	1.38
1	2A	2503	2MA	C2-N3	2.21	1.35	1.31
54	1w	54	5MU	C4-C5	2.20	1.48	1.44
55	1x	54	5MU	C6-N1	-2.20	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.19	1.34	1.38
55	2x	8	4SU	O2-C2	2.19	1.27	1.23
54	2w	8	4SU	C5-C4	-2.18	1.39	1.42
32	2a	1404	5MC	C6-N1	-2.17	1.34	1.38
54	1w	8	4SU	C2-N3	-2.14	1.34	1.38
55	1x	8	4SU	O2-C2	2.14	1.27	1.23
54	2w	8	4SU	C6-C5	2.13	1.40	1.35
32	2a	967	5MC	C6-N1	-2.12	1.34	1.38
54	1y	46	7MG	C6-N1	-2.12	1.34	1.38
55	2x	8	4SU	C2-N1	2.12	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C6-N1	-2.11	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.11	1.34	1.37
54	1y	8	4SU	C2-N3	-2.11	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.10	1.34	1.38
55	1x	54	5MU	C2-N3	-2.10	1.34	1.38
54	2y	39	PSU	C4-C5	2.09	1.50	1.44
32	1a	967	5MC	C6-N1	-2.09	1.34	1.38
54	2w	54	5MU	C2-N3	-2.09	1.34	1.38
54	1y	46	7MG	C4-N9	-2.09	1.35	1.37
54	1w	8	4SU	C2-N1	2.08	1.41	1.38
1	2A	2552	2MU	C2-N3	-2.08	1.34	1.38
55	1x	54	5MU	C4-C5	2.08	1.48	1.44
1	2A	2552	2MU	C5-C4	2.07	1.48	1.43
32	1a	1407	5MC	C6-N1	-2.06	1.34	1.38
54	1y	54	5MU	C4-C5	2.06	1.48	1.44
32	2a	1402	4OC	C6-C5	2.05	1.39	1.35
1	1A	1915	5MU	C4-C5	2.04	1.48	1.44
54	1w	54	5MU	C2-N3	-2.03	1.34	1.38

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	17.35	133.84	102.44
54	2y	46	7MG	N9-C4-N3	9.35	139.45	125.47
54	1y	46	7MG	N9-C4-N3	9.27	139.33	125.47
54	1w	46	7MG	N9-C4-N3	9.01	138.94	125.47
32	1a	527	7MG	N9-C4-N3	8.80	138.64	125.47
32	2a	527	7MG	N9-C4-N3	8.28	137.86	125.47
54	2w	46	7MG	N9-C4-N3	8.03	137.47	125.47
54	1w	37	MIA	C12-C13-C14	-7.98	111.61	127.14
54	2y	8	4SU	C4-N3-C2	-6.41	121.11	127.34
32	1a	516	PSU	N1-C2-N3	6.22	122.18	115.13
1	2A	2605	PSU	N1-C2-N3	6.18	122.13	115.13
54	1w	39	PSU	N1-C2-N3	6.17	122.12	115.13
1	2A	1917	PSU	N1-C2-N3	6.11	122.05	115.13
54	2y	55	PSU	N1-C2-N3	6.10	122.04	115.13
32	2a	1498	UR3	C4-N3-C2	-6.07	118.85	124.56
1	1A	2605	PSU	N1-C2-N3	6.05	121.99	115.13
54	2y	39	PSU	N1-C2-N3	6.04	121.98	115.13
54	1w	8	4SU	C5-C4-N3	6.04	120.29	114.69
54	1w	32	PSU	N1-C2-N3	6.02	121.95	115.13
1	1A	1917	PSU	N1-C2-N3	6.01	121.94	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	55	PSU	N1-C2-N3	5.99	121.92	115.13
55	2x	55	PSU	N1-C2-N3	5.99	121.91	115.13
54	1y	39	PSU	N1-C2-N3	5.98	121.90	115.13
55	1x	55	PSU	N1-C2-N3	5.91	121.83	115.13
1	1A	1911	PSU	N1-C2-N3	5.90	121.82	115.13
54	1w	55	PSU	N1-C2-N3	5.85	121.76	115.13
54	2w	55	PSU	N1-C2-N3	5.84	121.75	115.13
32	2a	516	PSU	N1-C2-N3	5.81	121.71	115.13
54	1w	8	4SU	C4-N3-C2	-5.77	121.73	127.34
32	2a	527	7MG	N9-C8-N7	-5.76	95.15	103.38
1	1A	2552	2MU	N3-C2-N1	5.75	122.53	114.89
54	2w	32	PSU	N1-C2-N3	5.71	121.60	115.13
54	2w	46	7MG	N9-C8-N7	-5.71	95.22	103.38
54	1y	32	PSU	N1-C2-N3	5.69	121.58	115.13
54	1y	46	7MG	C5-C4-N3	-5.68	117.31	128.13
54	2y	32	PSU	N1-C2-N3	5.66	121.54	115.13
54	2y	46	7MG	C5-C4-N3	-5.62	117.43	128.13
32	1a	1498	UR3	C4-N3-C2	-5.59	119.30	124.56
54	2y	8	4SU	C5-C4-N3	5.49	119.79	114.69
1	2A	1915	5MU	C4-N3-C2	-5.46	120.28	127.35
1	1A	1939	5MU	C5-C4-N3	5.46	119.97	115.31
32	1a	527	7MG	C5-C4-N3	-5.44	117.76	128.13
54	1w	46	7MG	N9-C8-N7	-5.43	95.61	103.38
1	2A	1911	PSU	N1-C2-N3	5.43	121.28	115.13
1	1A	1915	5MU	C4-N3-C2	-5.41	120.35	127.35
54	2w	8	4SU	C4-N3-C2	-5.39	122.11	127.34
54	1y	8	4SU	C5-C4-N3	5.36	119.66	114.69
1	1A	1915	5MU	O4-C4-C5	-5.31	118.75	124.90
1	1A	1939	5MU	C4-N3-C2	-5.30	120.49	127.35
54	1w	46	7MG	C5-C4-N3	-5.23	118.15	128.13
54	1y	8	4SU	C4-N3-C2	-5.20	122.29	127.34
1	2A	1915	5MU	C5-C4-N3	5.20	119.75	115.31
1	2A	1939	5MU	C4-N3-C2	-5.19	120.64	127.35
32	2a	527	7MG	C5-C4-N3	-5.01	118.59	128.13
54	2w	46	7MG	C5-C4-N3	-4.96	118.68	128.13
32	1a	527	7MG	N9-C8-N7	-4.93	96.33	103.38
54	1y	46	7MG	N9-C8-N7	-4.90	96.38	103.38
1	1A	1915	5MU	N3-C2-N1	4.89	121.38	114.89
1	1A	1939	5MU	O4-C4-C5	-4.82	119.31	124.90
54	2y	46	7MG	N9-C8-N7	-4.82	96.48	103.38
1	1A	1939	5MU	N3-C2-N1	4.80	121.27	114.89
54	2w	8	4SU	C5-C4-N3	4.77	119.11	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	54	5MU	O4-C4-C5	-4.77	119.38	124.90
1	1A	1915	5MU	C5-C4-N3	4.77	119.38	115.31
55	2x	54	5MU	N3-C2-N1	4.76	121.21	114.89
1	2A	1915	5MU	N3-C2-N1	4.75	121.19	114.89
54	1y	54	5MU	C5-C4-N3	4.66	119.29	115.31
1	2A	1939	5MU	N3-C2-N1	4.65	121.06	114.89
54	1w	54	5MU	C4-N3-C2	-4.63	121.35	127.35
1	2A	2552	2MU	N3-C2-N1	4.60	120.99	114.89
54	2y	54	5MU	C4-N3-C2	-4.59	121.40	127.35
55	2x	54	5MU	C4-N3-C2	-4.56	121.44	127.35
54	1w	54	5MU	C5-C4-N3	4.56	119.20	115.31
54	2w	39	PSU	N1-C2-N3	4.52	120.25	115.13
54	2w	46	7MG	C2-N3-C4	4.52	120.35	112.30
1	1A	2552	2MU	C4-N3-C2	-4.50	120.64	126.58
54	2y	54	5MU	C5-C4-N3	4.50	119.15	115.31
55	2x	8	4SU	C5-C4-N3	4.49	118.85	114.69
54	2y	46	7MG	C2-N3-C4	4.44	120.22	112.30
54	1y	46	7MG	C2-N3-C4	4.42	120.17	112.30
54	1y	54	5MU	C4-N3-C2	-4.40	121.65	127.35
1	2A	1939	5MU	O4-C4-C5	-4.32	119.89	124.90
1	1A	1939	5MU	C5-C6-N1	-4.29	118.93	123.34
1	2A	1939	5MU	C5-C4-N3	4.28	118.96	115.31
54	2y	54	5MU	N3-C2-N1	4.26	120.54	114.89
54	1w	54	5MU	N3-C2-N1	4.24	120.52	114.89
55	1x	54	5MU	C4-N3-C2	-4.24	121.86	127.35
1	2A	2605	PSU	C4-N3-C2	-4.23	120.24	126.34
1	1A	2605	PSU	C4-N3-C2	-4.19	120.30	126.34
54	1w	39	PSU	C4-N3-C2	-4.15	120.36	126.34
1	2A	1915	5MU	O4-C4-C5	-4.15	120.09	124.90
1	2A	1915	5MU	C5-C6-N1	-4.14	119.08	123.34
54	1w	37	MIA	C15-C14-C13	-4.14	110.69	122.65
32	1a	527	7MG	C2-N3-C4	4.14	119.67	112.30
54	1y	54	5MU	N3-C2-N1	4.13	120.37	114.89
32	1a	516	PSU	C4-N3-C2	-4.12	120.40	126.34
1	2A	1939	5MU	C5-C6-N1	-4.12	119.10	123.34
54	2y	8	4SU	N3-C2-N1	4.11	120.35	114.89
55	2x	55	PSU	C4-N3-C2	-4.09	120.44	126.34
1	2A	1962	5MC	C5-C6-N1	-4.09	119.13	123.34
43	2l	92	0TD	CSB-SB-CB	-4.09	95.04	102.44
55	1x	54	5MU	N3-C2-N1	4.08	120.31	114.89
54	1w	32	PSU	C4-N3-C2	-4.07	120.47	126.34
32	2a	527	7MG	C2-N3-C4	4.07	119.54	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C2-N3-C4	4.06	120.92	115.32
54	2w	54	5MU	C4-N3-C2	-4.06	122.10	127.35
55	1x	54	5MU	C5-C4-N3	4.06	118.77	115.31
55	2x	8	4SU	C1'-N1-C2	4.05	124.90	117.57
54	1y	39	PSU	O2-C2-N1	-4.05	118.33	122.79
1	1A	2552	2MU	O2-C2-N1	-4.04	117.41	122.79
54	2w	54	5MU	C5-C4-N3	4.04	118.76	115.31
1	2A	1917	PSU	C4-N3-C2	-4.03	120.53	126.34
1	1A	1911	PSU	C4-N3-C2	-4.03	120.54	126.34
54	1w	46	7MG	C2-N3-C4	4.02	119.46	112.30
55	1x	55	PSU	C4-N3-C2	-4.00	120.57	126.34
54	1w	54	5MU	O4-C4-C5	-3.96	120.31	124.90
32	2a	516	PSU	C4-N3-C2	-3.95	120.65	126.34
55	1x	55	PSU	O2-C2-N1	-3.95	118.45	122.79
54	2y	39	PSU	O2-C2-N1	-3.94	118.45	122.79
54	2y	54	5MU	O4-C4-C5	-3.94	120.33	124.90
1	2A	2552	2MU	C4-N3-C2	-3.94	121.38	126.58
32	2a	1400	5MC	C5-C6-N1	-3.93	119.30	123.34
54	1w	55	PSU	O2-C2-N1	-3.92	118.47	122.79
1	1A	1917	PSU	C4-N3-C2	-3.92	120.69	126.34
54	2w	54	5MU	N3-C2-N1	3.90	120.07	114.89
55	1x	32	5MC	C5-C6-N1	-3.90	119.33	123.34
54	2y	39	PSU	C4-N3-C2	-3.89	120.73	126.34
54	1y	32	PSU	C4-N3-C2	-3.89	120.73	126.34
54	2y	55	PSU	O2-C2-N1	-3.89	118.51	122.79
54	2w	8	4SU	N3-C2-N1	3.88	120.04	114.89
1	2A	1942	5MC	C5-C6-N1	-3.87	119.36	123.34
1	2A	1911	PSU	C4-N3-C2	-3.87	120.76	126.34
54	1w	37	MIA	C5-C6-N1	-3.87	117.60	120.81
54	1y	39	PSU	C4-N3-C2	-3.85	120.80	126.34
55	1x	54	5MU	O4-C4-C5	-3.82	120.47	124.90
54	2y	55	PSU	C4-N3-C2	-3.80	120.86	126.34
54	2y	8	4SU	C5-C4-S4	-3.78	119.59	124.47
54	2y	32	PSU	C4-N3-C2	-3.74	120.94	126.34
32	2a	1518	MA6	C4-C5-N7	-3.74	105.50	109.40
55	2x	54	5MU	C5-C4-N3	3.73	118.50	115.31
54	1w	39	PSU	O2-C2-N1	-3.72	118.70	122.79
32	2a	967	5MC	C5-C6-N1	-3.70	119.53	123.34
54	1w	37	MIA	C11-S10-C2	-3.69	99.51	102.27
54	1w	37	MIA	C16-C14-C13	-3.66	112.06	122.65
32	1a	1400	5MC	C5-C6-N1	-3.62	119.61	123.34
54	1y	55	PSU	C4-N3-C2	-3.61	121.13	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	C4-C5-N7	-3.60	105.64	109.40
54	1y	54	5MU	C5-C6-N1	-3.59	119.64	123.34
54	1y	55	PSU	O2-C2-N1	-3.59	118.84	122.79
54	1w	54	5MU	C5-C6-N1	-3.57	119.67	123.34
54	2y	37	MIA	N3-C2-N1	-3.57	123.10	128.68
32	1a	1407	5MC	C5-C6-N1	-3.57	119.67	123.34
54	2w	55	PSU	C4-N3-C2	-3.56	121.21	126.34
1	1A	1911	PSU	O2-C2-N1	-3.56	118.88	122.79
32	2a	1519	MA6	C4-C5-N7	-3.56	105.69	109.40
54	2w	32	PSU	C4-N3-C2	-3.54	121.24	126.34
1	1A	1942	5MC	C5-C6-N1	-3.54	119.70	123.34
55	2x	32	5MC	C5-C6-N1	-3.54	119.70	123.34
32	2a	1518	MA6	N3-C2-N1	-3.52	123.17	128.68
54	1w	55	PSU	C4-N3-C2	-3.52	121.27	126.34
54	2w	54	5MU	O4-C4-C5	-3.52	120.83	124.90
55	2x	54	5MU	O4-C4-C5	-3.50	120.85	124.90
32	2a	516	PSU	O2-C2-N1	-3.50	118.94	122.79
54	2w	55	PSU	O2-C2-N1	-3.49	118.95	122.79
54	2w	37	MIA	N3-C2-N1	-3.48	123.24	128.68
32	1a	1404	5MC	C5-C6-N1	-3.46	119.77	123.34
54	2w	32	PSU	O2-C2-N1	-3.45	118.99	122.79
32	2a	1404	5MC	C5-C6-N1	-3.44	119.80	123.34
1	1A	1917	PSU	O2-C2-N1	-3.38	119.07	122.79
54	1y	37	MIA	N3-C2-N1	-3.37	123.41	128.68
54	2y	32	PSU	O2-C2-N1	-3.36	119.09	122.79
32	2a	1518	MA6	C9-N6-C6	-3.36	109.35	119.51
32	1a	967	5MC	C5-C6-N1	-3.32	119.92	123.34
54	1w	8	4SU	N3-C2-N1	3.32	119.30	114.89
54	1y	32	PSU	O2-C2-N1	-3.30	119.15	122.79
54	1y	8	4SU	N3-C2-N1	3.30	119.27	114.89
32	1a	1519	MA6	C9-N6-C6	-3.29	109.55	119.51
54	2w	54	5MU	C5-C6-N1	-3.26	119.98	123.34
55	1x	54	5MU	C5-C6-N1	-3.25	120.00	123.34
54	1w	8	4SU	C5-C4-S4	-3.23	120.30	124.47
1	1A	1915	5MU	C5-C6-N1	-3.23	120.02	123.34
32	2a	1519	MA6	N3-C2-N1	-3.22	123.64	128.68
54	1w	32	PSU	O2-C2-N1	-3.19	119.28	122.79
43	2l	92	0TD	OD2-CG-CB	3.19	120.04	113.15
1	2A	1911	PSU	O2-C2-N1	-3.17	119.30	122.79
32	1a	1519	MA6	C4-C5-N7	-3.16	106.11	109.40
32	1a	1518	MA6	N3-C2-N1	-3.10	123.84	128.68
32	2a	1519	MA6	C9-N6-C6	-3.09	110.16	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	C6-C5-C4	-3.07	117.29	119.95
32	1a	1518	MA6	C9-N6-C6	-3.07	110.22	119.51
1	2A	1917	PSU	O2-C2-N1	-3.04	119.44	122.79
54	2w	39	PSU	C4-N3-C2	-3.04	121.96	126.34
43	1l	92	0TD	OD2-CG-CB	3.03	119.71	113.15
32	1a	516	PSU	O2-C2-N1	-3.03	119.46	122.79
32	1a	1519	MA6	N1-C6-N6	3.02	120.24	117.06
54	2w	46	7MG	C5-C6-N1	3.00	116.28	110.99
55	2x	55	PSU	O2-C2-N1	-3.00	119.49	122.79
1	1A	1942	5MC	C5-C4-N3	-2.99	118.44	121.67
32	2a	1407	5MC	C5-C6-N1	-2.99	120.27	123.34
32	1a	1519	MA6	N3-C2-N1	-2.96	124.05	128.68
54	2y	54	5MU	C5-C6-N1	-2.89	120.36	123.34
1	2A	2605	PSU	O2-C2-N1	-2.89	119.61	122.79
54	1w	37	MIA	C2-N1-C6	2.88	122.34	117.19
55	2x	8	4SU	C6-C5-C4	-2.87	117.47	119.95
1	1A	2503	2MA	C8-N7-C5	2.86	108.44	102.99
55	2x	54	5MU	C5-C6-N1	-2.85	120.41	123.34
54	1y	8	4SU	C5-C4-S4	-2.83	120.83	124.47
54	2w	37	MIA	C4-C5-N7	-2.82	106.46	109.40
1	1A	1962	5MC	C5-C6-N1	-2.81	120.45	123.34
32	1a	1404	5MC	C5-C4-N3	-2.80	118.65	121.67
1	1A	2552	2MU	C2'-C1'-N1	-2.79	108.80	114.22
32	2a	1407	5MC	C5-C4-N3	-2.79	118.66	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.79	117.70	123.86
1	2A	2552	2MU	C5-C4-N3	2.78	118.99	114.84
32	2a	527	7MG	C5-C6-N1	2.76	115.86	110.99
32	1a	1407	5MC	C5-C4-N3	-2.75	118.71	121.67
32	2a	1402	4OC	C6-C5-C4	2.73	120.30	116.96
1	1A	1920	4OC	O2-C2-N3	-2.72	117.91	122.33
1	1A	2503	2MA	C5-C6-N1	2.70	118.69	114.02
54	2y	37	MIA	C4-C5-N7	-2.67	106.62	109.40
54	1y	37	MIA	C4-C5-N7	-2.65	106.64	109.40
54	1w	46	7MG	C5-C4-N9	-2.65	102.91	106.35
55	1x	32	5MC	C5-C4-N3	-2.65	118.81	121.67
1	1A	1915	5MU	O2-C2-N1	-2.64	119.28	122.79
54	1w	46	7MG	C5-C6-N1	2.64	115.64	110.99
55	1x	8	4SU	O2-C2-N1	2.64	126.29	122.79
54	1w	37	MIA	C4-C5-N7	-2.63	106.66	109.40
32	1a	1402	4OC	C6-C5-C4	2.63	120.17	116.96
32	2a	1519	MA6	N1-C6-N6	2.62	119.81	117.06
55	2x	32	5MC	C5-C4-N3	-2.61	118.85	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2251	OMG	C5-C6-N1	2.60	118.55	113.95
1	2A	2552	2MU	O4-C4-C5	-2.56	120.66	125.16
54	1y	46	7MG	C5-C6-N1	2.56	115.49	110.99
54	2y	8	4SU	C1'-N1-C2	2.55	122.19	117.57
32	1a	1207	2MG	C8-N7-C5	2.55	107.84	102.99
54	2w	46	7MG	O4'-C1'-N9	-2.55	105.83	109.30
32	2a	1498	UR3	C3U-N3-C2	2.54	121.77	117.31
1	2A	2251	OMG	C8-N7-C5	2.54	107.82	102.99
1	1A	2605	PSU	O2-C2-N3	-2.52	117.06	121.82
1	2A	2503	2MA	C5-C6-N1	2.52	118.36	114.02
43	2l	92	0TD	OD1-CG-CB	-2.51	117.19	122.44
54	1w	37	MIA	C12-N6-C6	-2.50	118.84	122.55
54	2w	8	4SU	C5-C4-S4	-2.50	121.25	124.47
54	2y	54	5MU	C1'-N1-C2	2.50	122.09	117.57
54	2w	39	PSU	C6-C5-C4	-2.49	116.45	118.20
54	2y	46	7MG	C5-C4-N9	-2.49	103.12	106.35
32	1a	1400	5MC	C5-C4-N3	-2.48	119.00	121.67
32	1a	527	7MG	C5-C6-N1	2.48	115.36	110.99
1	1A	1962	5MC	C5-C4-N3	-2.46	119.02	121.67
32	2a	1207	2MG	C8-N7-C5	2.45	107.67	102.99
1	2A	2503	2MA	C8-N7-C5	2.43	107.62	102.99
55	1x	8	4SU	C5-C4-N3	2.42	116.94	114.69
32	2a	1404	5MC	C5-C4-N3	-2.41	119.07	121.67
1	2A	1942	5MC	O2-C2-N3	-2.40	118.42	122.33
54	2y	54	5MU	C5M-C5-C4	2.40	121.41	118.77
54	2y	46	7MG	C5-C6-N1	2.40	115.22	110.99
55	1x	8	4SU	C1'-N1-C2	2.39	121.91	117.57
32	2a	1400	5MC	C5-C4-N3	-2.39	119.09	121.67
1	2A	2605	PSU	C5-C6-N1	-2.38	118.53	122.11
32	1a	967	5MC	C5-C4-N3	-2.37	119.12	121.67
1	2A	1939	5MU	O2-C2-N1	-2.36	119.65	122.79
32	2a	1207	2MG	CM2-N2-C2	-2.35	118.66	123.86
55	2x	54	5MU	O2-C2-N1	-2.34	119.68	122.79
32	2a	1404	5MC	O2-C2-N3	-2.33	118.53	122.33
32	2a	967	5MC	C5-C4-N3	-2.33	119.16	121.67
55	2x	32	5MC	O2-C2-N3	-2.33	118.54	122.33
1	2A	1917	PSU	C5-C6-N1	-2.31	118.64	122.11
55	2x	8	4SU	C1'-N1-C6	-2.31	115.81	120.84
54	1y	46	7MG	C5-C4-N9	-2.30	103.36	106.35
1	1A	2251	OMG	C5-C6-N1	2.30	118.01	113.95
1	1A	2605	PSU	C5-C6-N1	-2.30	118.67	122.11
1	2A	1962	5MC	C5-C4-N3	-2.28	119.22	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	46	7MG	O6-C6-C5	-2.27	121.98	127.54
32	1a	1498	UR3	C3U-N3-C2	2.27	121.28	117.31
54	1w	37	MIA	N3-C2-N1	-2.26	122.82	126.98
55	2x	54	5MU	C5M-C5-C4	2.26	121.26	118.77
32	1a	1518	MA6	C10-N6-C6	-2.26	112.68	119.51
32	2a	966	M2G	C8-N7-C5	2.24	107.26	102.99
1	1A	2251	OMG	C8-N7-C5	2.24	107.25	102.99
54	1w	46	7MG	O6-C6-C5	-2.23	122.08	127.54
32	2a	1518	MA6	C10-N6-C9	-2.23	108.95	116.12
1	1A	2552	2MU	O4-C4-C5	-2.22	121.26	125.16
54	1y	8	4SU	C1'-N1-C2	2.20	121.56	117.57
1	2A	2552	2MU	O2-C2-N1	-2.20	119.86	122.79
32	1a	1400	5MC	O2-C2-N3	-2.20	118.76	122.33
54	2y	54	5MU	C1'-N1-C6	-2.18	117.50	121.12
1	2A	1920	4OC	O2-C2-N3	-2.18	118.79	122.33
32	2a	1407	5MC	O2-C2-N3	-2.18	118.79	122.33
32	2a	527	7MG	C5-C4-N9	-2.17	103.53	106.35
32	2a	516	PSU	O4'-C1'-C2'	2.15	108.18	105.14
32	2a	966	M2G	C5-C6-N1	2.15	117.75	113.95
32	1a	966	M2G	C8-N7-C5	2.15	107.08	102.99
1	1A	2552	2MU	C5-C4-N3	2.13	118.03	114.84
32	1a	516	PSU	O4'-C1'-C2'	2.13	108.15	105.14
32	1a	1518	MA6	C10-N6-C9	-2.13	109.26	116.12
1	2A	1942	5MC	C5-C4-N3	-2.12	119.39	121.67
32	1a	527	7MG	O6-C6-C5	-2.12	122.34	127.54
54	1w	39	PSU	C5-C6-N1	-2.11	118.94	122.11
32	1a	527	7MG	C5-C4-N9	-2.11	103.60	106.35
1	2A	1962	5MC	CM5-C5-C6	-2.11	120.03	122.85
32	1a	966	M2G	C5-C6-N1	2.09	117.64	113.95
1	2A	1915	5MU	O2-C2-N1	-2.09	120.01	122.79
55	1x	54	5MU	O2-C2-N1	-2.07	120.03	122.79
54	2w	54	5MU	C5M-C5-C4	2.07	121.05	118.77
32	2a	967	5MC	CM5-C5-C6	-2.07	120.08	122.85
54	1w	32	PSU	C5-C6-N1	-2.07	119.01	122.11
32	2a	1207	2MG	C5-C6-N1	2.05	117.57	113.95
54	1y	32	PSU	C5-C6-N1	-2.05	119.04	122.11
1	2A	2552	2MU	C2'-C1'-N1	-2.04	110.26	114.22
1	1A	1911	PSU	C5-C6-N1	-2.03	119.07	122.11
55	1x	55	PSU	C5-C6-N1	-2.02	119.07	122.11
32	2a	1400	5MC	O2-C2-N3	-2.01	119.06	122.33
54	2y	46	7MG	O6-C6-C5	-2.01	122.61	127.54
54	1y	46	7MG	O6-C6-C5	-2.01	122.62	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	32	5MC	C1'-N1-C6	-2.00	117.79	121.12

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	1498	UR3	O4'-C4'-C5'-O5'
32	2a	1498	UR3	C3'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C16
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	C3'-C4'-C5'-O5'
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	1y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C6
54	2w	46	7MG	O4'-C1'-N9-C4
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C10
54	1w	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	1y	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
32	2a	1400	5MC	O4'-C1'-N1-C6
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1400	5MC	C2'-C1'-N1-C2
54	2w	46	7MG	O4'-C1'-N9-C8
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	1400	5MC	O4'-C1'-N1-C2
54	1y	55	PSU	O4'-C1'-C5-C4
32	1a	967	5MC	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
32	2a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	1911	PSU	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C8
1	1A	1920	4OC	C2'-C1'-N1-C2
1	1A	1962	5MC	C2'-C1'-N1-C6
54	1y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
1	2A	1920	4OC	C2'-C1'-N1-C2
55	2x	8	4SU	C2'-C1'-N1-C2
54	1y	8	4SU	C2'-C1'-N1-C2
54	2y	54	5MU	C2'-C1'-N1-C2
54	1w	46	7MG	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C1'-N1-C6

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 (i)

Of 2312 ligands modelled in this entry, 2306 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
61	FME	2x	3003	55	8,9,10	0.51	0	7,9,11	1.38	1 (14%)
60	SF4	1d	501	35	0,12,12	-	-	-		
57	4M2	2A	3670	-	56,62,62	3.11	11 (19%)	61,90,90	2.06	12 (19%)
61	FME	1x	115	55	8,9,10	0.37	0	7,9,11	1.61	1 (14%)
60	SF4	2d	501	35	0,12,12	-	-	-		
57	4M2	1A	3894	-	56,62,62	3.15	8 (14%)	61,90,90	2.06	11 (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
61	FME	2x	3003	55	-	4/7/9/11	-
60	SF4	1d	501	35	-	-	0/6/5/5
57	4M2	2A	3670	-	-	6/31/93/93	0/6/6/6
61	FME	1x	115	55	-	4/7/9/11	-
60	SF4	2d	501	35	-	-	0/6/5/5
57	4M2	1A	3894	-	-	13/31/93/93	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	3894	4M2	CAN-CBI	21.04	1.56	1.34
57	2A	3670	4M2	CAN-CBI	20.81	1.56	1.34
57	2A	3670	4M2	C2-N3	4.52	1.39	1.32
57	1A	3894	4M2	CBX-CBT	-4.27	1.47	1.52
57	1A	3894	4M2	C2-N3	4.04	1.38	1.32
57	1A	3894	4M2	OBF-CBX	-3.98	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3670	4M2	CAV-CBK	3.05	1.52	1.48
57	2A	3670	4M2	CBM-CAN	-3.02	1.41	1.46
57	1A	3894	4M2	C2-N1	2.96	1.39	1.33
57	2A	3670	4M2	OBH-CCC	2.94	1.45	1.41
57	2A	3670	4M2	C2-N1	2.74	1.39	1.33
57	1A	3894	4M2	CBM-CAN	-2.73	1.41	1.46
57	2A	3670	4M2	C5-C4	-2.47	1.34	1.40
57	2A	3670	4M2	CBX-CBT	-2.46	1.49	1.52
57	1A	3894	4M2	C5-C4	-2.29	1.34	1.40
57	2A	3670	4M2	CBK-CBL	-2.27	1.32	1.35
57	2A	3670	4M2	OBF-CBX	-2.08	1.38	1.41
57	2A	3670	4M2	CBV-CBZ	-2.06	1.50	1.53
57	1A	3894	4M2	CAV-CBK	2.01	1.51	1.48

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2A	3670	4M2	N3-C2-N1	-7.39	117.12	128.68
57	1A	3894	4M2	CBN-OBF-CBX	-7.34	107.03	117.79
57	2A	3670	4M2	CBN-OBF-CBX	-7.24	107.18	117.79
57	1A	3894	4M2	N3-C2-N1	-6.86	117.96	128.68
57	1A	3894	4M2	OBE-CBX-CBT	-5.07	97.41	105.81
57	2A	3670	4M2	CAA-OBA-CBK	-4.38	110.56	119.20
57	2A	3670	4M2	CCC-N9-C4	-4.35	119.00	126.64
57	1A	3894	4M2	OBH-CBW-CBZ	-4.26	97.97	104.06
57	1A	3894	4M2	OBF-CBX-CBT	4.17	113.84	106.78
57	2A	3670	4M2	OBF-CBX-CBT	4.07	113.67	106.78
57	2A	3670	4M2	C4-C5-N7	-3.83	105.41	109.40
57	2A	3670	4M2	OBE-CBX-CBT	-3.75	99.59	105.81
57	1A	3894	4M2	CAA-OBA-CBK	-3.74	111.84	119.20
57	2A	3670	4M2	OBH-CBW-CBZ	-3.55	98.97	104.06
57	1A	3894	4M2	CBT-CBS-CBL	-3.46	98.78	102.08
57	1A	3894	4M2	CAC-OBC-CCB	-3.24	106.03	114.52
61	1x	115	FME	CA-N-CN	-3.23	117.85	122.82
57	1A	3894	4M2	C4-C5-N7	-3.12	106.15	109.40
57	1A	3894	4M2	CBM-CAN-CBI	-2.91	123.72	129.33
57	1A	3894	4M2	CAE-CBR-CCA	-2.79	109.15	113.41
57	2A	3670	4M2	CBM-CAN-CBI	-2.39	124.73	129.33
61	2x	3003	FME	CA-N-CN	-2.16	119.49	122.82
57	2A	3670	4M2	OBG-CBY-OBD	-2.12	104.94	109.97
57	2A	3670	4M2	CAE-CBR-CCA	-2.05	110.28	113.41
57	2A	3670	4M2	CBT-CBS-CBL	-2.03	100.15	102.08

There are no chirality outliers.

All (27) torsion outliers are listed below:

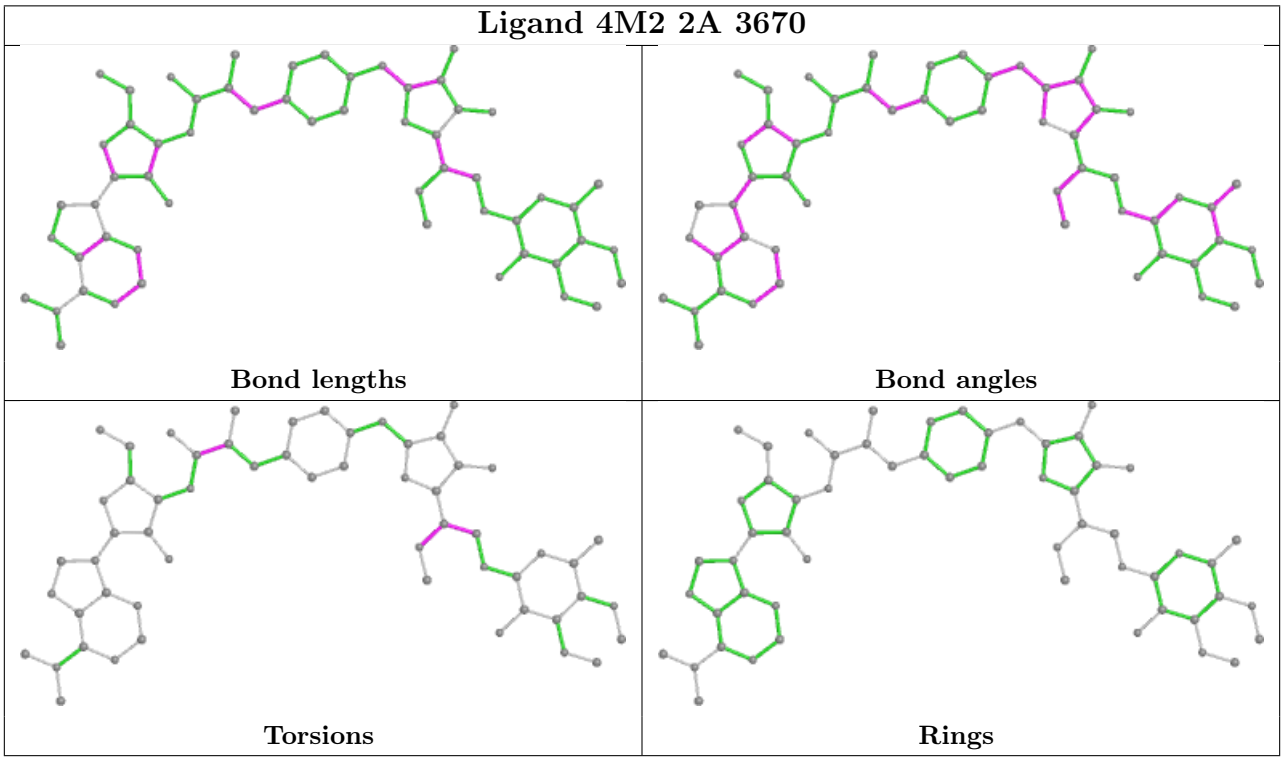
Mol	Chain	Res	Type	Atoms
57	1A	3894	4M2	C5-C6-N6-CAF
57	1A	3894	4M2	CAV-CBK-OBA-CAA
57	1A	3894	4M2	CBL-CBK-OBA-CAA
57	2A	3670	4M2	CAV-CBK-OBA-CAA
61	1x	115	FME	O1-CN-N-CA
61	1x	115	FME	C-CA-CB-CG
61	1x	115	FME	CA-CB-CG-SD
61	2x	3003	FME	O1-CN-N-CA
61	2x	3003	FME	CB-CA-N-CN
61	2x	3003	FME	C-CA-CB-CG
57	1A	3894	4M2	OAI-CAU-CBW-OBH
61	2x	3003	FME	N-CA-CB-CG
57	1A	3894	4M2	C5-C6-N6-CAG
57	1A	3894	4M2	OBD-CAV-CBK-OBA
57	1A	3894	4M2	CAR-CBN-OBF-CBX
57	1A	3894	4M2	CAN-CBI-CBJ-OAH
57	1A	3894	4M2	CAN-CBI-CBJ-NAZ
57	2A	3670	4M2	CAN-CBI-CBJ-OAH
57	2A	3670	4M2	CAN-CBI-CBJ-NAZ
57	2A	3670	4M2	OBD-CAV-CBK-OBA
57	1A	3894	4M2	CAD-CBI-CBJ-OAH
57	1A	3894	4M2	CAD-CBI-CBJ-NAZ
57	2A	3670	4M2	CAD-CBI-CBJ-OAH
57	2A	3670	4M2	CAD-CBI-CBJ-NAZ
57	1A	3894	4M2	CAS-CBN-OBF-CBX
61	1x	115	FME	N-CA-CB-CG
57	1A	3894	4M2	OAI-CAU-CBW-CBZ

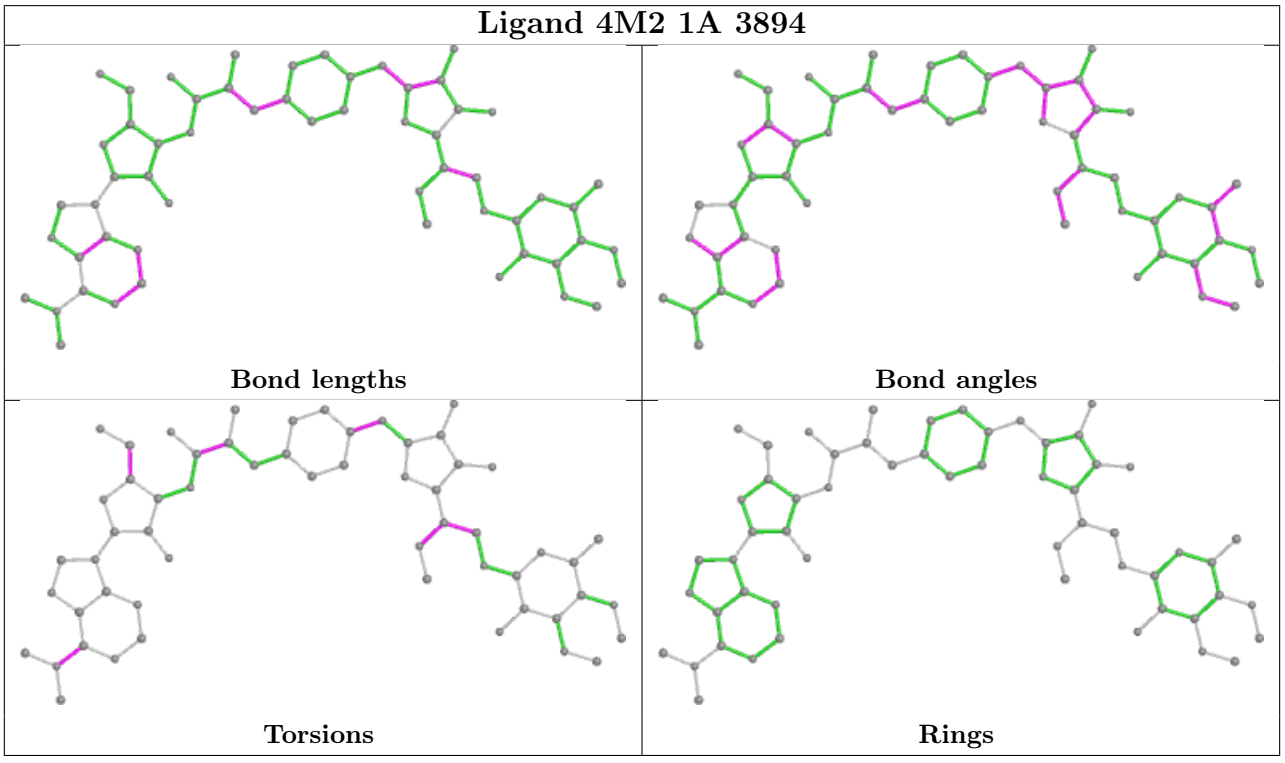
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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	1A	2860/2915 (98%)	0.26	65 (2%) 60 56	22, 42, 92, 106	0
1	2A	2789/2915 (95%)	-0.24	64 (2%) 60 56	26, 46, 90, 104	0
2	1B	120/121 (99%)	0.01	0 100 100	37, 59, 71, 89	0
2	2B	120/121 (99%)	-0.39	0 100 100	46, 66, 77, 90	0
3	1D	275/276 (99%)	0.50	3 (1%) 80 79	21, 42, 59, 79	0
3	2D	275/276 (99%)	0.38	7 (2%) 57 53	23, 44, 61, 80	0
4	1E	204/206 (99%)	0.21	0 100 100	20, 45, 65, 78	0
4	2E	204/206 (99%)	-0.04	1 (0%) 91 91	21, 49, 68, 79	0
5	1F	203/210 (96%)	0.53	5 (2%) 57 53	23, 51, 73, 89	0
5	2F	203/210 (96%)	0.42	12 (5%) 22 19	25, 56, 75, 91	0
6	1G	181/182 (99%)	0.90	16 (8%) 10 8	48, 67, 80, 92	0
6	2G	181/182 (99%)	2.30	88 (48%) 0 0	52, 71, 82, 95	0
7	1H	174/180 (96%)	0.31	1 (0%) 89 89	48, 65, 75, 82	0
7	2H	174/180 (96%)	1.62	57 (32%) 0 0	52, 70, 80, 83	0
8	1I	146/148 (98%)	0.22	0 100 100	47, 74, 83, 89	0
8	2I	146/148 (98%)	-0.24	1 (0%) 87 87	49, 74, 84, 86	0
9	1N	140/140 (100%)	0.28	0 100 100	31, 48, 69, 79	0
9	2N	140/140 (100%)	0.06	1 (0%) 87 87	36, 53, 72, 80	0
10	1O	122/122 (100%)	0.06	0 100 100	25, 38, 58, 63	0
10	2O	122/122 (100%)	0.85	10 (8%) 11 9	39, 57, 72, 76	0
11	1P	149/150 (99%)	0.23	0 100 100	23, 52, 75, 81	0
11	2P	149/150 (99%)	-0.06	1 (0%) 87 87	26, 58, 78, 83	0
12	1Q	141/141 (100%)	1.01	13 (9%) 9 7	30, 49, 64, 80	0
12	2Q	141/141 (100%)	1.28	30 (21%) 0 1	37, 54, 68, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.31	0 100 100	30, 40, 55, 67	0
13	2R	118/118 (100%)	0.17	0 100 100	32, 43, 57, 69	0
14	1S	110/112 (98%)	0.27	0 100 100	45, 59, 71, 75	0
14	2S	110/112 (98%)	-0.12	1 (0%) 84 83	52, 64, 74, 77	0
15	1T	131/146 (89%)	0.25	1 (0%) 86 85	37, 50, 73, 84	0
15	2T	131/146 (89%)	0.08	0 100 100	41, 53, 74, 84	0
16	1U	116/118 (98%)	0.30	0 100 100	26, 42, 58, 75	0
16	2U	116/118 (98%)	0.12	2 (1%) 70 67	32, 47, 62, 77	0
17	1V	101/101 (100%)	0.41	2 (1%) 65 60	29, 51, 66, 77	0
17	2V	101/101 (100%)	0.14	2 (1%) 65 60	33, 58, 70, 77	0
18	1W	112/113 (99%)	0.18	1 (0%) 84 83	25, 37, 59, 86	0
18	2W	112/113 (99%)	0.20	1 (0%) 84 83	29, 40, 61, 88	0
19	1X	95/96 (98%)	0.05	0 100 100	22, 35, 60, 84	0
19	2X	95/96 (98%)	0.65	4 (4%) 36 33	40, 60, 75, 82	0
20	1Y	107/110 (97%)	0.17	0 100 100	44, 59, 72, 85	0
20	2Y	107/110 (97%)	0.87	12 (11%) 5 3	49, 62, 75, 87	0
21	1Z	154/206 (74%)	1.56	48 (31%) 0 0	46, 71, 88, 93	0
21	2Z	160/206 (77%)	2.44	86 (53%) 0 0	52, 76, 90, 94	0
22	10	83/85 (97%)	0.81	7 (8%) 11 8	25, 36, 66, 88	0
22	20	83/85 (97%)	0.85	8 (9%) 8 6	47, 65, 77, 91	0
23	11	97/98 (98%)	0.49	3 (3%) 49 45	30, 47, 69, 79	0
23	21	97/98 (98%)	-0.03	1 (1%) 82 81	30, 51, 72, 80	0
24	12	70/72 (97%)	0.20	0 100 100	39, 56, 67, 77	0
24	22	70/72 (97%)	0.06	1 (1%) 75 73	45, 61, 69, 77	0
25	13	59/60 (98%)	0.38	0 100 100	33, 46, 68, 76	0
25	23	59/60 (98%)	0.52	3 (5%) 28 25	38, 52, 70, 79	0
26	14	69/71 (97%)	0.69	10 (14%) 2 1	47, 72, 90, 94	0
26	24	69/71 (97%)	2.96	38 (55%) 0 0	73, 86, 96, 98	0
27	15	59/60 (98%)	0.05	1 (1%) 70 67	19, 32, 51, 62	0
27	25	59/60 (98%)	0.08	0 100 100	32, 49, 66, 73	0
28	16	53/54 (98%)	0.33	1 (1%) 66 63	28, 39, 56, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.17	0 100 100	41, 58, 70, 77	0
29	17	48/49 (97%)	0.39	1 (2%) 63 59	24, 30, 58, 73	0
29	27	48/49 (97%)	1.00	6 (12%) 3 2	25, 33, 60, 75	0
30	18	64/65 (98%)	0.27	0 100 100	30, 41, 49, 58	0
30	28	64/65 (98%)	-0.28	0 100 100	35, 45, 53, 59	0
31	19	37/37 (100%)	0.53	1 (2%) 54 50	39, 49, 63, 67	0
31	29	37/37 (100%)	0.71	3 (8%) 12 9	43, 55, 65, 70	0
32	1a	1488/1521 (97%)	-0.04	23 (1%) 73 71	41, 69, 92, 105	0
32	2a	1491/1521 (98%)	-0.22	27 (1%) 68 65	45, 72, 93, 104	0
33	1b	231/256 (90%)	-0.29	0 100 100	67, 82, 90, 96	0
33	2b	231/256 (90%)	-0.32	0 100 100	70, 84, 90, 96	0
34	1c	206/239 (86%)	0.09	2 (0%) 82 81	64, 76, 85, 95	0
34	2c	206/239 (86%)	1.35	58 (28%) 0 0	68, 79, 86, 95	0
35	1d	208/209 (99%)	0.09	2 (0%) 82 81	55, 70, 80, 86	0
35	2d	208/209 (99%)	0.83	25 (12%) 4 3	58, 71, 81, 86	0
36	1e	148/162 (91%)	0.09	0 100 100	58, 70, 79, 91	0
36	2e	148/162 (91%)	0.29	5 (3%) 45 41	61, 73, 82, 90	0
37	1f	100/101 (99%)	0.27	0 100 100	54, 66, 77, 83	0
37	2f	100/101 (99%)	-0.18	0 100 100	54, 68, 77, 83	0
38	1g	155/156 (99%)	0.85	20 (12%) 3 2	63, 73, 85, 97	0
38	2g	155/156 (99%)	1.03	23 (14%) 2 1	66, 75, 87, 98	0
39	1h	137/138 (99%)	0.12	0 100 100	61, 72, 79, 85	0
39	2h	137/138 (99%)	-0.05	2 (1%) 73 71	62, 75, 81, 86	0
40	1i	127/128 (99%)	-0.12	0 100 100	49, 75, 83, 92	0
40	2i	127/128 (99%)	0.46	9 (7%) 16 12	73, 84, 92, 96	0
41	1j	97/105 (92%)	-0.30	0 100 100	45, 75, 86, 93	0
41	2j	96/105 (91%)	0.60	13 (13%) 3 2	72, 85, 93, 98	0
42	1k	114/129 (88%)	1.01	10 (8%) 10 8	46, 68, 80, 86	0
42	2k	114/129 (88%)	0.37	4 (3%) 44 40	48, 70, 81, 89	0
43	1l	121/132 (91%)	0.48	3 (2%) 57 53	44, 58, 70, 74	0
43	2l	121/132 (91%)	1.02	16 (13%) 3 2	47, 61, 72, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.49	8 (6%) 18 16	51, 67, 77, 85	0
44	2m	122/126 (96%)	2.81	75 (61%) 0 0	70, 83, 88, 92	0
45	1n	60/61 (98%)	0.31	1 (1%) 70 67	50, 62, 73, 76	0
45	2n	60/61 (98%)	2.27	31 (51%) 0 0	75, 83, 90, 93	0
46	1o	88/89 (98%)	0.38	7 (7%) 12 9	50, 68, 79, 82	0
46	2o	88/89 (98%)	0.19	2 (2%) 60 56	53, 69, 80, 83	0
47	1p	82/88 (93%)	0.21	2 (2%) 59 54	58, 70, 77, 82	0
47	2p	82/88 (93%)	0.38	1 (1%) 79 77	57, 70, 78, 84	0
48	1q	99/105 (94%)	0.74	3 (3%) 50 47	59, 71, 79, 83	0
48	2q	99/105 (94%)	1.27	25 (25%) 0 0	59, 73, 80, 83	0
49	1r	68/88 (77%)	0.82	10 (14%) 2 1	52, 64, 78, 81	0
49	2r	68/88 (77%)	-0.06	0 100 100	60, 74, 83, 87	0
50	1s	83/93 (89%)	1.20	14 (16%) 1 1	66, 75, 83, 95	0
50	2s	83/93 (89%)	2.47	47 (56%) 0 0	70, 78, 85, 96	0
51	1t	96/106 (90%)	1.43	29 (30%) 0 0	57, 70, 82, 88	0
51	2t	96/106 (90%)	0.88	13 (13%) 3 2	59, 70, 83, 85	0
52	1u	23/27 (85%)	0.61	2 (8%) 10 8	64, 70, 77, 79	0
52	2u	23/27 (85%)	2.32	14 (60%) 0 0	68, 74, 78, 81	0
53	1v	14/27 (51%)	0.80	3 (21%) 0 1	51, 71, 93, 96	0
53	2v	13/27 (48%)	0.61	0 100 100	56, 68, 87, 96	0
54	1w	67/76 (88%)	2.47	34 (50%) 0 0	62, 87, 96, 105	0
54	1y	67/76 (88%)	1.59	21 (31%) 0 0	41, 93, 98, 100	0
54	2w	66/76 (86%)	2.60	37 (56%) 0 0	66, 88, 96, 99	0
54	2y	66/76 (86%)	1.54	24 (36%) 0 0	44, 94, 99, 100	0
55	1x	72/77 (93%)	0.90	8 (11%) 5 3	25, 59, 82, 92	0
55	2x	72/77 (93%)	0.71	5 (6%) 16 13	43, 79, 90, 94	0
All	All	20877/21754 (95%)	0.31	1277 (6%) 21 18	19, 62, 88, 106	0

All (1277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	1w	20	U	12.5
22	20	2	ALA	11.9

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Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	11.6
1	1A	885	C	11.4
22	10	7	LEU	10.9
22	20	3	HIS	10.5
1	1A	884	C	10.4
22	10	2	ALA	10.4
26	24	50	VAL	10.3
1	1A	896	A	9.9
22	10	6	GLY	9.5
7	2H	45	VAL	9.4
44	2m	123	ALA	9.3
22	20	7	LEU	9.2
22	10	5	LYS	9.0
38	2g	83	ALA	8.9
21	2Z	155	LEU	8.9
26	24	49	PHE	8.9
1	1A	883	G	8.8
1	2A	896	A	8.6
54	2w	76	A	8.4
38	1g	83	ALA	8.3
6	2G	48	GLU	8.2
22	10	3	HIS	8.1
44	2m	4	ILE	8.0
54	1w	73	A	8.0
54	1w	44	G	7.9
26	24	63	TYR	7.8
26	24	56	VAL	7.7
1	1A	887	A	7.6
38	2g	81	GLY	7.6
1	2A	888	C	7.6
1	2A	1509	C	7.4
32	1a	1030(B)	C	7.4
6	2G	139	LEU	7.4
50	2s	71	LEU	7.4
54	2w	75	C	7.3
44	2m	124	PRO	7.3
44	2m	5	ALA	7.3
6	2G	2	PRO	7.2
32	1a	1030(D)	A	7.2
21	2Z	141	VAL	7.2
21	2Z	144	LEU	7.1
50	2s	69	HIS	7.1

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Mol	Chain	Res	Type	RSRZ
44	2m	90	LEU	7.1
1	1A	888	C	7.1
38	1g	85	TYR	7.0
26	24	40	HIS	7.0
21	1Z	1	MET	7.0
22	20	5	LYS	7.0
26	24	45	GLY	6.9
45	2n	35	ARG	6.9
45	2n	34	TYR	6.9
45	2n	39	LEU	6.9
26	24	57	GLU	6.8
54	2w	71	G	6.8
6	2G	140	ILE	6.8
26	24	53	GLU	6.8
38	2g	82	GLY	6.8
43	2l	64	TYR	6.7
22	20	4	LYS	6.7
1	2A	884	C	6.7
6	2G	152	LEU	6.7
1	1A	897	C	6.6
54	1w	74	C	6.6
26	24	68	ARG	6.6
7	2H	49	VAL	6.6
1	1A	1509	C	6.6
26	24	51	ASP	6.5
32	2a	1030(B)	C	6.5
6	1G	49	ASP	6.5
1	2A	883	G	6.5
1	2A	885	C	6.4
38	1g	80	VAL	6.4
38	1g	81	GLY	6.4
21	2Z	170	THR	6.4
54	2w	73	A	6.3
21	1Z	149	SER	6.3
44	1m	124	PRO	6.3
50	2s	27	GLU	6.2
7	2H	44	VAL	6.2
6	2G	157	ILE	6.2
1	1A	1078	U	6.2
29	27	48	LYS	6.2
54	1w	72	C	6.2
26	24	59	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
44	2m	102	ARG	6.1
54	1w	70	G	6.1
6	2G	62	LEU	6.1
34	2c	87	LEU	6.1
7	2H	6	ARG	6.1
1	2A	886	C	6.0
21	1Z	168	GLU	6.0
44	2m	78	ILE	6.0
23	11	2	SER	6.0
44	2m	92	HIS	6.0
6	2G	144	ILE	6.0
45	2n	25	VAL	5.9
6	2G	146	TYR	5.9
1	2A	2155	G	5.9
7	2H	51	ARG	5.9
55	1x	47	U	5.9
21	2Z	140	ASP	5.9
54	1w	76	A	5.8
54	2w	1	G	5.8
54	1w	71	G	5.8
50	2s	35	SER	5.7
21	2Z	4	ARG	5.7
22	20	6	GLY	5.7
54	2w	44	G	5.7
7	2H	13	LYS	5.7
1	1A	1064	C	5.7
1	1A	882	G	5.7
6	2G	149	VAL	5.6
44	2m	12	ASN	5.6
22	10	4	LYS	5.6
3	1D	275	LYS	5.6
44	2m	60	VAL	5.5
1	1A	898	C	5.5
44	2m	23	TYR	5.5
1	2A	887	A	5.5
23	21	2	SER	5.4
1	1A	886	C	5.4
44	2m	66	LEU	5.4
6	2G	34	LEU	5.4
54	2w	70	G	5.4
54	2w	74	C	5.4
32	1a	1030(A)	G	5.4

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Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	5.4
6	1G	146	TYR	5.4
6	2G	28	VAL	5.3
50	2s	13	ASP	5.3
54	2w	45	U	5.3
26	24	32	TYR	5.3
6	2G	135	LEU	5.3
29	27	46	VAL	5.3
32	1a	1030(C)	G	5.3
44	2m	7	VAL	5.3
51	1t	47	GLY	5.3
38	2g	85	TYR	5.3
1	1A	895	U	5.3
32	2a	1034	G	5.3
44	2m	94	ARG	5.2
6	2G	115	ARG	5.2
21	2Z	122	ARG	5.2
7	2H	72	ILE	5.2
21	2Z	147	GLY	5.2
21	2Z	153	SER	5.2
54	2w	72	C	5.2
6	2G	136	ARG	5.2
21	2Z	50	GLN	5.2
34	2c	155	GLY	5.1
6	2G	19	LEU	5.1
55	1x	67	C	5.1
54	2w	14	A	5.1
26	24	19	GLY	5.1
32	1a	1031	G	5.1
21	2Z	139	VAL	5.1
50	1s	60	VAL	5.1
26	24	42	PHE	5.0
54	1y	35	A	5.0
54	2w	13	C	5.0
52	2u	16	GLY	5.0
44	2m	57	ARG	5.0
1	1A	1066	U	5.0
38	1g	79	ARG	4.9
6	2G	3	LEU	4.9
21	2Z	137	ILE	4.9
1	1A	1508	A	4.9
1	2A	2154	G	4.9

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Mol	Chain	Res	Type	RSRZ
45	2n	38	GLY	4.9
1	1A	1057	A	4.9
7	2H	35	VAL	4.9
21	1Z	100	VAL	4.9
50	2s	15	LEU	4.9
21	2Z	151	HIS	4.9
44	2m	77	ASN	4.9
21	2Z	161	VAL	4.8
1	1A	1081	U	4.8
44	2m	122	LYS	4.8
21	2Z	173	ALA	4.8
54	1y	36	A	4.8
35	2d	158	ILE	4.8
44	2m	6	GLY	4.8
34	2c	51	GLY	4.8
20	2Y	1	MET	4.8
32	2a	1036	G	4.8
50	2s	14	HIS	4.8
21	2Z	106	GLY	4.8
6	1G	48	GLU	4.8
32	2a	1030(A)	G	4.8
34	2c	101	LEU	4.8
38	2g	84	ASN	4.7
21	2Z	96	VAL	4.7
32	1a	1030	C	4.7
34	2c	8	ILE	4.7
54	1w	75	C	4.7
21	2Z	156	LYS	4.7
45	2n	53	LEU	4.7
21	2Z	51	ALA	4.7
21	2Z	53	ILE	4.7
54	1y	47	U	4.7
21	1Z	104	PHE	4.7
7	2H	115	VAL	4.7
44	2m	96	LEU	4.7
42	2k	13	GLN	4.7
32	1a	1027	C	4.7
51	1t	95	ALA	4.7
40	2i	115	GLY	4.7
1	1A	1087	G	4.6
6	2G	133	LEU	4.6
21	1Z	122	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
52	2u	24	ARG	4.6
34	2c	91	LEU	4.6
54	1y	45	U	4.6
44	2m	65	LYS	4.6
50	2s	47	HIS	4.6
44	2m	87	TYR	4.6
44	2m	120	LYS	4.6
3	2D	2	ALA	4.6
21	2Z	48	PHE	4.6
6	2G	181	ARG	4.5
26	24	52	THR	4.5
50	2s	80	TYR	4.5
6	2G	35	GLU	4.5
50	2s	24	ALA	4.5
44	2m	84	ILE	4.5
44	2m	76	ALA	4.5
50	2s	81	ARG	4.5
52	2u	11	GLY	4.5
5	2F	21	ALA	4.5
6	2G	37	VAL	4.5
21	1Z	152	ALA	4.5
12	2Q	63	LYS	4.5
7	2H	46	GLU	4.4
44	2m	71	ARG	4.4
50	2s	41	VAL	4.4
54	2y	53	G	4.4
29	27	47	ARG	4.4
54	2y	36	A	4.4
21	1Z	151	HIS	4.4
26	24	43	TYR	4.4
50	2s	62	ILE	4.4
6	2G	41	GLN	4.4
21	1Z	66	SER	4.4
44	2m	88	ARG	4.4
52	2u	17	THR	4.4
45	2n	42	ILE	4.4
26	24	54	GLY	4.3
45	2n	54	PRO	4.3
21	2Z	150	LEU	4.3
1	1A	881	G	4.3
1	2A	881	G	4.3
22	10	8	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
38	2g	154	TYR	4.3
21	2Z	68	PRO	4.3
1	1A	892	G	4.3
41	2j	88	LEU	4.3
21	2Z	152	ALA	4.3
34	2c	124	ILE	4.3
1	1A	1058	G	4.3
54	2y	47	U	4.3
45	2n	12	ARG	4.2
20	2Y	106	LEU	4.2
1	2A	882	G	4.2
1	1A	1077	A	4.2
38	1g	156	TRP	4.2
44	2m	24	GLY	4.2
1	1A	1097	U	4.2
1	2A	890	A	4.2
43	2l	28	LYS	4.2
6	2G	178	PHE	4.2
21	2Z	121	HIS	4.2
50	2s	52	TYR	4.2
1	1A	894	C	4.2
1	1A	1059	G	4.2
54	2y	22	G	4.2
48	2q	23	VAL	4.2
21	2Z	102	LEU	4.2
44	2m	75	ALA	4.2
19	2X	92	LEU	4.1
3	2D	276	LYS	4.1
21	1Z	170	THR	4.1
7	2H	82	GLY	4.1
3	2D	38	LYS	4.1
51	2t	55	ILE	4.1
54	1y	24	G	4.1
44	2m	72	ALA	4.1
42	2k	49	GLY	4.1
21	1Z	171	ILE	4.1
21	1Z	169	GLU	4.1
1	2A	899	A	4.1
1	2A	2173	A	4.1
51	1t	100	ILE	4.1
6	2G	102	PHE	4.1
6	2G	80	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
6	2G	151	ALA	4.1
45	2n	31	ARG	4.0
6	1G	139	LEU	4.0
26	24	18	CYS	4.0
1	1A	1082	U	4.0
51	1t	83	ARG	4.0
52	2u	6	ARG	4.0
21	2Z	146	ILE	4.0
35	2d	152	SER	4.0
54	2w	4	C	4.0
44	2m	61	GLU	4.0
54	2y	52	G	4.0
36	2e	17	ALA	4.0
6	2G	138	GLN	4.0
44	2m	101	GLN	4.0
1	1A	1176	G	4.0
34	2c	185	GLY	4.0
21	2Z	91	LEU	4.0
44	2m	56	LEU	4.0
50	2s	79	THR	4.0
34	2c	49	SER	4.0
54	2w	47	U	4.0
1	2A	892	G	4.0
7	2H	52	VAL	4.0
41	2j	65	LEU	3.9
6	2G	113	ARG	3.9
44	2m	15	VAL	3.9
26	24	44	THR	3.9
26	24	67	TYR	3.9
44	2m	67	GLU	3.9
38	1g	155	ARG	3.9
6	2G	141	PHE	3.9
1	1A	1076	C	3.9
54	2w	6	G	3.9
21	2Z	172	ALA	3.9
31	29	37	GLY	3.9
21	1Z	137	ILE	3.9
26	24	46	GLN	3.9
21	1Z	166	SER	3.9
32	2a	1030(C)	G	3.9
54	2w	15	G	3.9
54	2w	23	A	3.9

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Mol	Chain	Res	Type	RSRZ
21	2Z	148	ASP	3.8
54	1y	20	U	3.8
38	2g	80	VAL	3.8
54	1w	19	G	3.8
54	2w	69	G	3.8
12	2Q	33	GLY	3.8
35	2d	110	PHE	3.8
44	2m	42	ALA	3.8
44	1m	90	LEU	3.8
1	2A	2166	G	3.7
1	1A	1080	C	3.7
54	1y	13	C	3.7
55	2x	47	U	3.7
38	1g	84	ASN	3.7
44	2m	93	ARG	3.7
6	2G	161	THR	3.7
21	2Z	1	MET	3.7
12	1Q	60	ARG	3.7
54	2y	45	U	3.7
1	1A	889	C	3.7
54	1w	15	G	3.7
6	2G	43	LEU	3.7
21	2Z	125	LEU	3.7
1	1A	1084	A	3.7
12	2Q	6	ARG	3.7
32	2a	1001(A)	G	3.7
6	1G	51	ARG	3.7
34	2c	55	VAL	3.7
54	1y	23	A	3.7
29	27	1	MET	3.7
32	2a	1257	U	3.7
51	1t	45	GLN	3.7
45	2n	10	ALA	3.7
6	2G	116	ASP	3.7
7	2H	2	SER	3.7
35	2d	166	LYS	3.7
50	1s	28	LYS	3.7
7	2H	8	PRO	3.7
21	2Z	49	ARG	3.6
21	1Z	141	VAL	3.6
35	2d	167	GLY	3.6
38	1g	154	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
6	2G	155	MET	3.6
12	2Q	5	ARG	3.6
45	2n	37	PHE	3.6
50	1s	15	LEU	3.6
21	1Z	161	VAL	3.6
34	2c	184	TYR	3.6
44	2m	8	GLU	3.6
38	2g	32	ARG	3.6
21	1Z	156	LYS	3.6
54	1w	1	G	3.6
1	1A	1095	A	3.6
21	2Z	46	LYS	3.6
50	2s	16	LEU	3.6
6	2G	42	GLY	3.6
1	2A	2165	G	3.6
21	2Z	169	GLU	3.6
35	2d	180	GLY	3.6
12	2Q	60	ARG	3.6
26	24	13	ARG	3.6
1	2A	897	C	3.6
12	2Q	22	LYS	3.6
21	2Z	154	ASP	3.6
21	2Z	71	VAL	3.6
50	2s	51	VAL	3.6
50	1s	27	GLU	3.6
7	2H	138	LYS	3.6
26	24	58	ARG	3.6
34	2c	189	ALA	3.6
21	2Z	124	ILE	3.6
1	2A	889	C	3.6
20	2Y	55	TYR	3.6
21	2Z	162	GLU	3.6
38	1g	86	GLN	3.6
32	1a	1025	U	3.6
54	1w	5	G	3.6
54	2w	10	G	3.6
21	2Z	126	VAL	3.6
6	2G	134	GLY	3.6
44	2m	13	LYS	3.6
34	2c	196	LEU	3.6
44	2m	80	ARG	3.5
44	2m	64	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
50	2s	32	LYS	3.5
50	2s	38	SER	3.5
21	1Z	124	ILE	3.5
26	24	15	ILE	3.5
44	2m	97	PRO	3.5
21	1Z	147	GLY	3.5
25	23	26	LEU	3.5
6	2G	137	GLU	3.5
32	1a	1001(A)	G	3.5
29	27	45	ALA	3.5
26	24	55	ARG	3.5
48	2q	77	VAL	3.5
50	2s	49	ILE	3.5
42	1k	25	TYR	3.5
1	1A	1063	G	3.5
5	2F	15	SER	3.5
19	2X	68	ARG	3.5
54	1w	10	G	3.5
54	2y	35	A	3.5
6	2G	112	PRO	3.5
1	1A	1065	U	3.5
50	2s	12	ASP	3.5
12	2Q	20	ALA	3.5
6	2G	39	ILE	3.5
21	1Z	139	VAL	3.5
35	2d	176	LEU	3.5
51	1t	38	LYS	3.5
52	2u	23	PRO	3.5
51	1t	80	ARG	3.5
43	1l	64	TYR	3.5
5	2F	12	LEU	3.5
7	2H	105	LEU	3.5
26	24	31	ILE	3.5
54	1w	3	C	3.4
34	2c	182	ILE	3.4
51	1t	55	ILE	3.4
1	2A	880	G	3.4
1	2A	2127	G	3.4
34	2c	198	VAL	3.4
44	2m	70	LEU	3.4
54	2y	19	G	3.4
35	2d	160	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
49	1r	42	ARG	3.4
51	2t	9	ASN	3.4
7	2H	7	LEU	3.4
21	2Z	104	PHE	3.4
34	2c	22	TRP	3.4
6	2G	12	TYR	3.4
54	2y	59	U	3.4
1	1A	1075	C	3.4
22	20	8	GLY	3.4
26	14	54	GLY	3.4
1	2A	2153	G	3.4
6	2G	7	LEU	3.4
26	24	35	VAL	3.4
21	2Z	57	ILE	3.4
1	1A	899	A	3.4
1	2A	2159	G	3.4
40	2i	124	GLN	3.4
48	2q	65	ILE	3.4
48	2q	84	LEU	3.4
50	2s	84	GLY	3.4
12	2Q	104	PHE	3.3
54	1w	57	G	3.3
26	14	51	ASP	3.3
21	1Z	138	GLU	3.3
7	2H	37	VAL	3.3
44	2m	54	VAL	3.3
1	2A	2116	G	3.3
1	2A	2157	G	3.3
54	1w	45	U	3.3
7	2H	41	MET	3.3
12	1Q	61	GLY	3.3
35	1d	167	GLY	3.3
6	2G	159	VAL	3.3
7	2H	19	VAL	3.3
21	2Z	128	VAL	3.3
6	2G	169	ALA	3.3
54	2w	19	G	3.3
54	2w	49	C	3.3
38	2g	147	ALA	3.3
44	2m	68	GLY	3.3
54	1y	12	U	3.3
5	1F	15	SER	3.3

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Mol	Chain	Res	Type	RSRZ
40	2i	36	TYR	3.3
6	2G	179	PRO	3.3
49	1r	85	LEU	3.3
7	2H	43	VAL	3.3
21	2Z	56	VAL	3.3
43	2l	39	VAL	3.3
45	2n	7	ILE	3.3
44	2m	73	GLU	3.3
1	2A	2131	G	3.3
32	1a	1003	G	3.3
36	2e	12	LEU	3.3
21	2Z	149	SER	3.2
54	1w	13	C	3.2
43	2l	95	GLY	3.2
7	2H	47	GLU	3.2
6	2G	156	ASP	3.2
21	2Z	24	LEU	3.2
50	2s	45	VAL	3.2
1	2A	2174	C	3.2
20	2Y	75	ILE	3.2
6	2G	29	TRP	3.2
7	2H	36	PRO	3.2
32	2a	1030	C	3.2
48	2q	90	ILE	3.2
45	2n	50	LYS	3.2
21	2Z	99	TYR	3.2
21	1Z	148	ASP	3.2
1	2A	2156	G	3.2
21	2Z	55	HIS	3.2
29	27	23	ARG	3.2
1	1A	879	G	3.2
29	17	48	LYS	3.2
5	2F	145	GLU	3.2
43	2l	69	TYR	3.2
21	2Z	163	LEU	3.2
35	2d	188	LEU	3.2
38	2g	115	ARG	3.2
50	2s	48	THR	3.2
1	2A	1719	G	3.2
1	2A	2125	G	3.2
21	2Z	157	LEU	3.2
50	2s	30	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
38	1g	153	HIS	3.1
1	2A	2167	U	3.1
35	2d	157	LEU	3.1
44	2m	110	ARG	3.1
6	2G	15	VAL	3.1
6	2G	109	VAL	3.1
32	1a	1257	U	3.1
40	2i	109	VAL	3.1
12	1Q	79	LEU	3.1
32	1a	1029	C	3.1
38	2g	119	ARG	3.1
45	2n	29	ARG	3.1
44	2m	48	LEU	3.1
20	2Y	91	GLU	3.1
51	1t	68	LYS	3.1
12	1Q	81	VAL	3.1
6	2G	51	ARG	3.1
34	2c	80	GLY	3.1
6	2G	114	ILE	3.1
21	2Z	93	ASP	3.1
7	2H	123	PHE	3.1
52	2u	22	ARG	3.1
1	1A	271(K)	U	3.1
7	2H	10	PRO	3.1
34	2c	45	LYS	3.1
50	2s	53	ASN	3.1
7	2H	9	ILE	3.1
36	2e	13	ILE	3.1
54	2w	5	G	3.1
51	2t	86	ARG	3.1
34	2c	199	LYS	3.1
48	2q	11	VAL	3.1
34	2c	65	ALA	3.1
1	1A	1060	U	3.1
6	2G	95	ARG	3.1
32	1a	204	U	3.1
50	2s	28	LYS	3.1
6	1G	76	SER	3.1
12	2Q	2	LEU	3.1
21	2Z	95	PRO	3.1
21	2Z	133	ILE	3.1
44	2m	25	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
7	2H	159	GLU	3.1
21	2Z	138	GLU	3.1
21	2Z	145	GLU	3.1
12	1Q	112	GLU	3.0
34	2c	50	ALA	3.0
51	1t	42	GLN	3.0
54	1w	2	C	3.0
54	2w	2	C	3.0
54	2y	23	A	3.0
21	2Z	143	GLY	3.0
50	1s	18	LYS	3.0
5	2F	20	LEU	3.0
10	2O	49	ARG	3.0
48	2q	22	LEU	3.0
12	2Q	66	ILE	3.0
44	2m	39	ILE	3.0
47	1p	38	TYR	3.0
48	2q	42	TYR	3.0
7	2H	30	LYS	3.0
32	2a	1035	A	3.0
54	1y	21	A	3.0
44	2m	19	LEU	3.0
1	2A	2133	G	3.0
51	1t	74	LYS	3.0
54	1w	69	G	3.0
44	2m	74	VAL	3.0
49	1r	76	LEU	3.0
51	2t	13	LEU	3.0
51	1t	86	ARG	3.0
32	2a	1033	G	3.0
6	2G	173	LEU	3.0
6	2G	182	LYS	3.0
12	2Q	121	ALA	3.0
5	2F	131	GLY	3.0
34	2c	158	GLY	3.0
54	1w	21	A	3.0
54	2w	9	A	3.0
6	2G	58	GLN	3.0
34	2c	186	PHE	3.0
21	1Z	39	VAL	3.0
21	2Z	59	LEU	3.0
21	2Z	70	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
7	2H	48	GLY	3.0
54	1w	25	C	3.0
7	2H	3	ARG	3.0
1	1A	878	A	3.0
7	2H	25	LYS	3.0
44	2m	63	THR	3.0
6	2G	176	LEU	3.0
50	2s	82	GLY	3.0
6	2G	6	ALA	3.0
1	2A	1744	C	2.9
34	2c	57	ILE	2.9
1	1A	1175	U	2.9
21	1Z	121	HIS	2.9
51	1t	72	LEU	2.9
45	2n	11	LYS	2.9
26	14	52	THR	2.9
32	1a	1032	G	2.9
6	2G	90	LEU	2.9
12	1Q	59	ARG	2.9
34	2c	190	ARG	2.9
36	2e	10	MET	2.9
38	1g	78	ARG	2.9
48	2q	71	PHE	2.9
1	2A	898	C	2.9
34	2c	193	TYR	2.9
12	2Q	106	VAL	2.9
26	14	50	VAL	2.9
21	2Z	167	PRO	2.9
54	2w	22	G	2.9
54	1y	14	A	2.9
40	2i	125	TYR	2.9
50	2s	67	VAL	2.9
52	2u	21	TYR	2.9
6	2G	59	GLU	2.9
7	2H	128	PRO	2.9
32	1a	1002	G	2.9
1	2A	2158	A	2.9
34	2c	13	GLY	2.9
46	1o	89	GLY	2.9
48	2q	66	SER	2.9
54	2w	21	A	2.9
21	2Z	9	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
38	2g	156	TRP	2.9
54	1w	4	C	2.9
50	2s	54	GLY	2.9
1	2A	2160	G	2.9
7	2H	50	VAL	2.9
21	2Z	38	TYR	2.9
44	2m	17	VAL	2.9
50	2s	66	MET	2.9
45	2n	30	ALA	2.9
7	2H	23	ARG	2.9
12	2Q	59	ARG	2.9
38	2g	79	ARG	2.9
21	1Z	136	PHE	2.9
20	2Y	63	LYS	2.9
34	2c	64	VAL	2.9
41	2j	44	VAL	2.9
52	2u	10	ARG	2.9
55	2x	46	G	2.9
1	1A	1096	A	2.8
44	2m	9	ILE	2.8
1	2A	2146	C	2.8
45	2n	27	CYS	2.8
48	2q	80	GLY	2.8
54	2y	64	A	2.8
1	2A	2128	C	2.8
21	1Z	140	ASP	2.8
55	1x	66	C	2.8
34	2c	72	LYS	2.8
38	2g	109	ASN	2.8
44	2m	82	MET	2.8
44	2m	106	ASN	2.8
50	2s	65	ASN	2.8
6	2G	11	TYR	2.8
1	2A	2132	U	2.8
21	1Z	165	VAL	2.8
42	2k	94	ALA	2.8
54	2w	68	C	2.8
48	2q	92	ARG	2.8
7	2H	4	ILE	2.8
3	2D	37	LEU	2.8
1	2A	1508	A	2.8
1	2A	2126	A	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2793	G	2.8
12	2Q	136	ALA	2.8
32	1a	1036	G	2.8
32	1a	1531	A	2.8
54	2w	58	A	2.8
12	1Q	5	ARG	2.8
12	1Q	10	ARG	2.8
46	1o	68	ARG	2.8
6	2G	100	TRP	2.8
23	11	98	LEU	2.8
12	2Q	61	GLY	2.8
43	2l	68	ALA	2.8
9	2N	8	GLN	2.8
54	1y	27	G	2.8
54	2y	65	G	2.8
26	24	9	LEU	2.8
45	2n	36	PHE	2.8
6	2G	177	GLY	2.8
6	1G	75	LYS	2.8
6	1G	182	LYS	2.8
6	2G	175	LEU	2.8
20	2Y	89	PHE	2.8
21	1Z	155	LEU	2.8
54	1w	6	G	2.8
6	2G	118	ARG	2.8
10	2O	51	ALA	2.7
21	1Z	102	LEU	2.7
48	2q	100	LYS	2.7
41	2j	10	GLY	2.7
49	1r	79	LEU	2.7
6	1G	77	ILE	2.7
6	2G	22	ARG	2.7
41	2j	66	ARG	2.7
43	2l	59	ARG	2.7
7	2H	86	GLU	2.7
32	2a	1021	G	2.7
54	1w	56	C	2.7
6	2G	154	GLY	2.7
12	2Q	64	ILE	2.7
6	2G	145	THR	2.7
50	2s	77	THR	2.7
1	1A	1069	A	2.7

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Mol	Chain	Res	Type	RSRZ
43	2l	40	VAL	2.7
50	2s	58	VAL	2.7
45	2n	6	LEU	2.7
3	2D	4	LYS	2.7
41	2j	48	THR	2.7
7	2H	24	VAL	2.7
7	2H	169	VAL	2.7
26	24	34	GLU	2.7
54	2w	48	C	2.7
25	23	23	LEU	2.7
52	2u	14	TRP	2.7
6	2G	142	PRO	2.7
43	2l	56	ALA	2.7
6	2G	148	MET	2.7
50	1s	21	GLU	2.7
12	2Q	19	GLY	2.7
26	14	45	GLY	2.7
6	2G	23	PHE	2.7
40	2i	19	LEU	2.7
32	2a	1224	G	2.7
28	16	28	ARG	2.7
12	2Q	109	VAL	2.7
38	1g	89	MET	2.7
50	2s	44	MET	2.7
21	1Z	125	LEU	2.7
21	2Z	89	PHE	2.7
21	2Z	171	ILE	2.7
1	2A	1536	C	2.7
50	2s	29	ARG	2.7
34	2c	194	GLY	2.7
1	1A	1068	G	2.7
1	2A	879	G	2.7
21	1Z	146	ILE	2.7
26	14	55	ARG	2.7
26	14	68	ARG	2.7
43	2l	7	ILE	2.7
44	2m	104	ARG	2.7
45	2n	17	LYS	2.7
25	23	51	ALA	2.6
32	2a	1358	U	2.6
45	2n	51	GLY	2.6
54	2w	3	C	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	229	A	2.6
54	1y	38	A	2.6
6	2G	60	LEU	2.6
17	2V	35	LEU	2.6
49	1r	78	LEU	2.6
6	1G	80	PHE	2.6
12	2Q	32	TYR	2.6
6	1G	73	ALA	2.6
34	2c	53	ALA	2.6
41	2j	91	PRO	2.6
21	2Z	76	LEU	2.6
26	24	23	GLU	2.6
3	2D	275	LYS	2.6
21	2Z	88	PHE	2.6
54	2w	24	G	2.6
50	1s	58	VAL	2.6
54	2y	12	U	2.6
1	2A	1507	A	2.6
1	2A	1847	A	2.6
21	1Z	120	ILE	2.6
44	2m	95	GLY	2.6
44	2m	103	THR	2.6
38	1g	141	VAL	2.6
54	2y	6	G	2.6
48	2q	74	LEU	2.6
50	1s	71	LEU	2.6
1	2A	2161	C	2.6
34	2c	39	ILE	2.6
48	2q	59	ILE	2.6
10	2O	7	TYR	2.6
12	1Q	32	TYR	2.6
34	2c	60	ALA	2.6
1	1A	890	A	2.6
12	1Q	1	MET	2.6
21	2Z	5	LEU	2.6
7	2H	57	ASP	2.6
38	2g	77	SER	2.6
50	2s	43	GLU	2.6
7	2H	29	PRO	2.6
44	2m	11	ARG	2.6
47	1p	19	ILE	2.6
50	2s	34	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
34	2c	149	ALA	2.6
35	2d	170	VAL	2.6
46	2o	60	VAL	2.6
49	1r	40	LEU	2.6
54	2w	26	A	2.6
32	1a	1023	G	2.6
43	2l	94	PRO	2.6
42	1k	61	ALA	2.6
54	1w	48	C	2.6
55	1x	68	C	2.6
5	2F	196	LEU	2.6
35	2d	196	LEU	2.6
12	2Q	65	PHE	2.6
21	2Z	44	PHE	2.6
1	1A	1847	A	2.6
44	2m	91	ARG	2.6
21	2Z	62	PRO	2.5
21	2Z	101	PRO	2.5
44	2m	111	LYS	2.5
54	1w	47	U	2.5
12	2Q	53	ALA	2.5
45	2n	46	GLU	2.5
48	2q	58	GLU	2.5
12	1Q	2	LEU	2.5
42	1k	14	VAL	2.5
1	2A	2164	C	2.5
32	1a	1028	C	2.5
21	2Z	80	ARG	2.5
42	1k	64	ALA	2.5
44	1m	2	ALA	2.5
1	2A	2802	G	2.5
12	2Q	10	ARG	2.5
54	1y	34	G	2.5
54	2y	57	G	2.5
44	2m	69	GLU	2.5
34	2c	200	ALA	2.5
46	2o	87	ILE	2.5
21	1Z	150	LEU	2.5
32	2a	1286	A	2.5
34	2c	23	TYR	2.5
34	2c	52	LEU	2.5
44	2m	121	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
12	2Q	29	PHE	2.5
32	2a	1309	G	2.5
7	2H	121	ILE	2.5
38	2g	152	ALA	2.5
34	2c	21	ARG	2.5
44	2m	100	GLY	2.5
6	2G	131	TYR	2.5
16	2U	90	VAL	2.5
34	1c	87	LEU	2.5
46	1o	78	TYR	2.5
48	2q	60	ILE	2.5
50	2s	40	ILE	2.5
54	2y	56	C	2.5
55	2x	70	G	2.5
5	2F	140	LEU	2.5
51	1t	53	LEU	2.5
6	2G	117	PHE	2.5
6	2G	121	ASN	2.5
1	2A	878	A	2.5
12	2Q	28	ALA	2.5
51	1t	52	ALA	2.5
21	1Z	163	LEU	2.5
32	2a	1325	C	2.5
19	2X	69	TYR	2.5
32	2a	1003	G	2.5
35	2d	20	TYR	2.5
21	2Z	136	PHE	2.5
1	1A	1963	U	2.5
21	1Z	123	ASP	2.5
26	24	5	ILE	2.5
7	1H	7	LEU	2.5
21	1Z	157	LEU	2.5
50	1s	32	LYS	2.5
12	1Q	55	VAL	2.5
48	1q	11	VAL	2.5
41	2j	47	PHE	2.5
54	1y	56	C	2.5
1	1A	1094	U	2.4
44	2m	10	PRO	2.4
21	2Z	21	ALA	2.4
50	1s	48	THR	2.4
21	1Z	18	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
21	1Z	61	LEU	2.4
51	2t	62	LEU	2.4
51	2t	100	ILE	2.4
35	2d	115	ARG	2.4
54	2y	21	A	2.4
26	14	53	GLU	2.4
5	1F	16	GLY	2.4
44	2m	119	GLY	2.4
1	1A	2131	G	2.4
34	2c	187	ALA	2.4
54	1w	24	G	2.4
54	1y	44	G	2.4
54	2y	44	G	2.4
21	1Z	133	ILE	2.4
35	2d	174	LEU	2.4
43	2l	60	LEU	2.4
46	1o	87	ILE	2.4
21	2Z	60	GLU	2.4
42	1k	92	GLU	2.4
1	2A	894	C	2.4
32	2a	1029	C	2.4
21	1Z	70	LEU	2.4
21	2Z	33	LEU	2.4
1	1A	1074	G	2.4
1	2A	2124	G	2.4
45	2n	58	LYS	2.4
54	1y	22	G	2.4
54	2y	5	G	2.4
50	1s	61	TYR	2.4
34	2c	59	ARG	2.4
52	1u	6	ARG	2.4
5	2F	172	TRP	2.4
6	2G	180	PHE	2.4
32	1a	1026	G	2.4
5	1F	14	PRO	2.4
36	2e	107	ARG	2.4
45	1n	2	ALA	2.4
43	2l	100	ILE	2.4
53	1v	13	A	2.4
34	2c	74	GLY	2.4
38	2g	135	VAL	2.4
1	1A	1093	G	2.4

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Mol	Chain	Res	Type	RSRZ
6	2G	106	LEU	2.4
50	1s	30	LEU	2.4
50	2s	63	THR	2.4
54	2y	34	G	2.4
55	1x	70	G	2.4
51	2t	42	GLN	2.4
16	2U	88	ILE	2.4
35	2d	146	ILE	2.4
18	2W	112	GLY	2.4
38	2g	130	GLY	2.4
50	2s	23	ASN	2.4
27	15	60	VAL	2.4
1	1A	1070	A	2.4
53	1v	14	A	2.4
1	2A	1040	C	2.4
1	2A	1041	C	2.4
26	24	41	PRO	2.4
40	2i	123	PRO	2.4
20	2Y	90	LEU	2.4
21	1Z	69	THR	2.4
38	2g	116	ALA	2.4
38	2g	117	ALA	2.4
44	2m	105	THR	2.4
32	1a	1024	G	2.4
52	2u	13	ILE	2.4
21	2Z	79	ARG	2.4
51	2t	80	ARG	2.4
1	2A	2169	A	2.3
38	1g	73	MET	2.3
5	1F	21	ALA	2.3
34	2c	160	ALA	2.3
21	2Z	11	GLU	2.3
54	1y	5	G	2.3
6	1G	86	MET	2.3
45	2n	49	HIS	2.3
54	2y	51	U	2.3
48	2q	6	LEU	2.3
7	2H	14	GLY	2.3
42	1k	49	GLY	2.3
50	1s	84	GLY	2.3
54	1w	7	A	2.3
54	2w	61	C	2.3

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Mol	Chain	Res	Type	RSRZ
54	2y	62	C	2.3
51	2t	83	ARG	2.3
50	1s	40	ILE	2.3
51	1t	63	ILE	2.3
6	2G	92	VAL	2.3
10	2O	52	VAL	2.3
26	14	59	PHE	2.3
31	29	16	VAL	2.3
6	2G	97	ASP	2.3
21	1Z	99	TYR	2.3
21	2Z	66	SER	2.3
1	1A	893	C	2.3
31	19	7	VAL	2.3
42	1k	42	TRP	2.3
52	2u	5	ASP	2.3
34	2c	85	ARG	2.3
35	2d	130	GLY	2.3
44	2m	108	ARG	2.3
50	2s	20	LEU	2.3
1	1A	2113	U	2.3
32	2a	1220	G	2.3
41	2j	50	ILE	2.3
1	1A	2140	C	2.3
54	1y	49	C	2.3
7	2H	32	GLU	2.3
54	1w	23	A	2.3
12	2Q	56	ARG	2.3
44	2m	3	ARG	2.3
17	1V	101	GLY	2.3
26	24	29	PRO	2.3
21	2Z	69	THR	2.3
38	2g	86	GLN	2.3
45	2n	13	THR	2.3
51	1t	32	ALA	2.3
52	2u	12	LYS	2.3
6	2G	88	ILE	2.3
34	2c	14	ILE	2.3
5	2F	132	VAL	2.3
26	24	48	ARG	2.3
12	2Q	37	LEU	2.3
54	2w	31	A	2.3
7	2H	34	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
12	2Q	47	ILE	2.3
11	2P	125	VAL	2.3
21	2Z	72	ARG	2.3
42	1k	96	ARG	2.3
6	2G	49	ASP	2.3
51	1t	69	GLY	2.3
47	2p	48	TRP	2.3
12	2Q	113	GLN	2.3
19	2X	66	LEU	2.3
51	1t	36	LEU	2.3
51	2t	99	LEU	2.3
44	2m	51	ALA	2.3
42	1k	50	TYR	2.3
40	2i	127	LYS	2.3
6	1G	149	VAL	2.3
26	24	7	PRO	2.2
7	2H	18	GLU	2.2
12	2Q	112	GLU	2.2
44	2m	107	ALA	2.2
1	1A	1100	C	2.2
22	20	11	ARG	2.2
35	2d	141	ARG	2.2
51	1t	79	ARG	2.2
55	2x	71	C	2.2
48	2q	27	PHE	2.2
21	1Z	126	VAL	2.2
32	2a	1227	A	2.2
50	2s	11	VAL	2.2
53	1v	12	A	2.2
50	2s	56	GLN	2.2
54	1w	12	U	2.2
17	2V	1	MET	2.2
35	2d	184	LYS	2.2
35	2d	49	ARG	2.2
21	2Z	8	TYR	2.2
6	2G	125	PHE	2.2
12	1Q	33	GLY	2.2
20	2Y	59	GLY	2.2
1	1A	2793	G	2.2
5	2F	199	TRP	2.2
32	1a	161	A	2.2
35	2d	186	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
43	1l	60	LEU	2.2
44	1m	96	LEU	2.2
44	1m	121	LYS	2.2
51	1t	84	LEU	2.2
51	1t	98	PRO	2.2
49	1r	54	ARG	2.2
34	2c	159	GLY	2.2
41	2j	63	PHE	2.2
39	2h	134	ILE	2.2
6	2G	67	LYS	2.2
48	2q	9	VAL	2.2
1	1A	1079	C	2.2
55	1x	69	C	2.2
50	2s	78	ARG	2.2
32	2a	1030(D)	A	2.2
26	24	60	GLN	2.2
26	14	32	TYR	2.2
10	2O	86	ILE	2.2
20	2Y	45	VAL	2.2
46	1o	82	ILE	2.2
51	2t	41	ILE	2.2
21	1Z	52	SER	2.2
4	2E	52	LEU	2.2
6	2G	120	LEU	2.2
54	1y	48	C	2.2
3	1D	2	ALA	2.2
10	2O	41	ALA	2.2
1	2A	2308	G	2.2
3	2D	5	LYS	2.2
20	2Y	57	GLN	2.2
34	2c	19	GLU	2.2
55	1x	46	G	2.2
43	2l	32	PHE	2.2
7	2H	107	VAL	2.2
34	2c	40	ARG	2.2
46	1o	88	ARG	2.2
48	1q	63	ARG	2.2
10	2O	48	PRO	2.2
21	1Z	159	PRO	2.2
34	2c	188	LEU	2.2
35	1d	157	LEU	2.2
49	1r	44	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	1G	46	ALA	2.2
34	2c	61	ALA	2.2
49	1r	24	ALA	2.2
54	2w	56	C	2.2
7	2H	69	ARG	2.2
21	2Z	131	ARG	2.2
1	2A	2162	G	2.2
32	1a	1033	G	2.2
34	2c	201	TYR	2.2
41	2j	72	VAL	2.2
51	1t	75	ASN	2.2
41	2j	55	LYS	2.2
54	2w	7	A	2.2
6	2G	32	PRO	2.2
5	1F	17	ARG	2.2
6	2G	170	ARG	2.2
42	2k	25	TYR	2.1
10	2O	19	ILE	2.1
14	2S	32	LEU	2.1
1	2A	2115	G	2.1
32	2a	1310	G	2.1
6	2G	33	ARG	2.1
43	2l	61	THR	2.1
51	2t	8	ARG	2.1
24	22	37	PHE	2.1
32	2a	1322	C	2.1
54	1y	67	C	2.1
54	2w	11	C	2.1
1	1A	1083	U	2.1
20	2Y	24	VAL	2.1
21	1Z	128	VAL	2.1
38	1g	42	ILE	2.1
38	2g	120	ILE	2.1
39	2h	83	ILE	2.1
48	1q	59	ILE	2.1
6	1G	90	LEU	2.1
46	1o	57	LEU	2.1
38	2g	78	ARG	2.1
38	1g	144	MET	2.1
51	1t	81	LYS	2.1
26	24	10	VAL	2.1
50	2s	60	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
8	2I	38	LEU	2.1
54	1w	68	C	2.1
44	1m	122	LYS	2.1
5	2F	127	GLU	2.1
45	2n	2	ALA	2.1
51	2t	77	ALA	2.1
35	2d	165	MET	2.1
21	2Z	81	ARG	2.1
34	1c	190	ARG	2.1
34	2c	17	ASP	2.1
44	2m	99	ARG	2.1
48	2q	19	VAL	2.1
34	2c	82	GLU	2.1
35	2d	179	GLU	2.1
52	1u	14	TRP	2.1
7	2H	74	ASN	2.1
44	2m	62	ASN	2.1
44	2m	27	LYS	2.1
6	2G	4	ASP	2.1
31	29	12	ASP	2.1
7	2H	76	VAL	2.1
7	2H	133	VAL	2.1
17	1V	35	LEU	2.1
21	1Z	53	ILE	2.1
21	2Z	100	VAL	2.1
34	2c	43	LEU	2.1
34	2c	204	LEU	2.1
38	1g	151	TYR	2.1
45	2n	44	LEU	2.1
1	2A	900	A	2.1
1	2A	2175	C	2.1
51	1t	58	LYS	2.1
52	2u	4	GLY	2.1
7	2H	71	LEU	2.1
41	2j	68	HIS	2.1
42	1k	63	LEU	2.1
12	2Q	68	ILE	2.1
44	1m	87	TYR	2.1
1	2A	2117	A	2.1
7	2H	165	ALA	2.1
54	1w	58	A	2.1
54	2y	15	G	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	54	ARG	2.1
26	24	24	THR	2.1
49	1r	25	THR	2.1
1	1A	2138	C	2.1
34	2c	44	GLU	2.1
34	2c	56	ASP	2.1
7	2H	67	LEU	2.1
35	2d	120	LEU	2.1
21	1Z	167	PRO	2.1
43	2l	85	ILE	2.1
51	1t	49	ALA	2.1
51	1t	89	ARG	2.1
1	1A	1067	A	2.1
1	1A	1088	A	2.1
6	1G	102	PHE	2.1
32	2a	161	A	2.1
32	2a	250	A	2.1
32	2a	1001	A	2.1
40	2i	116	LYS	2.0
48	2q	89	LEU	2.0
43	1l	43	VAL	2.0
51	1t	90	GLN	2.0
6	2G	150	ASP	2.0
21	2Z	166	SER	2.0
35	2d	2	GLY	2.0
45	2n	15	LYS	2.0
50	2s	6	LYS	2.0
1	2A	2114	A	2.0
1	1A	652(U)	G	2.0
10	2O	98	VAL	2.0
32	2a	1221	G	2.0
45	2n	33	VAL	2.0
10	2O	22	ILE	2.0
54	2y	49	C	2.0
55	1x	65	C	2.0
55	2x	68	C	2.0
6	2G	61	ALA	2.0
15	1T	126	ALA	2.0
21	2Z	26	GLY	2.0
21	2Z	52	SER	2.0
34	2c	78	GLY	2.0
34	2c	28	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
44	1m	82	MET	2.0
7	2H	101	ARG	2.0
7	2H	124	GLU	2.0
45	2n	45	ARG	2.0
38	1g	120	ILE	2.0
48	2q	24	GLU	2.0
6	2G	73	ALA	2.0
7	2H	157	TYR	2.0
48	2q	95	TYR	2.0
1	1A	2145	C	2.0
18	1W	112	GLY	2.0
54	1w	61	C	2.0
23	11	26	ARG	2.0
51	1t	13	LEU	2.0
48	2q	73	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	2y	55	20/21	0.55	0.38	83,99,115,129	0
54	5MU	2y	54	21/22	0.63	0.42	87,93,116,137	0
54	PSU	1y	55	20/21	0.73	0.19	82,98,110,129	0
54	4SU	2y	8	20/21	0.78	0.24	87,95,107,114	0
54	MIA	2y	37	22/30	0.80	0.25	68,80,89,112	0
54	5MU	1y	54	21/22	0.82	0.25	80,93,103,130	0
54	7MG	1y	46	24/25	0.83	0.32	81,93,105,133	0
54	7MG	2y	46	24/25	0.83	0.28	82,95,104,125	0
54	4SU	1y	8	20/21	0.84	0.23	84,90,107,112	0
54	PSU	2y	39	20/21	0.85	0.26	75,87,93,93	0
54	7MG	1w	46	24/25	0.86	0.24	71,81,95,125	0
54	7MG	2w	46	24/25	0.87	0.38	69,93,102,115	0
54	4SU	2w	8	20/21	0.87	0.28	64,91,96,98	0
54	PSU	2y	32	20/21	0.87	0.18	79,88,94,98	0
32	M2G	2a	966	25/26	0.88	0.19	45,64,88,101	0
54	PSU	2w	55	20/21	0.89	0.29	57,80,90,92	0
54	MIA	2w	37	22/30	0.89	0.21	49,73,85,86	0
55	4SU	2x	8	20/21	0.89	0.19	66,80,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MIA	1y	37	22/30	0.90	0.25	74,81,87,100	0
32	2MG	2a	1207	24/25	0.90	0.20	72,87,94,98	0
54	PSU	2w	32	20/21	0.91	0.25	63,79,90,93	0
32	5MC	2a	967	21/22	0.91	0.17	60,75,80,91	0
43	0TD	1l	92	10/11	0.92	0.21	44,58,62,69	0
54	PSU	1w	55	20/21	0.92	0.24	55,77,90,90	0
54	PSU	1y	39	20/21	0.92	0.29	73,85,90,93	0
54	PSU	1y	32	20/21	0.92	0.23	75,86,94,98	0
54	4SU	1w	8	20/21	0.92	0.20	70,77,91,94	0
54	5MU	2w	54	21/22	0.92	0.20	60,71,83,85	0
55	5MU	2x	54	21/22	0.92	0.22	69,81,87,96	0
55	PSU	2x	55	20/21	0.92	0.18	63,78,85,86	0
43	0TD	2l	92	10/11	0.93	0.22	50,61,67,77	0
32	7MG	2a	527	24/25	0.94	0.15	53,64,78,82	0
32	PSU	2a	516	20/21	0.94	0.13	56,64,70,74	0
32	4OC	2a	1402	22/23	0.94	0.15	49,66,75,76	0
32	MA6	2a	1519	24/25	0.94	0.19	45,65,75,82	0
54	PSU	2w	39	20/21	0.94	0.25	63,72,81,83	0
32	MA6	2a	1518	24/25	0.95	0.23	53,67,73,75	0
1	5MU	1A	1915	21/22	0.95	0.19	50,58,65,70	0
1	5MU	2A	1915	21/22	0.95	0.19	56,63,68,75	0
55	5MC	2x	32	21/22	0.95	0.18	66,71,79,82	0
55	5MU	1x	54	21/22	0.95	0.20	52,64,69,72	0
1	4OC	2A	1920	21/23	0.95	0.21	45,51,56,64	0
32	5MC	2a	1404	21/22	0.95	0.18	52,59,71,74	0
32	UR3	2a	1498	21/22	0.96	0.20	41,54,63,70	0
54	PSU	1w	32	20/21	0.96	0.17	59,74,84,92	0
1	5MC	2A	1962	21/22	0.96	0.17	34,40,48,53	0
1	PSU	2A	1911	20/21	0.96	0.16	40,51,56,58	0
32	5MC	2a	1400	21/22	0.96	0.17	61,72,78,82	0
55	4SU	1x	8	20/21	0.96	0.19	43,54,68,74	0
32	2MG	1a	1207	24/25	0.96	0.16	48,66,70,78	0
32	PSU	1a	516	20/21	0.96	0.16	53,61,67,70	0
54	5MU	1w	54	21/22	0.96	0.26	51,64,74,75	0
32	5MC	2a	1407	21/22	0.96	0.17	36,55,59,60	0
55	PSU	1x	55	20/21	0.96	0.19	51,62,74,75	0
54	PSU	1w	39	20/21	0.96	0.21	58,68,76,78	0
1	5MU	2A	1939	21/22	0.97	0.19	26,34,39,41	0
1	5MC	2A	1942	21/22	0.97	0.18	44,47,58,74	0
32	M2G	1a	966	25/26	0.97	0.17	37,51,54,61	0
1	PSU	1A	1917	20/21	0.97	0.22	47,53,60,62	0
32	4OC	1a	1402	22/23	0.97	0.18	33,44,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	1a	1404	21/22	0.97	0.20	23,37,50,52	0
32	5MC	1a	1407	21/22	0.97	0.20	27,38,45,47	0
1	4OC	1A	1920	21/23	0.97	0.24	38,47,52,61	0
55	5MC	1x	32	21/22	0.97	0.20	35,48,56,75	0
1	5MC	1A	1942	21/22	0.97	0.21	38,47,55,63	0
1	PSU	1A	1911	20/21	0.97	0.20	41,47,54,55	0
1	PSU	2A	1917	20/21	0.97	0.17	47,56,61,63	0
32	7MG	1a	527	24/25	0.97	0.14	33,43,56,62	0
54	MIA	1w	37	29/30	0.97	0.22	44,56,67,77	0
32	5MC	1a	1400	21/22	0.98	0.18	36,44,55,65	0
1	2MU	1A	2552	21/23	0.98	0.19	25,34,40,43	0
1	PSU	1A	2605	20/21	0.98	0.18	21,29,35,36	0
1	5MU	1A	1939	21/22	0.98	0.24	21,29,37,41	0
1	OMG	2A	2251	24/25	0.98	0.17	27,33,39,39	0
1	2MU	2A	2552	21/23	0.98	0.17	27,37,41,43	0
1	PSU	2A	2605	20/21	0.98	0.16	25,32,38,39	0
32	UR3	1a	1498	21/22	0.98	0.19	30,40,45,52	0
32	MA6	1a	1518	24/25	0.98	0.20	32,41,49,57	0
32	MA6	1a	1519	24/25	0.98	0.21	27,43,51,60	0
1	5MC	1A	1962	21/22	0.98	0.20	29,38,43,46	0
1	OMG	1A	2251	24/25	0.98	0.21	19,30,34,37	0
32	5MC	1a	967	21/22	0.98	0.18	42,51,61,68	0
1	2MA	1A	2503	23/24	0.98	0.22	17,22,30,33	0
1	2MA	2A	2503	23/24	0.99	0.19	21,25,31,36	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
56	MG	2A	3599	1/1	0.25	0.08	78,78,78,78	0
56	MG	1A	3388	1/1	0.37	0.17	55,55,55,55	0
56	MG	1A	3768	1/1	0.38	0.10	61,61,61,61	0
56	MG	1A	3799	1/1	0.41	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3767	1/1	0.50	0.22	63,63,63,63	0
56	MG	1A	3720	1/1	0.50	0.19	66,66,66,66	0
56	MG	2A	3575	1/1	0.53	0.11	62,62,62,62	0
56	MG	2A	3279	1/1	0.54	0.11	46,46,46,46	0
56	MG	2A	3087	1/1	0.55	0.22	69,69,69,69	0
56	MG	1B	218	1/1	0.55	0.24	64,64,64,64	0
56	MG	1A	3235	1/1	0.56	0.19	64,64,64,64	0
56	MG	1a	1819	1/1	0.56	0.09	91,91,91,91	0
56	MG	2a	1745	1/1	0.56	0.26	72,72,72,72	0
56	MG	2a	1793	1/1	0.56	0.19	86,86,86,86	0
56	MG	2f	3002	1/1	0.56	0.17	85,85,85,85	0
59	ZN	2n	501	1/1	0.56	0.17	152,152,152,152	0
56	MG	2A	3547	1/1	0.57	0.11	70,70,70,70	0
56	MG	1A	3622	1/1	0.59	0.11	55,55,55,55	0
56	MG	2j	8001	1/1	0.59	0.09	76,76,76,76	0
56	MG	1F	308	1/1	0.59	0.40	63,63,63,63	0
56	MG	2A	3632	1/1	0.60	0.88	66,66,66,66	0
56	MG	1A	3575	1/1	0.61	0.18	31,31,31,31	0
56	MG	1A	3621	1/1	0.61	0.13	56,56,56,56	0
56	MG	2A	3538	1/1	0.61	0.26	82,82,82,82	0
56	MG	2A	3033	1/1	0.61	0.32	53,53,53,53	0
56	MG	2a	1797	1/1	0.62	0.17	89,89,89,89	0
56	MG	2a	1693	1/1	0.62	0.17	69,69,69,69	0
56	MG	2A	3557	1/1	0.62	0.12	55,55,55,55	0
56	MG	15	104	1/1	0.62	0.24	55,55,55,55	0
56	MG	1A	3495	1/1	0.63	0.17	48,48,48,48	0
56	MG	1A	3813	1/1	0.63	0.14	63,63,63,63	0
56	MG	2a	1760	1/1	0.64	0.18	79,79,79,79	0
56	MG	1A	3838	1/1	0.64	0.18	40,40,40,40	0
56	MG	2F	301	1/1	0.64	0.16	54,54,54,54	0
56	MG	2A	3526	1/1	0.65	0.21	60,60,60,60	0
56	MG	2A	3085	1/1	0.65	0.18	56,56,56,56	0
56	MG	2a	1607	1/1	0.65	0.16	67,67,67,67	0
56	MG	2A	3590	1/1	0.65	0.16	65,65,65,65	0
56	MG	2a	1705	1/1	0.65	0.24	69,69,69,69	0
56	MG	2A	3309	1/1	0.65	0.15	39,39,39,39	0
56	MG	1A	3342	1/1	0.66	0.61	48,48,48,48	0
56	MG	2A	3505	1/1	0.66	0.15	72,72,72,72	0
56	MG	1A	3453	1/1	0.66	0.26	34,34,34,34	0
56	MG	2A	3541	1/1	0.67	0.24	67,67,67,67	0
56	MG	1y	3006	1/1	0.67	0.25	82,82,82,82	0
56	MG	1A	3015	1/1	0.67	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3641	1/1	0.67	0.95	57,57,57,57	0
56	MG	1v	3001	1/1	0.67	0.15	58,58,58,58	0
56	MG	1A	3686	1/1	0.68	0.24	62,62,62,62	0
56	MG	10	105	1/1	0.68	0.12	63,63,63,63	0
56	MG	1A	3316	1/1	0.68	0.17	57,57,57,57	0
56	MG	2a	1623	1/1	0.69	0.28	80,80,80,80	0
56	MG	2a	1657	1/1	0.69	0.20	76,76,76,76	0
56	MG	2a	1684	1/1	0.69	0.17	76,76,76,76	0
56	MG	2A	3537	1/1	0.69	0.14	67,67,67,67	0
56	MG	1a	1616	1/1	0.69	0.27	68,68,68,68	0
56	MG	1a	1792	1/1	0.69	0.12	82,82,82,82	0
56	MG	2A	3655	1/1	0.70	0.09	41,41,41,41	0
56	MG	1A	3459	1/1	0.70	0.15	42,42,42,42	0
56	MG	2A	3531	1/1	0.70	0.17	66,66,66,66	0
56	MG	2A	3404	1/1	0.70	0.14	39,39,39,39	0
56	MG	1A	3685	1/1	0.70	0.12	49,49,49,49	0
56	MG	2A	3508	1/1	0.71	0.12	44,44,44,44	0
56	MG	2A	3219	1/1	0.71	0.30	69,69,69,69	0
56	MG	2a	1782	1/1	0.71	0.18	90,90,90,90	0
56	MG	1A	3936	1/1	0.71	0.36	61,61,61,61	0
56	MG	1A	3781	1/1	0.71	0.13	69,69,69,69	0
56	MG	2A	3315	1/1	0.71	0.12	36,36,36,36	0
56	MG	1a	1827	1/1	0.71	0.17	63,63,63,63	0
56	MG	1A	3296	1/1	0.71	0.24	56,56,56,56	0
56	MG	1A	3752	1/1	0.72	0.19	62,62,62,62	0
56	MG	2A	3072	1/1	0.72	0.17	47,47,47,47	0
56	MG	1A	3014	1/1	0.72	0.16	46,46,46,46	0
56	MG	2a	1726	1/1	0.72	0.12	68,68,68,68	0
56	MG	1A	3182	1/1	0.72	0.17	52,52,52,52	0
59	ZN	16	101	1/1	0.72	0.36	91,91,91,91	0
59	ZN	24	501	1/1	0.72	0.10	185,185,185,185	0
56	MG	2A	3328	1/1	0.72	0.11	47,47,47,47	0
56	MG	2a	1602	1/1	0.73	0.13	70,70,70,70	0
56	MG	2A	3515	1/1	0.73	0.09	45,45,45,45	0
56	MG	1A	3063	1/1	0.73	0.16	52,52,52,52	0
56	MG	1A	3512	1/1	0.73	0.09	66,66,66,66	0
56	MG	1A	3153	1/1	0.73	0.19	52,52,52,52	0
56	MG	2A	3163	1/1	0.73	0.63	59,59,59,59	0
56	MG	1A	3872	1/1	0.74	0.18	50,50,50,50	0
56	MG	2B	3010	1/1	0.74	0.16	63,63,63,63	0
56	MG	2a	1691	1/1	0.74	0.17	80,80,80,80	0
56	MG	1A	3423	1/1	0.74	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3126	1/1	0.74	0.18	59,59,59,59	0
56	MG	1A	3640	1/1	0.74	0.40	82,82,82,82	0
56	MG	2a	1613	1/1	0.74	0.17	59,59,59,59	0
56	MG	1a	1615	1/1	0.74	0.17	60,60,60,60	0
56	MG	2B	3011	1/1	0.75	0.15	72,72,72,72	0
56	MG	1A	3696	1/1	0.75	0.22	50,50,50,50	0
56	MG	2A	3585	1/1	0.75	0.16	64,64,64,64	0
56	MG	1x	102	1/1	0.75	0.18	62,62,62,62	0
56	MG	1A	3301	1/1	0.75	0.17	45,45,45,45	0
56	MG	2A	3466	1/1	0.75	0.60	49,49,49,49	0
56	MG	1A	3104	1/1	0.75	0.24	71,71,71,71	0
56	MG	2a	1675	1/1	0.75	0.12	64,64,64,64	0
56	MG	1a	1822	1/1	0.75	0.07	79,79,79,79	0
56	MG	2a	1690	1/1	0.75	0.14	69,69,69,69	0
56	MG	2B	3009	1/1	0.75	0.16	60,60,60,60	0
56	MG	1A	3134	1/1	0.75	0.26	56,56,56,56	0
56	MG	10	103	1/1	0.76	0.14	61,61,61,61	0
56	MG	2a	1710	1/1	0.76	0.20	65,65,65,65	0
56	MG	2A	3239	1/1	0.76	0.15	58,58,58,58	0
56	MG	1A	3905	1/1	0.76	0.30	46,46,46,46	0
56	MG	1A	3233	1/1	0.76	0.17	60,60,60,60	0
56	MG	2A	3528	1/1	0.76	0.09	73,73,73,73	0
56	MG	1A	3396	1/1	0.76	0.16	42,42,42,42	0
56	MG	1A	3713	1/1	0.76	0.15	71,71,71,71	0
56	MG	1w	3001	1/1	0.76	0.13	52,52,52,52	0
56	MG	2A	3411	1/1	0.76	0.20	57,57,57,57	0
56	MG	2A	3544	1/1	0.76	0.33	75,75,75,75	0
56	MG	1a	1668	1/1	0.76	0.11	44,44,44,44	0
56	MG	2a	1700	1/1	0.76	0.12	57,57,57,57	0
56	MG	2B	3021	1/1	0.77	0.14	76,76,76,76	0
56	MG	2a	1686	1/1	0.77	0.12	82,82,82,82	0
56	MG	1A	3268	1/1	0.77	0.14	63,63,63,63	0
56	MG	1A	3306	1/1	0.77	0.23	62,62,62,62	0
56	MG	2A	3222	1/1	0.77	0.16	46,46,46,46	0
56	MG	2a	1699	1/1	0.77	0.14	49,49,49,49	0
56	MG	1A	3402	1/1	0.77	0.17	27,27,27,27	0
56	MG	2A	3246	1/1	0.77	0.22	61,61,61,61	0
56	MG	1A	3852	1/1	0.77	0.09	70,70,70,70	0
56	MG	2A	3292	1/1	0.77	0.19	47,47,47,47	0
56	MG	2A	3105	1/1	0.78	0.14	52,52,52,52	0
56	MG	2A	3639	1/1	0.78	0.08	44,44,44,44	0
56	MG	1P	203	1/1	0.78	0.48	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1V	203	1/1	0.78	0.22	64,64,64,64	0
56	MG	2A	3403	1/1	0.78	0.34	25,25,25,25	0
56	MG	1a	1746	1/1	0.78	0.12	52,52,52,52	0
56	MG	1a	1768	1/1	0.78	0.09	66,66,66,66	0
56	MG	2a	1706	1/1	0.78	0.07	68,68,68,68	0
56	MG	2a	1709	1/1	0.78	0.11	92,92,92,92	0
56	MG	1A	3615	1/1	0.78	0.26	34,34,34,34	0
56	MG	2A	3467	1/1	0.78	0.19	51,51,51,51	0
56	MG	2A	3469	1/1	0.78	0.64	53,53,53,53	0
56	MG	2A	3498	1/1	0.78	0.36	56,56,56,56	0
56	MG	1A	3229	1/1	0.78	0.16	56,56,56,56	0
56	MG	2A	3586	1/1	0.78	0.16	73,73,73,73	0
56	MG	2a	1649	1/1	0.78	0.11	65,65,65,65	0
56	MG	1A	3862	1/1	0.78	0.13	54,54,54,54	0
56	MG	2a	1668	1/1	0.78	0.15	66,66,66,66	0
56	MG	1A	3184	1/1	0.78	0.11	59,59,59,59	0
56	MG	2a	1683	1/1	0.78	0.12	82,82,82,82	0
56	MG	2A	3608	1/1	0.78	0.13	64,64,64,64	0
56	MG	2A	3356	1/1	0.79	0.14	48,48,48,48	0
56	MG	2A	3643	1/1	0.79	0.16	63,63,63,63	0
56	MG	2A	3396	1/1	0.79	0.13	50,50,50,50	0
56	MG	2A	3667	1/1	0.79	0.23	64,64,64,64	0
56	MG	1A	3502	1/1	0.79	0.14	71,71,71,71	0
56	MG	1a	1722	1/1	0.79	0.12	64,64,64,64	0
56	MG	1x	107	1/1	0.79	0.28	75,75,75,75	0
56	MG	2A	3231	1/1	0.79	0.23	59,59,59,59	0
56	MG	1A	3216	1/1	0.79	0.13	65,65,65,65	0
56	MG	2Q	3002	1/1	0.79	0.12	52,52,52,52	0
56	MG	2Z	8001	1/1	0.79	0.45	90,90,90,90	0
56	MG	2A	3571	1/1	0.79	0.10	56,56,56,56	0
56	MG	1A	3322	1/1	0.79	0.13	57,57,57,57	0
56	MG	1A	3005	1/1	0.79	0.11	59,59,59,59	0
56	MG	1A	3417	1/1	0.79	0.10	36,36,36,36	0
56	MG	1A	3773	1/1	0.79	0.24	48,48,48,48	0
56	MG	1a	1633	1/1	0.79	0.13	66,66,66,66	0
56	MG	1a	1667	1/1	0.79	0.35	76,76,76,76	0
56	MG	2A	3620	1/1	0.79	0.13	70,70,70,70	0
56	MG	2A	3341	1/1	0.79	0.16	41,41,41,41	0
56	MG	2A	3529	1/1	0.79	0.13	58,58,58,58	0
56	MG	1A	3310	1/1	0.80	0.16	52,52,52,52	0
56	MG	1A	3198	1/1	0.80	0.23	43,43,43,43	0
56	MG	2a	1651	1/1	0.80	0.28	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3075	1/1	0.80	0.14	47,47,47,47	0
56	MG	2A	3225	1/1	0.80	0.41	49,49,49,49	0
56	MG	2A	3521	1/1	0.80	0.13	52,52,52,52	0
56	MG	1A	3538	1/1	0.80	0.13	45,45,45,45	0
56	MG	2a	1769	1/1	0.80	0.14	65,65,65,65	0
56	MG	2A	3236	1/1	0.80	0.14	65,65,65,65	0
56	MG	2A	3086	1/1	0.80	0.17	51,51,51,51	0
56	MG	2A	3243	1/1	0.80	0.19	66,66,66,66	0
56	MG	1A	3248	1/1	0.80	0.14	63,63,63,63	0
56	MG	2a	1692	1/1	0.80	0.13	72,72,72,72	0
56	MG	2A	3257	1/1	0.80	0.16	61,61,61,61	0
56	MG	1A	3154	1/1	0.80	0.12	53,53,53,53	0
56	MG	1A	3830	1/1	0.80	0.15	60,60,60,60	0
56	MG	2E	304	1/1	0.81	0.16	43,43,43,43	0
56	MG	1A	3659	1/1	0.81	0.16	41,41,41,41	0
56	MG	1A	3783	1/1	0.81	0.11	51,51,51,51	0
56	MG	2R	201	1/1	0.81	0.19	58,58,58,58	0
56	MG	12	101	1/1	0.81	0.18	54,54,54,54	0
56	MG	1A	3785	1/1	0.81	0.21	65,65,65,65	0
56	MG	1A	3241	1/1	0.81	0.17	50,50,50,50	0
56	MG	2A	3094	1/1	0.81	0.10	50,50,50,50	0
56	MG	2a	1618	1/1	0.81	0.10	68,68,68,68	0
56	MG	2A	3104	1/1	0.81	0.16	72,72,72,72	0
56	MG	2a	1629	1/1	0.81	0.22	66,66,66,66	0
56	MG	1A	3347	1/1	0.81	0.12	46,46,46,46	0
56	MG	2A	3117	1/1	0.81	0.17	52,52,52,52	0
56	MG	2a	1655	1/1	0.81	0.14	56,56,56,56	0
56	MG	1A	3583	1/1	0.81	0.09	64,64,64,64	0
56	MG	1a	1641	1/1	0.81	0.12	49,49,49,49	0
56	MG	2A	3168	1/1	0.81	0.23	59,59,59,59	0
56	MG	2a	1677	1/1	0.81	0.19	67,67,67,67	0
56	MG	2a	1680	1/1	0.81	0.15	72,72,72,72	0
56	MG	2A	3175	1/1	0.81	0.22	47,47,47,47	0
56	MG	2A	3187	1/1	0.81	0.21	42,42,42,42	0
56	MG	1a	1659	1/1	0.81	0.31	59,59,59,59	0
56	MG	1A	3699	1/1	0.81	0.11	65,65,65,65	0
56	MG	1A	3712	1/1	0.81	0.24	36,36,36,36	0
56	MG	1a	1698	1/1	0.81	0.36	72,72,72,72	0
56	MG	1a	1708	1/1	0.81	0.25	60,60,60,60	0
56	MG	1a	1718	1/1	0.81	0.11	49,49,49,49	0
56	MG	1A	3584	1/1	0.81	0.46	70,70,70,70	0
56	MG	1A	3867	1/1	0.81	0.08	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3587	1/1	0.81	0.11	59,59,59,59	0
56	MG	1A	3868	1/1	0.81	0.15	37,37,37,37	0
56	MG	1A	3466	1/1	0.81	0.08	64,64,64,64	0
56	MG	1A	3725	1/1	0.81	0.11	49,49,49,49	0
56	MG	1A	3750	1/1	0.81	0.09	51,51,51,51	0
56	MG	1B	210	1/1	0.81	0.10	53,53,53,53	0
56	MG	1A	3386	1/1	0.81	0.09	42,42,42,42	0
56	MG	2A	3339	1/1	0.81	0.14	42,42,42,42	0
56	MG	1B	223	1/1	0.81	0.20	58,58,58,58	0
56	MG	1E	306	1/1	0.81	0.15	61,61,61,61	0
56	MG	1A	3419	1/1	0.81	0.06	53,53,53,53	0
56	MG	1y	3004	1/1	0.81	0.28	73,73,73,73	0
56	MG	1A	3630	1/1	0.81	0.12	62,62,62,62	0
56	MG	1A	3294	1/1	0.81	0.25	63,63,63,63	0
56	MG	2A	3456	1/1	0.81	0.12	42,42,42,42	0
56	MG	1A	3239	1/1	0.82	0.14	63,63,63,63	0
56	MG	2A	3179	1/1	0.82	0.23	56,56,56,56	0
56	MG	1A	3273	1/1	0.82	0.14	59,59,59,59	0
56	MG	1A	3285	1/1	0.82	0.12	57,57,57,57	0
56	MG	1y	3001	1/1	0.82	0.09	73,73,73,73	0
56	MG	1A	3433	1/1	0.82	0.18	54,54,54,54	0
56	MG	2A	3226	1/1	0.82	0.51	60,60,60,60	0
56	MG	1A	3341	1/1	0.82	0.28	68,68,68,68	0
56	MG	2A	3646	1/1	0.82	0.11	46,46,46,46	0
56	MG	1a	1681	1/1	0.82	0.14	58,58,58,58	0
56	MG	1A	3195	1/1	0.82	0.23	46,46,46,46	0
56	MG	1A	3244	1/1	0.82	0.34	52,52,52,52	0
56	MG	2A	3244	1/1	0.82	0.17	46,46,46,46	0
56	MG	1A	3855	1/1	0.82	0.10	69,69,69,69	0
56	MG	1A	3299	1/1	0.82	0.20	41,41,41,41	0
56	MG	1a	1735	1/1	0.82	0.12	66,66,66,66	0
56	MG	1A	3247	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3103	1/1	0.82	0.27	46,46,46,46	0
56	MG	1A	3674	1/1	0.82	0.12	48,48,48,48	0
56	MG	2X	101	1/1	0.82	0.15	42,42,42,42	0
56	MG	15	101	1/1	0.82	0.23	48,48,48,48	0
56	MG	2a	1752	1/1	0.82	0.20	78,78,78,78	0
56	MG	2A	3546	1/1	0.82	0.19	72,72,72,72	0
56	MG	1A	3302	1/1	0.82	0.15	65,65,65,65	0
56	MG	2a	1608	1/1	0.82	0.45	73,73,73,73	0
56	MG	2a	1788	1/1	0.82	0.19	81,81,81,81	0
56	MG	2A	3121	1/1	0.82	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3350	1/1	0.82	0.11	30,30,30,30	0
56	MG	1A	3901	1/1	0.82	0.16	36,36,36,36	0
56	MG	2A	3374	1/1	0.82	0.10	47,47,47,47	0
56	MG	2a	1648	1/1	0.82	0.13	55,55,55,55	0
56	MG	1A	3181	1/1	0.82	0.25	56,56,56,56	0
56	MG	1a	1623	1/1	0.82	0.12	54,54,54,54	0
56	MG	2A	3304	1/1	0.83	0.17	59,59,59,59	0
56	MG	1A	3756	1/1	0.83	0.16	67,67,67,67	0
56	MG	1a	1753	1/1	0.83	0.11	67,67,67,67	0
56	MG	2A	3321	1/1	0.83	0.18	59,59,59,59	0
56	MG	1A	3076	1/1	0.83	0.27	66,66,66,66	0
56	MG	2A	3338	1/1	0.83	0.15	43,43,43,43	0
56	MG	1A	3438	1/1	0.83	0.21	40,40,40,40	0
56	MG	1a	1810	1/1	0.83	0.16	77,77,77,77	0
56	MG	1a	1608	1/1	0.83	0.16	56,56,56,56	0
56	MG	2A	3132	1/1	0.83	0.18	51,51,51,51	0
56	MG	2A	3144	1/1	0.83	0.12	49,49,49,49	0
56	MG	2A	3384	1/1	0.83	0.15	61,61,61,61	0
56	MG	2a	1682	1/1	0.83	0.14	64,64,64,64	0
56	MG	1A	3577	1/1	0.83	0.16	43,43,43,43	0
56	MG	1A	3231	1/1	0.83	0.24	61,61,61,61	0
56	MG	2A	3637	1/1	0.83	0.07	58,58,58,58	0
56	MG	1A	3210	1/1	0.83	0.15	45,45,45,45	0
56	MG	1A	3934	1/1	0.83	0.23	84,84,84,84	0
56	MG	1A	3139	1/1	0.83	0.49	45,45,45,45	0
56	MG	2A	3212	1/1	0.83	0.16	66,66,66,66	0
56	MG	1a	1642	1/1	0.83	0.19	60,60,60,60	0
56	MG	1a	1657	1/1	0.83	0.11	50,50,50,50	0
56	MG	2A	3671	1/1	0.83	0.22	52,52,52,52	0
56	MG	2A	3482	1/1	0.83	0.07	77,77,77,77	0
56	MG	2A	3497	1/1	0.83	0.48	64,64,64,64	0
56	MG	1A	3348	1/1	0.83	0.14	33,33,33,33	0
56	MG	1A	3318	1/1	0.83	0.15	60,60,60,60	0
56	MG	2a	1732	1/1	0.83	0.09	77,77,77,77	0
56	MG	1A	3827	1/1	0.83	0.16	68,68,68,68	0
56	MG	2a	1746	1/1	0.83	0.11	55,55,55,55	0
56	MG	1A	3828	1/1	0.83	0.15	43,43,43,43	0
56	MG	2F	302	1/1	0.83	0.22	53,53,53,53	0
56	MG	2a	1763	1/1	0.83	0.10	75,75,75,75	0
56	MG	2A	3237	1/1	0.83	0.55	63,63,63,63	0
56	MG	1A	3425	1/1	0.83	0.17	52,52,52,52	0
56	MG	1A	3520	1/1	0.83	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3845	1/1	0.83	0.13	68,68,68,68	0
56	MG	1A	3531	1/1	0.83	0.15	61,61,61,61	0
56	MG	2a	1604	1/1	0.83	0.18	76,76,76,76	0
56	MG	2A	3089	1/1	0.83	0.21	58,58,58,58	0
56	MG	2w	3001	1/1	0.83	0.16	58,58,58,58	0
56	MG	1A	3755	1/1	0.83	0.14	32,32,32,32	0
56	MG	2A	3096	1/1	0.83	0.14	57,57,57,57	0
56	MG	2a	1616	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3407	1/1	0.84	0.11	24,24,24,24	0
56	MG	1A	3251	1/1	0.84	0.15	47,47,47,47	0
56	MG	2A	3614	1/1	0.84	0.17	47,47,47,47	0
56	MG	2A	3421	1/1	0.84	0.14	51,51,51,51	0
56	MG	2a	1662	1/1	0.84	0.40	67,67,67,67	0
56	MG	2A	3623	1/1	0.84	0.13	52,52,52,52	0
56	MG	2a	1670	1/1	0.84	0.11	66,66,66,66	0
56	MG	2A	3625	1/1	0.84	0.07	62,62,62,62	0
56	MG	2A	3423	1/1	0.84	0.21	36,36,36,36	0
56	MG	1A	3462	1/1	0.84	0.19	58,58,58,58	0
56	MG	1A	3173	1/1	0.84	0.21	41,41,41,41	0
56	MG	1A	3870	1/1	0.84	0.17	49,49,49,49	0
56	MG	1A	3550	1/1	0.84	0.20	49,49,49,49	0
56	MG	1A	3810	1/1	0.84	0.24	63,63,63,63	0
56	MG	1A	3745	1/1	0.84	0.10	64,64,64,64	0
56	MG	1a	1790	1/1	0.84	0.23	62,62,62,62	0
56	MG	1A	3478	1/1	0.84	0.12	29,29,29,29	0
56	MG	2A	3251	1/1	0.84	0.10	59,59,59,59	0
56	MG	1A	3487	1/1	0.84	0.12	48,48,48,48	0
56	MG	1A	3215	1/1	0.84	0.25	43,43,43,43	0
56	MG	2B	3015	1/1	0.84	0.19	53,53,53,53	0
56	MG	1a	1637	1/1	0.84	0.13	44,44,44,44	0
56	MG	1A	3113	1/1	0.84	0.47	47,47,47,47	0
56	MG	2E	307	1/1	0.84	0.35	51,51,51,51	0
56	MG	1B	222	1/1	0.84	0.14	78,78,78,78	0
56	MG	2a	1727	1/1	0.84	0.14	54,54,54,54	0
56	MG	1A	3612	1/1	0.84	0.15	43,43,43,43	0
56	MG	2A	3152	1/1	0.84	0.30	50,50,50,50	0
56	MG	1a	1658	1/1	0.84	0.15	59,59,59,59	0
56	MG	2a	1751	1/1	0.84	0.17	70,70,70,70	0
56	MG	1A	3290	1/1	0.84	0.21	68,68,68,68	0
56	MG	2A	3174	1/1	0.84	0.09	63,63,63,63	0
56	MG	20	103	1/1	0.84	0.09	65,65,65,65	0
56	MG	2a	1601	1/1	0.84	0.11	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3706	1/1	0.84	0.14	55,55,55,55	0
56	MG	1O	8001	1/1	0.84	0.07	63,63,63,63	0
56	MG	1A	3859	1/1	0.84	0.16	40,40,40,40	0
56	MG	2A	3358	1/1	0.84	0.19	50,50,50,50	0
56	MG	2A	3191	1/1	0.84	0.45	52,52,52,52	0
56	MG	1a	1688	1/1	0.84	0.20	57,57,57,57	0
56	MG	2A	3070	1/1	0.84	0.20	52,52,52,52	0
58	K	1A	3931	1/1	0.84	0.19	71,71,71,71	0
56	MG	2A	3220	1/1	0.84	0.16	56,56,56,56	0
56	MG	1A	3861	1/1	0.84	0.15	58,58,58,58	0
56	MG	2A	3597	1/1	0.84	0.14	65,65,65,65	0
56	MG	1A	3232	1/1	0.85	0.12	55,55,55,55	0
56	MG	1A	3669	1/1	0.85	0.25	58,58,58,58	0
56	MG	2A	3425	1/1	0.85	0.14	76,76,76,76	0
56	MG	2A	3426	1/1	0.85	0.23	44,44,44,44	0
56	MG	2A	3436	1/1	0.85	0.12	54,54,54,54	0
56	MG	2A	3439	1/1	0.85	0.10	60,60,60,60	0
56	MG	2A	3447	1/1	0.85	0.09	68,68,68,68	0
56	MG	20	102	1/1	0.85	0.08	61,61,61,61	0
56	MG	1A	3801	1/1	0.85	0.08	43,43,43,43	0
56	MG	2A	3461	1/1	0.85	0.30	57,57,57,57	0
56	MG	1a	1786	1/1	0.85	0.10	55,55,55,55	0
56	MG	1A	3424	1/1	0.85	0.17	51,51,51,51	0
56	MG	2a	1605	1/1	0.85	0.36	54,54,54,54	0
56	MG	2a	1606	1/1	0.85	0.08	60,60,60,60	0
56	MG	1R	202	1/1	0.85	0.15	71,71,71,71	0
56	MG	2A	3481	1/1	0.85	0.34	62,62,62,62	0
56	MG	1a	1804	1/1	0.85	0.12	65,65,65,65	0
56	MG	1A	3676	1/1	0.85	0.12	52,52,52,52	0
56	MG	2A	3206	1/1	0.85	0.18	48,48,48,48	0
56	MG	1a	1816	1/1	0.85	0.12	83,83,83,83	0
56	MG	2a	1624	1/1	0.85	0.20	62,62,62,62	0
56	MG	2A	3218	1/1	0.85	0.13	53,53,53,53	0
56	MG	2a	1636	1/1	0.85	0.14	62,62,62,62	0
56	MG	1A	3677	1/1	0.85	0.11	68,68,68,68	0
56	MG	1A	3095	1/1	0.85	0.24	56,56,56,56	0
56	MG	1A	3515	1/1	0.85	0.13	58,58,58,58	0
56	MG	1A	3837	1/1	0.85	0.13	56,56,56,56	0
56	MG	1A	3042	1/1	0.85	0.10	40,40,40,40	0
56	MG	1A	3190	1/1	0.85	0.14	47,47,47,47	0
56	MG	2A	3536	1/1	0.85	0.31	53,53,53,53	0
56	MG	1A	3442	1/1	0.85	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3444	1/1	0.85	0.16	26,26,26,26	0
56	MG	1A	3560	1/1	0.85	0.20	19,19,19,19	0
56	MG	1A	3719	1/1	0.85	0.15	48,48,48,48	0
56	MG	1A	3176	1/1	0.85	0.12	47,47,47,47	0
56	MG	2A	3044	1/1	0.85	0.17	46,46,46,46	0
56	MG	2A	3065	1/1	0.85	0.09	47,47,47,47	0
56	MG	1A	3457	1/1	0.85	0.13	35,35,35,35	0
56	MG	1A	3741	1/1	0.85	0.10	63,63,63,63	0
56	MG	2A	3582	1/1	0.85	0.13	46,46,46,46	0
56	MG	2A	3290	1/1	0.85	0.21	50,50,50,50	0
56	MG	1A	3243	1/1	0.85	0.14	66,66,66,66	0
56	MG	2A	3293	1/1	0.85	0.11	54,54,54,54	0
56	MG	2A	3294	1/1	0.85	0.11	60,60,60,60	0
56	MG	2A	3596	1/1	0.85	0.17	76,76,76,76	0
56	MG	1A	3291	1/1	0.85	0.12	52,52,52,52	0
56	MG	1A	3886	1/1	0.85	0.15	58,58,58,58	0
56	MG	1a	1663	1/1	0.85	0.20	68,68,68,68	0
56	MG	2A	3318	1/1	0.85	0.11	33,33,33,33	0
56	MG	1A	3593	1/1	0.85	0.14	38,38,38,38	0
56	MG	1A	3465	1/1	0.85	0.11	35,35,35,35	0
56	MG	2a	1743	1/1	0.85	0.12	92,92,92,92	0
56	MG	1a	1679	1/1	0.85	0.09	67,67,67,67	0
56	MG	1A	3412	1/1	0.85	0.13	44,44,44,44	0
56	MG	1a	1686	1/1	0.85	0.23	53,53,53,53	0
56	MG	2A	3343	1/1	0.85	0.16	40,40,40,40	0
56	MG	1A	3475	1/1	0.85	0.19	42,42,42,42	0
56	MG	2A	3108	1/1	0.85	0.59	37,37,37,37	0
56	MG	1A	3230	1/1	0.85	0.09	55,55,55,55	0
56	MG	2a	1776	1/1	0.85	0.07	78,78,78,78	0
56	MG	1A	3482	1/1	0.85	0.13	35,35,35,35	0
56	MG	2a	1783	1/1	0.85	0.14	68,68,68,68	0
56	MG	1B	220	1/1	0.85	0.09	56,56,56,56	0
56	MG	2A	3390	1/1	0.85	0.19	51,51,51,51	0
56	MG	2A	3129	1/1	0.85	0.17	47,47,47,47	0
56	MG	1A	3633	1/1	0.85	0.09	50,50,50,50	0
56	MG	2A	3137	1/1	0.85	0.15	62,62,62,62	0
56	MG	2j	8002	1/1	0.85	0.17	92,92,92,92	0
56	MG	2A	3138	1/1	0.85	0.16	29,29,29,29	0
56	MG	2B	3019	1/1	0.85	0.26	44,44,44,44	0
56	MG	1A	3051	1/1	0.85	0.15	58,58,58,58	0
56	MG	2D	302	1/1	0.85	0.27	70,70,70,70	0
56	MG	2A	3416	1/1	0.85	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3556	1/1	0.86	0.10	55,55,55,55	0
56	MG	1a	1622	1/1	0.86	0.08	59,59,59,59	0
56	MG	2A	3568	1/1	0.86	0.30	74,74,74,74	0
56	MG	1A	3726	1/1	0.86	0.12	38,38,38,38	0
56	MG	1a	1829	1/1	0.86	0.12	59,59,59,59	0
56	MG	1b	3002	1/1	0.86	0.08	85,85,85,85	0
56	MG	1r	3001	1/1	0.86	0.22	67,67,67,67	0
56	MG	2A	3180	1/1	0.86	0.38	54,54,54,54	0
56	MG	1a	1625	1/1	0.86	0.16	48,48,48,48	0
56	MG	1A	3812	1/1	0.86	0.11	61,61,61,61	0
56	MG	2A	3593	1/1	0.86	0.09	41,41,41,41	0
56	MG	1A	3314	1/1	0.86	0.33	68,68,68,68	0
56	MG	1A	3078	1/1	0.86	0.18	47,47,47,47	0
56	MG	2a	1665	1/1	0.86	0.22	66,66,66,66	0
56	MG	1B	213	1/1	0.86	0.10	49,49,49,49	0
56	MG	2A	3602	1/1	0.86	0.11	63,63,63,63	0
56	MG	2A	3413	1/1	0.86	0.19	56,56,56,56	0
56	MG	2A	3610	1/1	0.86	0.10	50,50,50,50	0
56	MG	1A	3747	1/1	0.86	0.14	30,30,30,30	0
56	MG	1A	3045	1/1	0.86	0.14	46,46,46,46	0
56	MG	1B	221	1/1	0.86	0.08	48,48,48,48	0
56	MG	1A	3320	1/1	0.86	0.14	52,52,52,52	0
56	MG	2A	3061	1/1	0.86	0.13	56,56,56,56	0
56	MG	2A	3230	1/1	0.86	0.31	60,60,60,60	0
56	MG	1A	3245	1/1	0.86	0.15	48,48,48,48	0
56	MG	1A	3340	1/1	0.86	0.27	48,48,48,48	0
56	MG	1a	1673	1/1	0.86	0.22	52,52,52,52	0
56	MG	2a	1697	1/1	0.86	0.12	64,64,64,64	0
56	MG	1F	304	1/1	0.86	0.18	50,50,50,50	0
56	MG	1A	3763	1/1	0.86	0.36	63,63,63,63	0
56	MG	1A	3284	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	3192	1/1	0.86	0.29	42,42,42,42	0
56	MG	2B	3003	1/1	0.86	0.09	69,69,69,69	0
56	MG	2A	3477	1/1	0.86	0.13	52,52,52,52	0
56	MG	2a	1722	1/1	0.86	0.17	59,59,59,59	0
56	MG	1Q	3002	1/1	0.86	0.20	43,43,43,43	0
56	MG	1A	3018	1/1	0.86	0.24	53,53,53,53	0
56	MG	2a	1729	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3485	1/1	0.86	0.16	47,47,47,47	0
56	MG	2A	3266	1/1	0.86	0.15	53,53,53,53	0
56	MG	2A	3278	1/1	0.86	0.13	40,40,40,40	0
56	MG	2A	3501	1/1	0.86	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1712	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3102	1/1	0.86	0.99	60,60,60,60	0
56	MG	1U	201	1/1	0.86	0.19	48,48,48,48	0
56	MG	2A	3518	1/1	0.86	0.43	57,57,57,57	0
56	MG	2Q	3001	1/1	0.86	0.09	47,47,47,47	0
56	MG	2a	1774	1/1	0.86	0.16	70,70,70,70	0
56	MG	1A	3249	1/1	0.86	0.21	69,69,69,69	0
56	MG	1A	3360	1/1	0.86	0.14	52,52,52,52	0
56	MG	1A	3568	1/1	0.86	0.16	31,31,31,31	0
56	MG	1A	3869	1/1	0.86	0.36	52,52,52,52	0
56	MG	2a	1789	1/1	0.86	0.10	62,62,62,62	0
56	MG	1A	3793	1/1	0.86	0.09	38,38,38,38	0
56	MG	2A	3535	1/1	0.86	0.09	55,55,55,55	0
56	MG	28	101	1/1	0.86	0.30	57,57,57,57	0
56	MG	1A	3795	1/1	0.86	0.12	32,32,32,32	0
56	MG	1a	1607	1/1	0.86	0.26	52,52,52,52	0
56	MG	2r	3001	1/1	0.86	0.13	84,84,84,84	0
56	MG	1A	3877	1/1	0.86	0.48	58,58,58,58	0
56	MG	1a	1611	1/1	0.86	0.16	62,62,62,62	0
56	MG	1A	3652	1/1	0.86	0.15	65,65,65,65	0
56	MG	1A	3572	1/1	0.86	0.16	41,41,41,41	0
56	MG	1a	1619	1/1	0.86	0.15	71,71,71,71	0
56	MG	2A	3401	1/1	0.87	0.18	64,64,64,64	0
56	MG	1A	3119	1/1	0.87	0.20	44,44,44,44	0
56	MG	1A	3435	1/1	0.87	0.16	29,29,29,29	0
56	MG	1N	3001	1/1	0.87	0.28	51,51,51,51	0
56	MG	2A	3591	1/1	0.87	0.10	54,54,54,54	0
56	MG	2A	3592	1/1	0.87	0.08	54,54,54,54	0
56	MG	1A	3127	1/1	0.87	0.20	62,62,62,62	0
56	MG	2A	3412	1/1	0.87	0.07	27,27,27,27	0
56	MG	2a	1656	1/1	0.87	0.15	54,54,54,54	0
56	MG	2A	3213	1/1	0.87	0.08	58,58,58,58	0
56	MG	2A	3214	1/1	0.87	0.08	57,57,57,57	0
56	MG	1x	112	1/1	0.87	0.17	68,68,68,68	0
56	MG	1A	3578	1/1	0.87	0.07	56,56,56,56	0
56	MG	1A	3684	1/1	0.87	0.15	72,72,72,72	0
56	MG	1Q	3005	1/1	0.87	0.16	58,58,58,58	0
56	MG	2A	3031	1/1	0.87	0.10	50,50,50,50	0
56	MG	2A	3621	1/1	0.87	0.13	48,48,48,48	0
56	MG	1A	3865	1/1	0.87	0.26	50,50,50,50	0
56	MG	2A	3624	1/1	0.87	0.14	58,58,58,58	0
56	MG	1A	3581	1/1	0.87	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1684	1/1	0.87	0.24	64,64,64,64	0
56	MG	1A	3778	1/1	0.87	0.15	65,65,65,65	0
56	MG	1W	3002	1/1	0.87	0.16	53,53,53,53	0
56	MG	1A	3398	1/1	0.87	0.18	36,36,36,36	0
56	MG	1a	1701	1/1	0.87	0.15	50,50,50,50	0
56	MG	2A	3080	1/1	0.87	0.26	45,45,45,45	0
56	MG	1a	1704	1/1	0.87	0.14	77,77,77,77	0
56	MG	1A	3694	1/1	0.87	0.14	27,27,27,27	0
56	MG	1A	3498	1/1	0.87	0.21	58,58,58,58	0
56	MG	1A	3589	1/1	0.87	0.20	64,64,64,64	0
56	MG	2B	3005	1/1	0.87	0.12	64,64,64,64	0
56	MG	1A	3399	1/1	0.87	0.14	59,59,59,59	0
56	MG	1a	1724	1/1	0.87	0.16	46,46,46,46	0
56	MG	1a	1604	1/1	0.87	0.09	64,64,64,64	0
56	MG	1A	3194	1/1	0.87	0.15	55,55,55,55	0
56	MG	2B	3018	1/1	0.87	0.12	62,62,62,62	0
56	MG	1A	3279	1/1	0.87	0.18	57,57,57,57	0
56	MG	2a	1734	1/1	0.87	0.15	64,64,64,64	0
56	MG	2a	1737	1/1	0.87	0.15	55,55,55,55	0
56	MG	1A	3022	1/1	0.87	0.12	52,52,52,52	0
56	MG	1A	3529	1/1	0.87	0.12	60,60,60,60	0
56	MG	2A	3308	1/1	0.87	0.14	38,38,38,38	0
56	MG	1B	201	1/1	0.87	0.26	53,53,53,53	0
56	MG	1a	1617	1/1	0.87	0.23	71,71,71,71	0
56	MG	1a	1802	1/1	0.87	0.16	54,54,54,54	0
56	MG	2F	305	1/1	0.87	0.12	48,48,48,48	0
56	MG	2a	1768	1/1	0.87	0.19	79,79,79,79	0
56	MG	1A	3024	1/1	0.87	0.10	57,57,57,57	0
56	MG	2A	3325	1/1	0.87	0.20	49,49,49,49	0
56	MG	1A	3142	1/1	0.87	0.51	47,47,47,47	0
56	MG	1a	1812	1/1	0.87	0.17	65,65,65,65	0
56	MG	1A	3092	1/1	0.87	0.10	49,49,49,49	0
56	MG	1A	3642	1/1	0.87	0.14	42,42,42,42	0
56	MG	2A	3149	1/1	0.87	0.12	41,41,41,41	0
56	MG	1A	3646	1/1	0.87	0.08	68,68,68,68	0
56	MG	2A	3551	1/1	0.87	0.10	33,33,33,33	0
56	MG	2A	3552	1/1	0.87	0.17	53,53,53,53	0
56	MG	1a	1823	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3469	1/1	0.87	0.15	48,48,48,48	0
56	MG	1A	3839	1/1	0.87	0.11	61,61,61,61	0
56	MG	2A	3570	1/1	0.87	0.17	51,51,51,51	0
56	MG	1a	1833	1/1	0.87	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3574	1/1	0.87	0.11	62,62,62,62	0
56	MG	1A	3237	1/1	0.87	0.14	57,57,57,57	0
56	MG	1a	1656	1/1	0.87	0.21	57,57,57,57	0
56	MG	1A	3840	1/1	0.88	0.17	65,65,65,65	0
56	MG	1x	114	1/1	0.88	0.13	57,57,57,57	0
56	MG	1a	1661	1/1	0.88	0.25	61,61,61,61	0
56	MG	1G	3001	1/1	0.88	0.14	59,59,59,59	0
56	MG	2a	1603	1/1	0.88	0.11	64,64,64,64	0
56	MG	1a	1665	1/1	0.88	0.34	73,73,73,73	0
56	MG	2A	3006	1/1	0.88	0.18	58,58,58,58	0
56	MG	2A	3258	1/1	0.88	0.13	35,35,35,35	0
56	MG	2A	3024	1/1	0.88	0.31	45,45,45,45	0
56	MG	2A	3270	1/1	0.88	0.12	38,38,38,38	0
56	MG	1A	3448	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3846	1/1	0.88	0.15	39,39,39,39	0
56	MG	2A	3285	1/1	0.88	0.12	68,68,68,68	0
56	MG	1A	3415	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3069	1/1	0.88	0.23	52,52,52,52	0
56	MG	2a	1625	1/1	0.88	0.11	72,72,72,72	0
56	MG	1Q	3004	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	3458	1/1	0.88	0.18	26,26,26,26	0
56	MG	1A	3690	1/1	0.88	0.09	48,48,48,48	0
56	MG	1S	8001	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3775	1/1	0.88	0.23	43,43,43,43	0
56	MG	2A	3310	1/1	0.88	0.13	36,36,36,36	0
56	MG	2A	3084	1/1	0.88	0.08	59,59,59,59	0
56	MG	1V	202	1/1	0.88	0.19	59,59,59,59	0
56	MG	1a	1703	1/1	0.88	0.19	49,49,49,49	0
56	MG	1A	3120	1/1	0.88	0.25	39,39,39,39	0
56	MG	1A	3780	1/1	0.88	0.14	62,62,62,62	0
56	MG	2A	3093	1/1	0.88	0.12	55,55,55,55	0
56	MG	2a	1673	1/1	0.88	0.22	55,55,55,55	0
56	MG	1A	3420	1/1	0.88	0.18	46,46,46,46	0
56	MG	1A	3379	1/1	0.88	0.11	48,48,48,48	0
56	MG	2a	1678	1/1	0.88	0.65	60,60,60,60	0
56	MG	11	102	1/1	0.88	0.17	54,54,54,54	0
56	MG	1A	3278	1/1	0.88	0.14	61,61,61,61	0
56	MG	1a	1731	1/1	0.88	0.27	79,79,79,79	0
56	MG	13	101	1/1	0.88	0.12	46,46,46,46	0
56	MG	2A	3600	1/1	0.88	0.12	45,45,45,45	0
56	MG	1a	1737	1/1	0.88	0.15	51,51,51,51	0
56	MG	2A	3112	1/1	0.88	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3386	1/1	0.88	0.19	33,33,33,33	0
56	MG	1A	3321	1/1	0.88	0.14	48,48,48,48	0
56	MG	2A	3616	1/1	0.88	0.21	64,64,64,64	0
56	MG	2A	3617	1/1	0.88	0.14	49,49,49,49	0
56	MG	1a	1747	1/1	0.88	0.15	53,53,53,53	0
56	MG	1a	1750	1/1	0.88	0.11	69,69,69,69	0
56	MG	1a	1752	1/1	0.88	0.30	66,66,66,66	0
56	MG	1A	3123	1/1	0.88	0.17	42,42,42,42	0
56	MG	2A	3135	1/1	0.88	0.13	36,36,36,36	0
56	MG	2a	1715	1/1	0.88	0.14	59,59,59,59	0
56	MG	1a	1761	1/1	0.88	0.20	51,51,51,51	0
56	MG	2a	1725	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3634	1/1	0.88	0.14	56,56,56,56	0
56	MG	1a	1602	1/1	0.88	0.17	60,60,60,60	0
56	MG	1a	1772	1/1	0.88	0.14	50,50,50,50	0
56	MG	1a	1603	1/1	0.88	0.17	60,60,60,60	0
56	MG	1a	1787	1/1	0.88	0.19	71,71,71,71	0
56	MG	1A	3885	1/1	0.88	0.08	64,64,64,64	0
56	MG	1a	1791	1/1	0.88	0.16	73,73,73,73	0
56	MG	2A	3661	1/1	0.88	0.21	61,61,61,61	0
56	MG	2A	3173	1/1	0.88	0.16	60,60,60,60	0
56	MG	2a	1749	1/1	0.88	0.11	59,59,59,59	0
56	MG	1A	3796	1/1	0.88	0.05	66,66,66,66	0
56	MG	2B	3002	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3899	1/1	0.88	0.40	50,50,50,50	0
56	MG	1A	3797	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3085	1/1	0.88	0.16	52,52,52,52	0
56	MG	1A	3913	1/1	0.88	0.42	54,54,54,54	0
56	MG	1A	3573	1/1	0.88	0.16	43,43,43,43	0
56	MG	1a	1818	1/1	0.88	0.12	72,72,72,72	0
56	MG	1A	3803	1/1	0.88	0.11	65,65,65,65	0
56	MG	1A	3808	1/1	0.88	0.19	46,46,46,46	0
56	MG	1A	3169	1/1	0.88	0.09	60,60,60,60	0
56	MG	1A	3439	1/1	0.88	0.10	54,54,54,54	0
56	MG	2a	1790	1/1	0.88	0.24	72,72,72,72	0
56	MG	1A	3667	1/1	0.88	0.20	51,51,51,51	0
56	MG	1a	1635	1/1	0.88	0.10	62,62,62,62	0
56	MG	1A	3489	1/1	0.88	0.16	31,31,31,31	0
56	MG	2A	3500	1/1	0.88	0.07	56,56,56,56	0
56	MG	1A	3746	1/1	0.88	0.19	31,31,31,31	0
56	MG	2p	3001	1/1	0.88	0.13	74,74,74,74	0
56	MG	1A	3672	1/1	0.88	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3001	1/1	0.88	0.23	60,60,60,60	0
56	MG	2A	3512	1/1	0.88	0.12	45,45,45,45	0
56	MG	1A	3675	1/1	0.88	0.20	50,50,50,50	0
56	MG	1x	106	1/1	0.88	0.23	59,59,59,59	0
56	MG	1A	3175	1/1	0.88	0.29	47,47,47,47	0
56	MG	2A	3509	1/1	0.89	0.14	35,35,35,35	0
56	MG	2A	3038	1/1	0.89	0.10	34,34,34,34	0
56	MG	2A	3043	1/1	0.89	0.16	44,44,44,44	0
56	MG	1A	3391	1/1	0.89	0.16	30,30,30,30	0
56	MG	1a	1728	1/1	0.89	0.16	67,67,67,67	0
56	MG	1A	3440	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3067	1/1	0.89	0.08	51,51,51,51	0
56	MG	1A	3847	1/1	0.89	0.15	51,51,51,51	0
56	MG	1a	1618	1/1	0.89	0.21	48,48,48,48	0
56	MG	1a	1745	1/1	0.89	0.13	81,81,81,81	0
56	MG	2A	3076	1/1	0.89	0.28	60,60,60,60	0
56	MG	1A	3287	1/1	0.89	0.17	57,57,57,57	0
56	MG	1A	3688	1/1	0.89	0.14	64,64,64,64	0
56	MG	2a	1611	1/1	0.89	0.16	68,68,68,68	0
56	MG	1a	1749	1/1	0.89	0.22	56,56,56,56	0
56	MG	2A	3542	1/1	0.89	0.14	48,48,48,48	0
56	MG	1A	3596	1/1	0.89	0.08	51,51,51,51	0
56	MG	1A	3036	1/1	0.89	0.12	54,54,54,54	0
56	MG	1a	1626	1/1	0.89	0.30	61,61,61,61	0
56	MG	2A	3550	1/1	0.89	0.07	70,70,70,70	0
56	MG	2a	1626	1/1	0.89	0.13	63,63,63,63	0
56	MG	2A	3299	1/1	0.89	0.23	54,54,54,54	0
56	MG	1A	3200	1/1	0.89	0.12	48,48,48,48	0
56	MG	2A	3553	1/1	0.89	0.06	45,45,45,45	0
56	MG	1a	1765	1/1	0.89	0.20	51,51,51,51	0
56	MG	1A	3863	1/1	0.89	0.23	56,56,56,56	0
56	MG	1a	1770	1/1	0.89	0.25	44,44,44,44	0
56	MG	1A	3170	1/1	0.89	0.28	64,64,64,64	0
56	MG	1a	1785	1/1	0.89	0.17	71,71,71,71	0
56	MG	2a	1661	1/1	0.89	0.28	62,62,62,62	0
56	MG	1a	1640	1/1	0.89	0.15	47,47,47,47	0
56	MG	2A	3323	1/1	0.89	0.07	47,47,47,47	0
56	MG	2A	3577	1/1	0.89	0.11	62,62,62,62	0
56	MG	2A	3324	1/1	0.89	0.16	45,45,45,45	0
56	MG	1A	3455	1/1	0.89	0.14	25,25,25,25	0
56	MG	2a	1674	1/1	0.89	0.13	62,62,62,62	0
56	MG	1A	3405	1/1	0.89	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3334	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3335	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3336	1/1	0.89	0.09	30,30,30,30	0
56	MG	2a	1681	1/1	0.89	0.13	84,84,84,84	0
56	MG	2A	3116	1/1	0.89	0.10	67,67,67,67	0
56	MG	1a	1655	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3120	1/1	0.89	0.19	57,57,57,57	0
56	MG	1A	3334	1/1	0.89	0.17	49,49,49,49	0
56	MG	2A	3122	1/1	0.89	0.16	47,47,47,47	0
56	MG	1a	1796	1/1	0.89	0.11	80,80,80,80	0
56	MG	1a	1800	1/1	0.89	0.15	56,56,56,56	0
56	MG	2A	3607	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3639	1/1	0.89	0.17	61,61,61,61	0
56	MG	1A	3236	1/1	0.89	0.14	58,58,58,58	0
56	MG	1A	3557	1/1	0.89	0.17	22,22,22,22	0
56	MG	1A	3254	1/1	0.89	0.10	54,54,54,54	0
56	MG	1A	3730	1/1	0.89	0.10	58,58,58,58	0
56	MG	1W	3001	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3893	1/1	0.89	0.14	71,71,71,71	0
56	MG	2A	3157	1/1	0.89	0.21	55,55,55,55	0
56	MG	2a	1721	1/1	0.89	0.13	54,54,54,54	0
56	MG	1A	3563	1/1	0.89	0.18	30,30,30,30	0
56	MG	1a	1669	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3900	1/1	0.89	0.34	35,35,35,35	0
56	MG	1a	1674	1/1	0.89	0.31	59,59,59,59	0
56	MG	11	101	1/1	0.89	0.16	44,44,44,44	0
56	MG	2A	3418	1/1	0.89	0.14	41,41,41,41	0
56	MG	1A	3052	1/1	0.89	0.17	40,40,40,40	0
56	MG	1A	3093	1/1	0.89	0.13	59,59,59,59	0
56	MG	1A	3227	1/1	0.89	0.12	63,63,63,63	0
56	MG	2A	3649	1/1	0.89	0.07	54,54,54,54	0
56	MG	2A	3189	1/1	0.89	0.18	54,54,54,54	0
56	MG	2A	3428	1/1	0.89	0.20	34,34,34,34	0
56	MG	2A	3664	1/1	0.89	0.08	43,43,43,43	0
56	MG	2A	3434	1/1	0.89	0.15	34,34,34,34	0
56	MG	1A	3919	1/1	0.89	0.32	46,46,46,46	0
56	MG	2A	3672	1/1	0.89	0.20	34,34,34,34	0
56	MG	2a	1764	1/1	0.89	0.15	67,67,67,67	0
56	MG	2A	3676	1/1	0.89	0.11	50,50,50,50	0
56	MG	2A	3681	1/1	0.89	0.40	50,50,50,50	0
56	MG	2a	1773	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3194	1/1	0.89	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1694	1/1	0.89	0.13	55,55,55,55	0
56	MG	2a	1780	1/1	0.89	0.14	69,69,69,69	0
56	MG	2A	3454	1/1	0.89	0.12	34,34,34,34	0
56	MG	1A	3749	1/1	0.89	0.16	39,39,39,39	0
56	MG	15	105	1/1	0.89	0.09	55,55,55,55	0
56	MG	1A	3056	1/1	0.89	0.11	43,43,43,43	0
56	MG	2A	3215	1/1	0.89	0.14	53,53,53,53	0
56	MG	2a	1791	1/1	0.89	0.09	75,75,75,75	0
56	MG	1A	3364	1/1	0.89	0.12	35,35,35,35	0
56	MG	2a	1794	1/1	0.89	0.11	94,94,94,94	0
56	MG	2A	3470	1/1	0.89	0.08	53,53,53,53	0
56	MG	2e	201	1/1	0.89	0.18	67,67,67,67	0
56	MG	2e	202	1/1	0.89	0.12	71,71,71,71	0
56	MG	1A	3313	1/1	0.89	0.10	56,56,56,56	0
56	MG	1y	3002	1/1	0.89	0.44	72,72,72,72	0
56	MG	1A	3060	1/1	0.89	0.17	44,44,44,44	0
56	MG	1a	1716	1/1	0.89	0.09	81,81,81,81	0
56	MG	1A	3758	1/1	0.89	0.13	33,33,33,33	0
56	MG	2A	3018	1/1	0.89	0.18	41,41,41,41	0
56	MG	1a	1719	1/1	0.89	0.11	62,62,62,62	0
56	MG	1a	1720	1/1	0.89	0.10	57,57,57,57	0
56	MG	1A	3196	1/1	0.89	0.12	61,61,61,61	0
56	MG	2A	3238	1/1	0.89	0.94	61,61,61,61	0
61	FME	2x	3003	10/11	0.89	0.43	43,53,58,59	10
56	MG	1A	3408	1/1	0.90	0.17	36,36,36,36	0
56	MG	1A	3410	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3317	1/1	0.90	0.14	48,48,48,48	0
56	MG	2a	1612	1/1	0.90	0.18	66,66,66,66	0
56	MG	1a	1672	1/1	0.90	0.21	55,55,55,55	0
56	MG	2a	1614	1/1	0.90	0.29	58,58,58,58	0
56	MG	2a	1615	1/1	0.90	0.15	60,60,60,60	0
56	MG	1a	1805	1/1	0.90	0.10	58,58,58,58	0
56	MG	2a	1617	1/1	0.90	0.17	51,51,51,51	0
56	MG	1Z	303	1/1	0.90	0.17	59,59,59,59	0
56	MG	1a	1811	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3634	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3560	1/1	0.90	0.17	47,47,47,47	0
56	MG	2A	3566	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3722	1/1	0.90	0.10	46,46,46,46	0
56	MG	2a	1632	1/1	0.90	0.16	63,63,63,63	0
56	MG	2A	3569	1/1	0.90	0.34	43,43,43,43	0
56	MG	2a	1643	1/1	0.90	0.22	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3802	1/1	0.90	0.10	56,56,56,56	0
56	MG	1a	1683	1/1	0.90	0.13	64,64,64,64	0
56	MG	2A	3134	1/1	0.90	0.23	54,54,54,54	0
56	MG	2A	3337	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3009	1/1	0.90	0.23	44,44,44,44	0
56	MG	1A	3281	1/1	0.90	0.17	52,52,52,52	0
56	MG	1A	3130	1/1	0.90	0.18	40,40,40,40	0
56	MG	1A	3643	1/1	0.90	0.11	55,55,55,55	0
56	MG	2A	3346	1/1	0.90	0.09	31,31,31,31	0
56	MG	2A	3147	1/1	0.90	0.15	55,55,55,55	0
56	MG	2A	3148	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3908	1/1	0.90	0.26	43,43,43,43	0
56	MG	2A	3369	1/1	0.90	0.14	64,64,64,64	0
56	MG	1A	3349	1/1	0.90	0.13	43,43,43,43	0
56	MG	2a	1676	1/1	0.90	0.12	58,58,58,58	0
56	MG	1c	3001	1/1	0.90	0.22	61,61,61,61	0
56	MG	1l	202	1/1	0.90	0.16	50,50,50,50	0
56	MG	19	503	1/1	0.90	0.12	37,37,37,37	0
56	MG	2A	3395	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3102	1/1	0.90	0.28	58,58,58,58	0
56	MG	1a	1706	1/1	0.90	0.12	72,72,72,72	0
56	MG	2A	3402	1/1	0.90	0.08	62,62,62,62	0
56	MG	2a	1685	1/1	0.90	0.22	62,62,62,62	0
56	MG	2A	3613	1/1	0.90	0.23	71,71,71,71	0
56	MG	2a	1688	1/1	0.90	0.09	65,65,65,65	0
56	MG	1A	3363	1/1	0.90	0.08	49,49,49,49	0
56	MG	1a	1709	1/1	0.90	0.12	62,62,62,62	0
56	MG	1A	3206	1/1	0.90	0.33	40,40,40,40	0
56	MG	2A	3619	1/1	0.90	0.46	47,47,47,47	0
56	MG	1A	3834	1/1	0.90	0.09	60,60,60,60	0
56	MG	1x	113	1/1	0.90	0.14	68,68,68,68	0
56	MG	1B	205	1/1	0.90	0.16	43,43,43,43	0
56	MG	2A	3193	1/1	0.90	0.13	48,48,48,48	0
56	MG	1a	1609	1/1	0.90	0.16	56,56,56,56	0
56	MG	2A	3198	1/1	0.90	0.18	52,52,52,52	0
56	MG	2A	3633	1/1	0.90	0.17	62,62,62,62	0
56	MG	1A	3836	1/1	0.90	0.11	48,48,48,48	0
56	MG	2A	3211	1/1	0.90	0.09	48,48,48,48	0
56	MG	1A	3317	1/1	0.90	0.52	43,43,43,43	0
56	MG	1A	3381	1/1	0.90	0.08	47,47,47,47	0
56	MG	2A	3642	1/1	0.90	0.19	65,65,65,65	0
56	MG	2A	3430	1/1	0.90	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1y	3007	1/1	0.90	0.09	79,79,79,79	0
56	MG	1a	1727	1/1	0.90	0.24	64,64,64,64	0
56	MG	2a	1733	1/1	0.90	0.12	78,78,78,78	0
56	MG	2A	3016	1/1	0.90	0.11	38,38,38,38	0
56	MG	1A	3189	1/1	0.90	0.16	47,47,47,47	0
56	MG	2A	3453	1/1	0.90	0.37	64,64,64,64	0
56	MG	1A	3250	1/1	0.90	0.32	57,57,57,57	0
56	MG	1A	3213	1/1	0.90	0.13	55,55,55,55	0
56	MG	2A	3223	1/1	0.90	0.11	56,56,56,56	0
56	MG	1A	3499	1/1	0.90	0.15	49,49,49,49	0
56	MG	1a	1740	1/1	0.90	0.12	60,60,60,60	0
56	MG	1D	308	1/1	0.90	0.45	51,51,51,51	0
56	MG	1A	3395	1/1	0.90	0.07	58,58,58,58	0
56	MG	2A	3046	1/1	0.90	0.17	50,50,50,50	0
56	MG	2A	3479	1/1	0.90	0.12	53,53,53,53	0
56	MG	2A	3057	1/1	0.90	0.12	54,54,54,54	0
56	MG	1E	308	1/1	0.90	0.15	49,49,49,49	0
56	MG	1A	3058	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3771	1/1	0.90	0.10	63,63,63,63	0
56	MG	2A	3068	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3856	1/1	0.90	0.12	41,41,41,41	0
56	MG	1G	3003	1/1	0.90	0.11	50,50,50,50	0
56	MG	1a	1754	1/1	0.90	0.20	84,84,84,84	0
56	MG	1A	3599	1/1	0.90	0.09	46,46,46,46	0
56	MG	1A	3860	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3604	1/1	0.90	0.22	32,32,32,32	0
56	MG	1A	3112	1/1	0.90	0.15	44,44,44,44	0
56	MG	1A	3613	1/1	0.90	0.12	34,34,34,34	0
56	MG	2a	1796	1/1	0.90	0.12	64,64,64,64	0
56	MG	2A	3282	1/1	0.90	0.14	41,41,41,41	0
56	MG	1a	1778	1/1	0.90	0.14	65,65,65,65	0
56	MG	2V	3001	1/1	0.90	0.47	62,62,62,62	0
56	MG	1A	3338	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	3144	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3701	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3534	1/1	0.90	0.12	58,58,58,58	0
56	MG	1A	3150	1/1	0.90	0.20	55,55,55,55	0
56	MG	2A	3296	1/1	0.90	0.33	52,52,52,52	0
56	MG	2w	3002	1/1	0.90	0.14	75,75,75,75	0
56	MG	1A	3623	1/1	0.90	0.12	59,59,59,59	0
59	ZN	14	501	1/1	0.90	0.10	90,90,90,90	0
56	MG	1a	1666	1/1	0.90	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3305	1/1	0.90	0.10	43,43,43,43	0
56	MG	1A	3871	1/1	0.90	0.20	69,69,69,69	0
56	MG	1a	1797	1/1	0.90	0.17	51,51,51,51	0
56	MG	1a	1601	1/1	0.91	0.10	68,68,68,68	0
56	MG	1A	3776	1/1	0.91	0.14	48,48,48,48	0
56	MG	1a	1725	1/1	0.91	0.11	63,63,63,63	0
56	MG	1A	3777	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3476	1/1	0.91	0.25	36,36,36,36	0
56	MG	2A	3489	1/1	0.91	0.20	73,73,73,73	0
56	MG	2A	3491	1/1	0.91	0.12	49,49,49,49	0
56	MG	2A	3494	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3224	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3888	1/1	0.91	0.19	46,46,46,46	0
56	MG	2A	3035	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	3111	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	3234	1/1	0.91	0.19	50,50,50,50	0
56	MG	1A	3582	1/1	0.91	0.11	42,42,42,42	0
56	MG	1a	1741	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3048	1/1	0.91	0.18	46,46,46,46	0
56	MG	2a	1609	1/1	0.91	0.09	47,47,47,47	0
56	MG	2A	3513	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	3681	1/1	0.91	0.16	37,37,37,37	0
56	MG	1A	3788	1/1	0.91	0.17	61,61,61,61	0
56	MG	1A	3483	1/1	0.91	0.17	27,27,27,27	0
56	MG	1A	3484	1/1	0.91	0.16	46,46,46,46	0
56	MG	2A	3249	1/1	0.91	0.13	45,45,45,45	0
56	MG	1A	3429	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3687	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3071	1/1	0.91	0.08	34,34,34,34	0
56	MG	1A	3385	1/1	0.91	0.06	68,68,68,68	0
56	MG	2A	3073	1/1	0.91	0.27	53,53,53,53	0
56	MG	2A	3275	1/1	0.91	0.10	31,31,31,31	0
56	MG	2a	1627	1/1	0.91	0.09	61,61,61,61	0
56	MG	2a	1628	1/1	0.91	0.15	66,66,66,66	0
56	MG	1A	3152	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3128	1/1	0.91	0.11	47,47,47,47	0
56	MG	2A	3077	1/1	0.91	0.14	51,51,51,51	0
56	MG	2a	1641	1/1	0.91	0.14	55,55,55,55	0
56	MG	1a	1629	1/1	0.91	0.14	69,69,69,69	0
56	MG	2A	3286	1/1	0.91	0.18	47,47,47,47	0
56	MG	2A	3081	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3043	1/1	0.91	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3806	1/1	0.91	0.08	67,67,67,67	0
56	MG	1A	3606	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3295	1/1	0.91	0.20	42,42,42,42	0
56	MG	2a	1658	1/1	0.91	0.12	81,81,81,81	0
56	MG	1A	3295	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3337	1/1	0.91	0.39	34,34,34,34	0
56	MG	1A	3614	1/1	0.91	0.17	23,23,23,23	0
56	MG	1a	1644	1/1	0.91	0.20	48,48,48,48	0
56	MG	1A	3825	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3099	1/1	0.91	0.26	50,50,50,50	0
56	MG	2A	3101	1/1	0.91	0.28	58,58,58,58	0
56	MG	1A	3826	1/1	0.91	0.14	55,55,55,55	0
56	MG	1E	302	1/1	0.91	0.30	35,35,35,35	0
56	MG	1a	1793	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3256	1/1	0.91	0.11	53,53,53,53	0
56	MG	1A	3617	1/1	0.91	0.07	41,41,41,41	0
56	MG	2A	3583	1/1	0.91	0.13	70,70,70,70	0
56	MG	2A	3110	1/1	0.91	0.14	31,31,31,31	0
56	MG	1A	3516	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3113	1/1	0.91	0.13	46,46,46,46	0
56	MG	2A	3329	1/1	0.91	0.17	35,35,35,35	0
56	MG	2A	3115	1/1	0.91	0.06	62,62,62,62	0
56	MG	1A	3267	1/1	0.91	0.19	63,63,63,63	0
56	MG	1A	3041	1/1	0.91	0.08	43,43,43,43	0
56	MG	2A	3119	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3626	1/1	0.91	0.07	44,44,44,44	0
56	MG	1A	3135	1/1	0.91	0.24	30,30,30,30	0
56	MG	1A	3732	1/1	0.91	0.13	55,55,55,55	0
56	MG	2a	1698	1/1	0.91	0.14	64,64,64,64	0
56	MG	1A	3734	1/1	0.91	0.14	58,58,58,58	0
56	MG	2A	3605	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3843	1/1	0.91	0.30	47,47,47,47	0
56	MG	1A	3535	1/1	0.91	0.11	40,40,40,40	0
56	MG	2A	3133	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3743	1/1	0.91	0.27	52,52,52,52	0
56	MG	2A	3364	1/1	0.91	0.18	55,55,55,55	0
56	MG	2a	1716	1/1	0.91	0.22	69,69,69,69	0
56	MG	1a	1820	1/1	0.91	0.21	72,72,72,72	0
56	MG	1a	1675	1/1	0.91	0.08	41,41,41,41	0
56	MG	2A	3618	1/1	0.91	0.33	45,45,45,45	0
56	MG	2A	3378	1/1	0.91	0.10	40,40,40,40	0
56	MG	1A	3536	1/1	0.91	0.17	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3637	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3622	1/1	0.91	0.59	49,49,49,49	0
56	MG	1A	3854	1/1	0.91	0.13	67,67,67,67	0
56	MG	1A	3277	1/1	0.91	0.18	49,49,49,49	0
56	MG	1a	1685	1/1	0.91	0.23	57,57,57,57	0
56	MG	2a	1738	1/1	0.91	0.29	70,70,70,70	0
56	MG	1A	3540	1/1	0.91	0.19	55,55,55,55	0
56	MG	2A	3153	1/1	0.91	0.28	59,59,59,59	0
56	MG	1d	502	1/1	0.91	0.37	58,58,58,58	0
56	MG	2A	3158	1/1	0.91	0.19	47,47,47,47	0
56	MG	2A	3405	1/1	0.91	0.20	58,58,58,58	0
56	MG	2A	3406	1/1	0.91	0.23	58,58,58,58	0
56	MG	2a	1759	1/1	0.91	0.11	75,75,75,75	0
56	MG	1f	3001	1/1	0.91	0.12	42,42,42,42	0
56	MG	2A	3409	1/1	0.91	0.16	46,46,46,46	0
56	MG	2A	3410	1/1	0.91	0.20	56,56,56,56	0
56	MG	2a	1766	1/1	0.91	0.12	48,48,48,48	0
56	MG	2a	1767	1/1	0.91	0.17	55,55,55,55	0
56	MG	2A	3166	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3650	1/1	0.91	0.13	55,55,55,55	0
56	MG	2a	1772	1/1	0.91	0.10	76,76,76,76	0
56	MG	1A	3081	1/1	0.91	0.41	35,35,35,35	0
56	MG	2A	3170	1/1	0.91	0.20	68,68,68,68	0
56	MG	1A	3311	1/1	0.91	0.10	54,54,54,54	0
56	MG	1Z	302	1/1	0.91	0.17	48,48,48,48	0
56	MG	2A	3419	1/1	0.91	0.17	60,60,60,60	0
56	MG	1a	1699	1/1	0.91	0.19	68,68,68,68	0
56	MG	2a	1785	1/1	0.91	0.15	58,58,58,58	0
56	MG	2a	1787	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3754	1/1	0.91	0.22	26,26,26,26	0
56	MG	1x	103	1/1	0.91	0.59	54,54,54,54	0
56	MG	2A	3186	1/1	0.91	0.16	51,51,51,51	0
56	MG	1A	3644	1/1	0.91	0.09	51,51,51,51	0
56	MG	2a	1792	1/1	0.91	0.23	76,76,76,76	0
56	MG	1A	3355	1/1	0.91	0.23	51,51,51,51	0
56	MG	2B	3007	1/1	0.91	0.18	74,74,74,74	0
56	MG	1x	110	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3651	1/1	0.91	0.11	62,62,62,62	0
56	MG	2d	502	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3463	1/1	0.91	0.18	57,57,57,57	0
56	MG	2B	3012	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3446	1/1	0.91	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3357	1/1	0.91	0.21	60,60,60,60	0
56	MG	2A	3203	1/1	0.91	0.27	42,42,42,42	0
56	MG	1A	3662	1/1	0.91	0.19	45,45,45,45	0
56	MG	2A	3208	1/1	0.91	0.08	52,52,52,52	0
56	MG	2t	3001	1/1	0.91	0.06	57,57,57,57	0
56	MG	1A	3140	1/1	0.91	0.57	47,47,47,47	0
56	MG	1A	3059	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3089	1/1	0.91	0.22	54,54,54,54	0
56	MG	1A	3874	1/1	0.91	0.21	27,27,27,27	0
56	MG	2A	3001	1/1	0.91	0.30	63,63,63,63	0
56	MG	2G	3001	1/1	0.91	0.11	58,58,58,58	0
56	MG	2O	201	1/1	0.91	0.22	54,54,54,54	0
61	FME	1x	115	10/11	0.91	0.43	38,46,53,57	10
56	MG	2A	3471	1/1	0.91	0.14	48,48,48,48	0
56	MG	1a	1814	1/1	0.92	0.22	74,74,74,74	0
56	MG	1A	3655	1/1	0.92	0.15	28,28,28,28	0
56	MG	1A	3167	1/1	0.92	0.21	50,50,50,50	0
56	MG	1a	1678	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3114	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3661	1/1	0.92	0.11	51,51,51,51	0
56	MG	1a	1680	1/1	0.92	0.15	48,48,48,48	0
56	MG	2A	3301	1/1	0.92	0.10	58,58,58,58	0
56	MG	2A	3303	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3252	1/1	0.92	0.46	47,47,47,47	0
56	MG	1a	1824	1/1	0.92	0.11	69,69,69,69	0
56	MG	1A	3663	1/1	0.92	0.12	43,43,43,43	0
56	MG	1A	3376	1/1	0.92	0.21	51,51,51,51	0
56	MG	1W	3004	1/1	0.92	0.11	41,41,41,41	0
56	MG	2A	3539	1/1	0.92	0.07	63,63,63,63	0
56	MG	2A	3311	1/1	0.92	0.18	46,46,46,46	0
56	MG	1b	3001	1/1	0.92	0.27	68,68,68,68	0
56	MG	2a	1622	1/1	0.92	0.11	42,42,42,42	0
56	MG	1Y	502	1/1	0.92	0.23	60,60,60,60	0
56	MG	2A	3131	1/1	0.92	0.18	55,55,55,55	0
56	MG	2A	3319	1/1	0.92	0.13	40,40,40,40	0
56	MG	1A	3769	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	3485	1/1	0.92	0.28	51,51,51,51	0
56	MG	1A	3671	1/1	0.92	0.18	40,40,40,40	0
56	MG	1A	3377	1/1	0.92	0.16	42,42,42,42	0
56	MG	2A	3327	1/1	0.92	0.11	48,48,48,48	0
56	MG	1A	3488	1/1	0.92	0.23	32,32,32,32	0
56	MG	2a	1638	1/1	0.92	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1639	1/1	0.92	0.13	54,54,54,54	0
56	MG	2a	1640	1/1	0.92	0.16	48,48,48,48	0
56	MG	1t	3001	1/1	0.92	0.13	49,49,49,49	0
56	MG	2A	3563	1/1	0.92	0.36	62,62,62,62	0
56	MG	2A	3139	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3585	1/1	0.92	0.14	34,34,34,34	0
56	MG	2A	3146	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3587	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3319	1/1	0.92	0.33	51,51,51,51	0
56	MG	2A	3572	1/1	0.92	0.06	49,49,49,49	0
56	MG	1a	1707	1/1	0.92	0.27	49,49,49,49	0
56	MG	2a	1659	1/1	0.92	0.17	55,55,55,55	0
56	MG	1x	105	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3491	1/1	0.92	0.12	46,46,46,46	0
56	MG	2a	1664	1/1	0.92	0.11	60,60,60,60	0
56	MG	2A	3344	1/1	0.92	0.16	31,31,31,31	0
56	MG	1A	3017	1/1	0.92	0.15	53,53,53,53	0
56	MG	2a	1669	1/1	0.92	0.16	67,67,67,67	0
56	MG	1A	3437	1/1	0.92	0.15	24,24,24,24	0
56	MG	2A	3160	1/1	0.92	0.07	36,36,36,36	0
56	MG	1a	1714	1/1	0.92	0.23	61,61,61,61	0
56	MG	2A	3362	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3292	1/1	0.92	0.13	33,33,33,33	0
56	MG	2A	3167	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3790	1/1	0.92	0.09	48,48,48,48	0
56	MG	2a	1679	1/1	0.92	0.15	66,66,66,66	0
56	MG	2A	3375	1/1	0.92	0.06	51,51,51,51	0
56	MG	1A	3500	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	3607	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3255	1/1	0.92	0.28	44,44,44,44	0
56	MG	2A	3389	1/1	0.92	0.09	39,39,39,39	0
56	MG	1A	3332	1/1	0.92	0.18	50,50,50,50	0
56	MG	1A	3798	1/1	0.92	0.14	27,27,27,27	0
56	MG	1a	1726	1/1	0.92	0.10	87,87,87,87	0
56	MG	1A	3013	1/1	0.92	0.21	33,33,33,33	0
56	MG	1A	3697	1/1	0.92	0.27	64,64,64,64	0
56	MG	2A	3017	1/1	0.92	0.15	42,42,42,42	0
56	MG	1a	1612	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	3698	1/1	0.92	0.29	65,65,65,65	0
56	MG	1A	3926	1/1	0.92	0.25	44,44,44,44	0
56	MG	1A	3394	1/1	0.92	0.18	43,43,43,43	0
56	MG	2A	3034	1/1	0.92	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1702	1/1	0.92	0.20	64,64,64,64	0
56	MG	2a	1703	1/1	0.92	0.10	76,76,76,76	0
56	MG	1A	3447	1/1	0.92	0.21	20,20,20,20	0
56	MG	1A	3807	1/1	0.92	0.14	63,63,63,63	0
56	MG	1B	202	1/1	0.92	0.16	61,61,61,61	0
56	MG	1A	3702	1/1	0.92	0.18	26,26,26,26	0
56	MG	2A	3414	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3626	1/1	0.92	0.08	51,51,51,51	0
56	MG	2A	3415	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	3618	1/1	0.92	0.16	29,29,29,29	0
56	MG	1A	3016	1/1	0.92	0.07	39,39,39,39	0
56	MG	2A	3635	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3055	1/1	0.92	0.11	47,47,47,47	0
56	MG	1a	1628	1/1	0.92	0.27	43,43,43,43	0
56	MG	2a	1731	1/1	0.92	0.16	87,87,87,87	0
56	MG	1B	216	1/1	0.92	0.14	58,58,58,58	0
56	MG	1A	3219	1/1	0.92	0.19	57,57,57,57	0
56	MG	1A	3270	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3644	1/1	0.92	0.08	45,45,45,45	0
56	MG	1a	1762	1/1	0.92	0.18	64,64,64,64	0
56	MG	1A	3099	1/1	0.92	0.13	44,44,44,44	0
56	MG	2a	1744	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3432	1/1	0.92	0.12	37,37,37,37	0
56	MG	2A	3651	1/1	0.92	0.26	54,54,54,54	0
56	MG	2a	1748	1/1	0.92	0.13	59,59,59,59	0
56	MG	2A	3652	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3654	1/1	0.92	0.28	42,42,42,42	0
56	MG	1A	3629	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1756	1/1	0.92	0.14	78,78,78,78	0
56	MG	2A	3656	1/1	0.92	0.22	58,58,58,58	0
56	MG	2A	3435	1/1	0.92	0.15	45,45,45,45	0
56	MG	1A	3305	1/1	0.92	0.14	55,55,55,55	0
56	MG	2A	3666	1/1	0.92	0.13	47,47,47,47	0
56	MG	1D	301	1/1	0.92	0.23	40,40,40,40	0
56	MG	2A	3668	1/1	0.92	0.20	44,44,44,44	0
56	MG	1A	3344	1/1	0.92	0.26	40,40,40,40	0
56	MG	1a	1650	1/1	0.92	0.23	57,57,57,57	0
56	MG	2a	1771	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	1654	1/1	0.92	0.24	46,46,46,46	0
56	MG	1A	3542	1/1	0.92	0.19	33,33,33,33	0
56	MG	1A	3635	1/1	0.92	0.20	66,66,66,66	0
56	MG	1A	3067	1/1	0.92	0.58	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1778	1/1	0.92	0.23	78,78,78,78	0
56	MG	2A	3464	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3137	1/1	0.92	0.27	45,45,45,45	0
56	MG	2B	3008	1/1	0.92	0.21	61,61,61,61	0
56	MG	2A	3245	1/1	0.92	0.15	55,55,55,55	0
56	MG	2a	1786	1/1	0.92	0.14	64,64,64,64	0
56	MG	1A	3048	1/1	0.92	0.16	32,32,32,32	0
56	MG	2A	3248	1/1	0.92	0.13	43,43,43,43	0
56	MG	1a	1794	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3473	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3204	1/1	0.92	0.08	38,38,38,38	0
56	MG	2A	3254	1/1	0.92	0.15	36,36,36,36	0
56	MG	2B	3020	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3416	1/1	0.92	0.12	25,25,25,25	0
56	MG	1A	3571	1/1	0.92	0.21	33,33,33,33	0
56	MG	2D	304	1/1	0.92	0.54	38,38,38,38	0
56	MG	2a	1800	1/1	0.92	0.13	82,82,82,82	0
56	MG	2E	302	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3483	1/1	0.92	0.27	56,56,56,56	0
56	MG	2A	3095	1/1	0.92	0.75	65,65,65,65	0
56	MG	1A	3166	1/1	0.92	0.24	65,65,65,65	0
56	MG	2A	3273	1/1	0.92	0.12	47,47,47,47	0
56	MG	2A	3492	1/1	0.92	0.10	59,59,59,59	0
56	MG	2l	202	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3359	1/1	0.92	0.14	22,22,22,22	0
56	MG	2A	3495	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3850	1/1	0.92	0.12	54,54,54,54	0
56	MG	1a	1808	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	3207	1/1	0.92	0.15	50,50,50,50	0
56	MG	2A	3283	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3504	1/1	0.92	0.09	55,55,55,55	0
59	ZN	15	103	1/1	0.92	0.29	81,81,81,81	0
56	MG	1A	3853	1/1	0.92	0.12	37,37,37,37	0
56	MG	20	101	1/1	0.92	0.44	68,68,68,68	0
59	ZN	29	501	1/1	0.92	0.09	64,64,64,64	0
56	MG	2A	3507	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	3654	1/1	0.92	0.12	27,27,27,27	0
56	MG	2A	3288	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3464	1/1	0.93	0.10	57,57,57,57	0
56	MG	1a	1803	1/1	0.93	0.28	69,69,69,69	0
56	MG	1A	3100	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	3300	1/1	0.93	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3519	1/1	0.93	0.08	64,64,64,64	0
56	MG	2A	3520	1/1	0.93	0.16	56,56,56,56	0
56	MG	2A	3109	1/1	0.93	0.08	40,40,40,40	0
56	MG	1A	3217	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3527	1/1	0.93	0.15	34,34,34,34	0
56	MG	1A	3645	1/1	0.93	0.09	58,58,58,58	0
56	MG	1F	305	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3472	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3647	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3648	1/1	0.93	0.19	69,69,69,69	0
56	MG	2A	3306	1/1	0.93	0.12	30,30,30,30	0
56	MG	1A	3413	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3842	1/1	0.93	0.17	56,56,56,56	0
56	MG	1O	8003	1/1	0.93	0.22	54,54,54,54	0
56	MG	2a	1620	1/1	0.93	0.20	55,55,55,55	0
56	MG	2a	1621	1/1	0.93	0.08	80,80,80,80	0
56	MG	1a	1821	1/1	0.93	0.16	65,65,65,65	0
56	MG	2A	3314	1/1	0.93	0.13	39,39,39,39	0
56	MG	1A	3272	1/1	0.93	0.22	39,39,39,39	0
56	MG	2A	3123	1/1	0.93	0.52	52,52,52,52	0
56	MG	2A	3124	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3548	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3303	1/1	0.93	0.26	28,28,28,28	0
56	MG	1Q	3003	1/1	0.93	0.17	41,41,41,41	0
56	MG	2A	3322	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	1635	1/1	0.93	0.18	61,61,61,61	0
56	MG	2A	3130	1/1	0.93	0.14	66,66,66,66	0
56	MG	1A	3354	1/1	0.93	0.11	42,42,42,42	0
56	MG	1A	3658	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3558	1/1	0.93	0.10	64,64,64,64	0
56	MG	1A	3849	1/1	0.93	0.07	46,46,46,46	0
56	MG	2A	3562	1/1	0.93	0.10	60,60,60,60	0
56	MG	2a	1646	1/1	0.93	0.22	68,68,68,68	0
56	MG	2a	1647	1/1	0.93	0.10	68,68,68,68	0
56	MG	1a	1834	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3565	1/1	0.93	0.22	45,45,45,45	0
56	MG	1A	3197	1/1	0.93	0.17	44,44,44,44	0
56	MG	2a	1653	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3567	1/1	0.93	0.28	54,54,54,54	0
56	MG	1A	3275	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3220	1/1	0.93	0.21	31,31,31,31	0
56	MG	1A	3757	1/1	0.93	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3143	1/1	0.93	0.21	56,56,56,56	0
56	MG	1a	1687	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3221	1/1	0.93	0.27	30,30,30,30	0
56	MG	1a	1693	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3761	1/1	0.93	0.15	71,71,71,71	0
56	MG	2a	1666	1/1	0.93	0.13	63,63,63,63	0
56	MG	2A	3579	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3666	1/1	0.93	0.19	45,45,45,45	0
56	MG	1X	102	1/1	0.93	0.19	38,38,38,38	0
56	MG	2A	3584	1/1	0.93	0.08	36,36,36,36	0
56	MG	1w	3004	1/1	0.93	0.07	57,57,57,57	0
56	MG	2A	3352	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3764	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3588	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3361	1/1	0.93	0.20	55,55,55,55	0
56	MG	1x	104	1/1	0.93	0.19	50,50,50,50	0
56	MG	1A	3053	1/1	0.93	0.15	48,48,48,48	0
56	MG	2A	3164	1/1	0.93	0.60	40,40,40,40	0
56	MG	2A	3595	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3430	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3280	1/1	0.93	0.21	44,44,44,44	0
56	MG	2A	3377	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	3598	1/1	0.93	0.16	61,61,61,61	0
56	MG	2A	3379	1/1	0.93	0.12	35,35,35,35	0
56	MG	2A	3603	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3169	1/1	0.93	0.19	41,41,41,41	0
56	MG	1A	3114	1/1	0.93	0.26	41,41,41,41	0
56	MG	1A	3601	1/1	0.93	0.11	49,49,49,49	0
56	MG	1A	3282	1/1	0.93	0.25	58,58,58,58	0
56	MG	2A	3611	1/1	0.93	0.15	57,57,57,57	0
56	MG	2A	3612	1/1	0.93	0.32	56,56,56,56	0
56	MG	1A	3678	1/1	0.93	0.08	46,46,46,46	0
56	MG	2A	3176	1/1	0.93	0.20	37,37,37,37	0
56	MG	2A	3400	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3178	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3779	1/1	0.93	0.18	70,70,70,70	0
56	MG	2a	1707	1/1	0.93	0.15	43,43,43,43	0
56	MG	1A	3378	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3181	1/1	0.93	0.17	55,55,55,55	0
56	MG	2A	3183	1/1	0.93	0.13	29,29,29,29	0
56	MG	16	102	1/1	0.93	0.24	41,41,41,41	0
56	MG	2a	1720	1/1	0.93	0.13	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	19	502	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3408	1/1	0.93	0.14	54,54,54,54	0
56	MG	1a	1723	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3005	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3631	1/1	0.93	0.05	57,57,57,57	0
56	MG	1A	3875	1/1	0.93	0.13	22,22,22,22	0
56	MG	1A	3682	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3196	1/1	0.93	0.30	47,47,47,47	0
56	MG	1A	3203	1/1	0.93	0.23	45,45,45,45	0
56	MG	2A	3636	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3200	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3061	1/1	0.93	0.20	38,38,38,38	0
56	MG	1A	3787	1/1	0.93	0.14	62,62,62,62	0
56	MG	1a	1729	1/1	0.93	0.22	67,67,67,67	0
56	MG	1a	1606	1/1	0.93	0.23	57,57,57,57	0
56	MG	1a	1733	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3514	1/1	0.93	0.26	66,66,66,66	0
56	MG	1A	3441	1/1	0.93	0.13	50,50,50,50	0
56	MG	2a	1750	1/1	0.93	0.22	66,66,66,66	0
56	MG	1A	3141	1/1	0.93	0.55	44,44,44,44	0
56	MG	2A	3429	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3289	1/1	0.93	0.31	44,44,44,44	0
56	MG	1a	1744	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3691	1/1	0.93	0.11	60,60,60,60	0
56	MG	2a	1761	1/1	0.93	0.11	71,71,71,71	0
56	MG	1A	3524	1/1	0.93	0.14	32,32,32,32	0
56	MG	1A	3131	1/1	0.93	0.28	40,40,40,40	0
56	MG	2A	3438	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3059	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3323	1/1	0.93	0.23	55,55,55,55	0
56	MG	1A	3924	1/1	0.93	0.13	49,49,49,49	0
56	MG	2A	3452	1/1	0.93	0.15	32,32,32,32	0
56	MG	1A	3209	1/1	0.93	0.15	55,55,55,55	0
56	MG	1a	1621	1/1	0.93	0.12	70,70,70,70	0
56	MG	2A	3677	1/1	0.93	0.91	49,49,49,49	0
56	MG	2A	3069	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3454	1/1	0.93	0.16	24,24,24,24	0
56	MG	2A	3463	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3935	1/1	0.93	0.24	40,40,40,40	0
56	MG	1A	3143	1/1	0.93	0.18	48,48,48,48	0
56	MG	2a	1784	1/1	0.93	0.28	87,87,87,87	0
56	MG	1A	3804	1/1	0.93	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3468	1/1	0.93	0.26	43,43,43,43	0
56	MG	1A	3805	1/1	0.93	0.16	52,52,52,52	0
56	MG	1B	203	1/1	0.93	0.17	33,33,33,33	0
56	MG	1A	3335	1/1	0.93	0.19	63,63,63,63	0
56	MG	2A	3079	1/1	0.93	0.11	42,42,42,42	0
56	MG	2B	3017	1/1	0.93	0.18	59,59,59,59	0
56	MG	2A	3474	1/1	0.93	0.08	41,41,41,41	0
56	MG	1a	1775	1/1	0.93	0.24	58,58,58,58	0
56	MG	2A	3478	1/1	0.93	0.08	53,53,53,53	0
56	MG	1B	206	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3082	1/1	0.93	0.12	40,40,40,40	0
56	MG	2A	3255	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3632	1/1	0.93	0.31	40,40,40,40	0
56	MG	1a	1638	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3259	1/1	0.93	0.17	30,30,30,30	0
56	MG	1A	3293	1/1	0.93	0.20	60,60,60,60	0
56	MG	2A	3269	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3133	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3811	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3091	1/1	0.93	0.14	45,45,45,45	0
56	MG	2O	202	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3714	1/1	0.93	0.14	56,56,56,56	0
56	MG	2A	3499	1/1	0.93	0.29	35,35,35,35	0
56	MG	2Q	3003	1/1	0.93	0.28	48,48,48,48	0
56	MG	2x	3002	1/1	0.93	0.06	72,72,72,72	0
56	MG	1a	1648	1/1	0.93	0.12	48,48,48,48	0
56	MG	2T	3001	1/1	0.93	0.18	45,45,45,45	0
56	MG	1A	3554	1/1	0.93	0.12	42,42,42,42	0
56	MG	2V	3002	1/1	0.93	0.53	57,57,57,57	0
56	MG	1A	3823	1/1	0.93	0.12	67,67,67,67	0
56	MG	2A	3284	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3262	1/1	0.93	0.33	31,31,31,31	0
56	MG	1a	1798	1/1	0.93	0.10	67,67,67,67	0
56	MG	1A	3083	1/1	0.93	0.16	37,37,37,37	0
56	MG	2A	3451	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3199	1/1	0.94	0.39	60,60,60,60	0
56	MG	1A	3044	1/1	0.94	0.12	22,22,22,22	0
56	MG	1A	3387	1/1	0.94	0.16	18,18,18,18	0
56	MG	2A	3455	1/1	0.94	0.21	39,39,39,39	0
56	MG	1A	3679	1/1	0.94	0.15	61,61,61,61	0
56	MG	1y	3003	1/1	0.94	0.24	59,59,59,59	0
56	MG	1E	307	1/1	0.94	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3161	1/1	0.94	0.16	32,32,32,32	0
56	MG	1F	301	1/1	0.94	0.21	49,49,49,49	0
56	MG	1a	1690	1/1	0.94	0.16	35,35,35,35	0
56	MG	2A	3004	1/1	0.94	0.20	50,50,50,50	0
56	MG	2A	3216	1/1	0.94	0.19	57,57,57,57	0
56	MG	2A	3217	1/1	0.94	0.11	68,68,68,68	0
56	MG	1A	3162	1/1	0.94	0.23	39,39,39,39	0
56	MG	2U	202	1/1	0.94	0.28	44,44,44,44	0
56	MG	1A	3579	1/1	0.94	0.16	27,27,27,27	0
56	MG	1a	1696	1/1	0.94	0.17	47,47,47,47	0
56	MG	2V	3003	1/1	0.94	0.15	48,48,48,48	0
56	MG	2A	3476	1/1	0.94	0.17	41,41,41,41	0
56	MG	2A	3221	1/1	0.94	0.15	35,35,35,35	0
56	MG	1A	3199	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3032	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3480	1/1	0.94	0.09	52,52,52,52	0
56	MG	23	101	1/1	0.94	0.42	62,62,62,62	0
56	MG	25	502	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3022	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3023	1/1	0.94	0.36	43,43,43,43	0
56	MG	1A	3080	1/1	0.94	0.34	41,41,41,41	0
56	MG	2A	3025	1/1	0.94	0.76	60,60,60,60	0
56	MG	2A	3486	1/1	0.94	0.25	58,58,58,58	0
56	MG	2A	3028	1/1	0.94	0.33	40,40,40,40	0
56	MG	2A	3490	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3235	1/1	0.94	0.13	53,53,53,53	0
56	MG	1A	3168	1/1	0.94	0.09	44,44,44,44	0
56	MG	1N	3006	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3035	1/1	0.94	0.28	41,41,41,41	0
56	MG	1A	3329	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3037	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3814	1/1	0.94	0.12	39,39,39,39	0
56	MG	1A	3817	1/1	0.94	0.24	54,54,54,54	0
56	MG	1a	1711	1/1	0.94	0.19	68,68,68,68	0
56	MG	2A	3045	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3821	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3506	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3693	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3050	1/1	0.94	0.15	55,55,55,55	0
56	MG	2A	3054	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3404	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3003	1/1	0.94	0.28	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3514	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3333	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3516	1/1	0.94	0.17	46,46,46,46	0
56	MG	1T	202	1/1	0.94	0.14	43,43,43,43	0
56	MG	1A	3597	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3066	1/1	0.94	0.08	39,39,39,39	0
56	MG	2A	3271	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3522	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3525	1/1	0.94	0.09	64,64,64,64	0
56	MG	1U	202	1/1	0.94	0.47	40,40,40,40	0
56	MG	1V	201	1/1	0.94	0.21	55,55,55,55	0
56	MG	1A	3409	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3208	1/1	0.94	0.47	42,42,42,42	0
56	MG	1A	3486	1/1	0.94	0.23	27,27,27,27	0
56	MG	1A	3603	1/1	0.94	0.24	54,54,54,54	0
56	MG	1A	3709	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3074	1/1	0.94	0.14	50,50,50,50	0
56	MG	1X	101	1/1	0.94	0.17	38,38,38,38	0
56	MG	2a	1654	1/1	0.94	0.23	69,69,69,69	0
56	MG	1A	3711	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3411	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3078	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3172	1/1	0.94	0.23	41,41,41,41	0
56	MG	1a	1739	1/1	0.94	0.15	70,70,70,70	0
56	MG	1A	3336	1/1	0.94	0.21	28,28,28,28	0
56	MG	1A	3844	1/1	0.94	0.14	54,54,54,54	0
56	MG	2a	1663	1/1	0.94	0.21	55,55,55,55	0
56	MG	1A	3715	1/1	0.94	0.17	69,69,69,69	0
56	MG	2A	3300	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3608	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3105	1/1	0.94	0.21	39,39,39,39	0
56	MG	1A	3848	1/1	0.94	0.19	66,66,66,66	0
56	MG	2A	3554	1/1	0.94	0.11	44,44,44,44	0
56	MG	2a	1671	1/1	0.94	0.10	86,86,86,86	0
56	MG	2A	3555	1/1	0.94	0.11	47,47,47,47	0
56	MG	1a	1748	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3721	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3307	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3110	1/1	0.94	0.29	38,38,38,38	0
56	MG	1A	3724	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3497	1/1	0.94	0.12	26,26,26,26	0
56	MG	1A	3214	1/1	0.94	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3002	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	3086	1/1	0.94	0.15	51,51,51,51	0
56	MG	1a	1764	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3858	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3620	1/1	0.94	0.21	43,43,43,43	0
56	MG	1a	1769	1/1	0.94	0.26	58,58,58,58	0
56	MG	2A	3106	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3573	1/1	0.94	0.05	52,52,52,52	0
56	MG	1A	3422	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3507	1/1	0.94	0.10	60,60,60,60	0
56	MG	1A	3744	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3510	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	3087	1/1	0.94	0.20	63,63,63,63	0
56	MG	1A	3627	1/1	0.94	0.18	66,66,66,66	0
56	MG	2A	3332	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3298	1/1	0.94	0.23	53,53,53,53	0
56	MG	1a	1789	1/1	0.94	0.15	75,75,75,75	0
56	MG	1A	3006	1/1	0.94	0.14	42,42,42,42	0
56	MG	1a	1613	1/1	0.94	0.30	47,47,47,47	0
56	MG	1A	3185	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3116	1/1	0.94	0.71	51,51,51,51	0
56	MG	1A	3523	1/1	0.94	0.21	33,33,33,33	0
56	MG	2a	1713	1/1	0.94	0.19	52,52,52,52	0
56	MG	2A	3342	1/1	0.94	0.12	43,43,43,43	0
56	MG	1a	1795	1/1	0.94	0.19	50,50,50,50	0
56	MG	2a	1717	1/1	0.94	0.07	63,63,63,63	0
56	MG	2a	1719	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3259	1/1	0.94	0.20	37,37,37,37	0
56	MG	2A	3345	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3636	1/1	0.94	0.20	51,51,51,51	0
56	MG	2A	3348	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3356	1/1	0.94	0.16	26,26,26,26	0
56	MG	1A	3883	1/1	0.94	0.27	33,33,33,33	0
56	MG	1A	3759	1/1	0.94	0.23	43,43,43,43	0
56	MG	2a	1730	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3530	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3887	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3609	1/1	0.94	0.11	52,52,52,52	0
56	MG	1a	1627	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3224	1/1	0.94	0.17	32,32,32,32	0
56	MG	2A	3371	1/1	0.94	0.07	41,41,41,41	0
56	MG	2a	1741	1/1	0.94	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3372	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	3891	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3615	1/1	0.94	0.11	69,69,69,69	0
56	MG	1a	1632	1/1	0.94	0.10	78,78,78,78	0
56	MG	2a	1747	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3376	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3532	1/1	0.94	0.10	59,59,59,59	0
56	MG	2A	3142	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3534	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3380	1/1	0.94	0.09	48,48,48,48	0
56	MG	1a	1636	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3145	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3387	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3304	1/1	0.94	0.11	39,39,39,39	0
56	MG	1A	3226	1/1	0.94	0.23	57,57,57,57	0
56	MG	2A	3392	1/1	0.94	0.20	51,51,51,51	0
56	MG	2a	1765	1/1	0.94	0.16	61,61,61,61	0
56	MG	1A	3770	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3090	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3397	1/1	0.94	0.08	56,56,56,56	0
56	MG	2A	3399	1/1	0.94	0.09	58,58,58,58	0
56	MG	2A	3151	1/1	0.94	0.23	44,44,44,44	0
56	MG	1A	3307	1/1	0.94	0.24	33,33,33,33	0
56	MG	1a	1643	1/1	0.94	0.28	61,61,61,61	0
56	MG	1A	3541	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	3921	1/1	0.94	0.24	38,38,38,38	0
56	MG	2a	1777	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3159	1/1	0.94	0.27	44,44,44,44	0
56	MG	1A	3309	1/1	0.94	0.24	66,66,66,66	0
56	MG	2A	3645	1/1	0.94	0.19	72,72,72,72	0
56	MG	1A	3925	1/1	0.94	0.30	44,44,44,44	0
56	MG	1A	3545	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3546	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3366	1/1	0.94	0.13	38,38,38,38	0
56	MG	1A	3228	1/1	0.94	0.26	51,51,51,51	0
56	MG	2A	3653	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3555	1/1	0.94	0.25	40,40,40,40	0
56	MG	1A	3782	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3556	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3784	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3031	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3312	1/1	0.94	0.34	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1795	1/1	0.94	0.20	76,76,76,76	0
56	MG	1A	3562	1/1	0.94	0.16	29,29,29,29	0
56	MG	2A	3420	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3669	1/1	0.94	0.14	68,68,68,68	0
56	MG	1w	3002	1/1	0.94	0.06	37,37,37,37	0
56	MG	2A	3422	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3070	1/1	0.94	0.29	60,60,60,60	0
56	MG	1A	3565	1/1	0.94	0.20	29,29,29,29	0
56	MG	2g	8001	1/1	0.94	0.14	65,65,65,65	0
56	MG	2A	3678	1/1	0.94	0.93	49,49,49,49	0
56	MG	1A	3566	1/1	0.94	0.18	32,32,32,32	0
56	MG	2A	3184	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3567	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3094	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3431	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3383	1/1	0.94	0.13	31,31,31,31	0
56	MG	2A	3433	1/1	0.94	0.12	34,34,34,34	0
56	MG	2A	3190	1/1	0.94	0.26	37,37,37,37	0
57	4M2	2A	3670	57/57	0.94	0.29	26,50,69,76	0
56	MG	1A	3315	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3192	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3437	1/1	0.94	0.08	36,36,36,36	0
56	MG	1x	108	1/1	0.94	0.09	55,55,55,55	0
59	ZN	2Y	501	1/1	0.94	0.07	85,85,85,85	0
56	MG	1D	305	1/1	0.94	0.18	38,38,38,38	0
56	MG	2A	3443	1/1	0.94	0.07	45,45,45,45	0
56	MG	1D	307	1/1	0.94	0.21	40,40,40,40	0
56	MG	1a	1682	1/1	0.94	0.19	43,43,43,43	0
56	MG	2A	3450	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3819	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	3118	1/1	0.95	0.54	50,50,50,50	0
56	MG	2E	305	1/1	0.95	0.16	39,39,39,39	0
56	MG	1G	3002	1/1	0.95	0.11	34,34,34,34	0
56	MG	2A	3457	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3331	1/1	0.95	0.14	37,37,37,37	0
56	MG	1G	3005	1/1	0.95	0.15	40,40,40,40	0
56	MG	1a	1691	1/1	0.95	0.15	47,47,47,47	0
56	MG	2N	8001	1/1	0.95	0.08	53,53,53,53	0
56	MG	2A	3465	1/1	0.95	0.09	33,33,33,33	0
56	MG	2A	3003	1/1	0.95	0.20	31,31,31,31	0
56	MG	1a	1692	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3600	1/1	0.95	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3700	1/1	0.95	0.13	71,71,71,71	0
56	MG	2A	3012	1/1	0.95	0.16	43,43,43,43	0
56	MG	2A	3014	1/1	0.95	0.29	41,41,41,41	0
56	MG	2A	3472	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3492	1/1	0.95	0.09	40,40,40,40	0
56	MG	1O	8002	1/1	0.95	0.15	63,63,63,63	0
56	MG	1A	3151	1/1	0.95	0.23	36,36,36,36	0
56	MG	2A	3019	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3021	1/1	0.95	0.20	29,29,29,29	0
56	MG	1a	1700	1/1	0.95	0.20	57,57,57,57	0
56	MG	2A	3232	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3233	1/1	0.95	0.15	48,48,48,48	0
56	MG	21	101	1/1	0.95	0.13	43,43,43,43	0
56	MG	21	102	1/1	0.95	0.10	45,45,45,45	0
56	MG	1P	202	1/1	0.95	0.17	30,30,30,30	0
56	MG	1a	1702	1/1	0.95	0.06	67,67,67,67	0
56	MG	1A	3072	1/1	0.95	0.19	35,35,35,35	0
56	MG	2A	3027	1/1	0.95	0.46	45,45,45,45	0
56	MG	2A	3488	1/1	0.95	0.21	50,50,50,50	0
56	MG	1A	3707	1/1	0.95	0.23	38,38,38,38	0
56	MG	2A	3241	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3030	1/1	0.95	0.89	48,48,48,48	0
56	MG	1A	3026	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	3077	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	3158	1/1	0.95	0.15	39,39,39,39	0
56	MG	2A	3496	1/1	0.95	0.05	54,54,54,54	0
56	MG	1A	3610	1/1	0.95	0.15	30,30,30,30	0
56	MG	2A	3036	1/1	0.95	0.10	50,50,50,50	0
56	MG	1a	1710	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3611	1/1	0.95	0.16	22,22,22,22	0
56	MG	1T	201	1/1	0.95	0.11	62,62,62,62	0
56	MG	1A	3286	1/1	0.95	0.14	39,39,39,39	0
56	MG	1a	1715	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3505	1/1	0.95	0.18	55,55,55,55	0
56	MG	2A	3260	1/1	0.95	0.13	27,27,27,27	0
56	MG	2A	3262	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3263	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3511	1/1	0.95	0.07	62,62,62,62	0
56	MG	2A	3264	1/1	0.95	0.22	52,52,52,52	0
56	MG	2A	3265	1/1	0.95	0.12	33,33,33,33	0
56	MG	2A	3047	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3004	1/1	0.95	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1U	203	1/1	0.95	0.59	40,40,40,40	0
56	MG	2A	3051	1/1	0.95	0.09	53,53,53,53	0
56	MG	1U	204	1/1	0.95	0.43	55,55,55,55	0
56	MG	2a	1633	1/1	0.95	0.15	71,71,71,71	0
56	MG	2a	1634	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3508	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3277	1/1	0.95	0.08	38,38,38,38	0
56	MG	2a	1637	1/1	0.95	0.10	60,60,60,60	0
56	MG	1A	3616	1/1	0.95	0.14	45,45,45,45	0
56	MG	2A	3523	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3058	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3339	1/1	0.95	0.20	32,32,32,32	0
56	MG	1A	3079	1/1	0.95	0.16	38,38,38,38	0
56	MG	2A	3062	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3421	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3240	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3851	1/1	0.95	0.10	50,50,50,50	0
56	MG	2a	1650	1/1	0.95	0.17	39,39,39,39	0
56	MG	1A	3163	1/1	0.95	0.25	43,43,43,43	0
56	MG	1X	103	1/1	0.95	0.16	40,40,40,40	0
56	MG	1a	1732	1/1	0.95	0.20	60,60,60,60	0
56	MG	1A	3733	1/1	0.95	0.28	48,48,48,48	0
56	MG	1A	3518	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3740	1/1	0.95	0.13	34,34,34,34	0
56	MG	10	102	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	3624	1/1	0.95	0.08	32,32,32,32	0
56	MG	2A	3545	1/1	0.95	0.07	66,66,66,66	0
56	MG	1A	3242	1/1	0.95	0.06	83,83,83,83	0
56	MG	1a	1742	1/1	0.95	0.12	20,20,20,20	0
56	MG	1a	1743	1/1	0.95	0.13	38,38,38,38	0
56	MG	10	106	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3164	1/1	0.95	0.17	53,53,53,53	0
56	MG	2a	1667	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3426	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3205	1/1	0.95	0.56	41,41,41,41	0
56	MG	1A	3631	1/1	0.95	0.14	36,36,36,36	0
56	MG	1A	3165	1/1	0.95	0.14	51,51,51,51	0
56	MG	15	102	1/1	0.95	0.18	39,39,39,39	0
56	MG	2A	3313	1/1	0.95	0.20	55,55,55,55	0
56	MG	1a	1751	1/1	0.95	0.12	65,65,65,65	0
56	MG	2A	3088	1/1	0.95	0.19	38,38,38,38	0
56	MG	1A	3431	1/1	0.95	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3866	1/1	0.95	0.13	63,63,63,63	0
56	MG	1A	3101	1/1	0.95	0.10	61,61,61,61	0
56	MG	1a	1757	1/1	0.95	0.11	57,57,57,57	0
56	MG	1a	1760	1/1	0.95	0.18	59,59,59,59	0
56	MG	18	101	1/1	0.95	0.25	37,37,37,37	0
56	MG	1A	3753	1/1	0.95	0.16	33,33,33,33	0
56	MG	1A	3297	1/1	0.95	0.16	62,62,62,62	0
56	MG	2A	3326	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3020	1/1	0.95	0.08	40,40,40,40	0
56	MG	1a	1766	1/1	0.95	0.07	48,48,48,48	0
56	MG	2a	1689	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3007	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3008	1/1	0.95	0.13	29,29,29,29	0
56	MG	1A	3107	1/1	0.95	0.12	24,24,24,24	0
56	MG	2A	3107	1/1	0.95	0.25	42,42,42,42	0
56	MG	2a	1694	1/1	0.95	0.15	62,62,62,62	0
56	MG	2a	1696	1/1	0.95	0.13	66,66,66,66	0
56	MG	1a	1605	1/1	0.95	0.15	71,71,71,71	0
56	MG	1a	1774	1/1	0.95	0.15	81,81,81,81	0
56	MG	1A	3171	1/1	0.95	0.20	56,56,56,56	0
56	MG	2A	3111	1/1	0.95	0.05	51,51,51,51	0
56	MG	1a	1776	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3362	1/1	0.95	0.13	60,60,60,60	0
56	MG	2a	1704	1/1	0.95	0.14	50,50,50,50	0
56	MG	1a	1784	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3879	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3881	1/1	0.95	0.15	46,46,46,46	0
56	MG	1a	1610	1/1	0.95	0.26	59,59,59,59	0
56	MG	2A	3118	1/1	0.95	0.17	33,33,33,33	0
56	MG	2a	1712	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3543	1/1	0.95	0.07	54,54,54,54	0
56	MG	2a	1714	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3050	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3138	1/1	0.95	0.54	36,36,36,36	0
56	MG	1A	3365	1/1	0.95	0.17	45,45,45,45	0
56	MG	2a	1718	1/1	0.95	0.11	71,71,71,71	0
56	MG	1A	3449	1/1	0.95	0.13	27,27,27,27	0
56	MG	2A	3601	1/1	0.95	0.08	38,38,38,38	0
56	MG	2A	3363	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3889	1/1	0.95	0.11	40,40,40,40	0
56	MG	2a	1724	1/1	0.95	0.16	77,77,77,77	0
56	MG	2A	3604	1/1	0.95	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3890	1/1	0.95	0.17	42,42,42,42	0
56	MG	2A	3606	1/1	0.95	0.31	40,40,40,40	0
56	MG	2A	3127	1/1	0.95	0.18	47,47,47,47	0
56	MG	1A	3451	1/1	0.95	0.12	21,21,21,21	0
56	MG	1A	3064	1/1	0.95	0.33	38,38,38,38	0
56	MG	1A	3895	1/1	0.95	0.17	39,39,39,39	0
56	MG	1a	1799	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	3653	1/1	0.95	0.16	31,31,31,31	0
56	MG	1a	1801	1/1	0.95	0.21	59,59,59,59	0
56	MG	1A	3774	1/1	0.95	0.10	61,61,61,61	0
56	MG	2a	1740	1/1	0.95	0.16	66,66,66,66	0
56	MG	2A	3136	1/1	0.95	0.19	53,53,53,53	0
56	MG	2a	1742	1/1	0.95	0.06	70,70,70,70	0
56	MG	2A	3382	1/1	0.95	0.21	40,40,40,40	0
56	MG	2A	3383	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3370	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3258	1/1	0.95	0.28	29,29,29,29	0
56	MG	1A	3456	1/1	0.95	0.13	23,23,23,23	0
56	MG	2A	3388	1/1	0.95	0.10	46,46,46,46	0
56	MG	1a	1806	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3037	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3915	1/1	0.95	0.24	36,36,36,36	0
56	MG	1A	3564	1/1	0.95	0.18	52,52,52,52	0
56	MG	2a	1753	1/1	0.95	0.12	72,72,72,72	0
56	MG	2a	1755	1/1	0.95	0.12	67,67,67,67	0
56	MG	1A	3178	1/1	0.95	0.26	38,38,38,38	0
56	MG	2A	3630	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3923	1/1	0.95	0.35	43,43,43,43	0
56	MG	2A	3398	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	3263	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3664	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3665	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	3929	1/1	0.95	0.36	39,39,39,39	0
56	MG	1A	3264	1/1	0.95	0.15	53,53,53,53	0
56	MG	2A	3638	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3266	1/1	0.95	0.37	50,50,50,50	0
56	MG	1A	3569	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3937	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3040	1/1	0.95	0.21	38,38,38,38	0
56	MG	1a	1651	1/1	0.95	0.36	56,56,56,56	0
56	MG	1a	1653	1/1	0.95	0.28	50,50,50,50	0
56	MG	1A	3223	1/1	0.95	0.30	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3269	1/1	0.95	0.22	57,57,57,57	0
56	MG	2a	1779	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3574	1/1	0.95	0.19	47,47,47,47	0
56	MG	2a	1781	1/1	0.95	0.26	64,64,64,64	0
56	MG	1A	3025	1/1	0.95	0.38	34,34,34,34	0
56	MG	1A	3576	1/1	0.95	0.22	24,24,24,24	0
56	MG	1A	3470	1/1	0.95	0.18	58,58,58,58	0
56	MG	1l	201	1/1	0.95	0.19	40,40,40,40	0
56	MG	2A	3417	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3115	1/1	0.95	0.26	46,46,46,46	0
56	MG	2A	3657	1/1	0.95	0.09	59,59,59,59	0
56	MG	1l	203	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3663	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	3680	1/1	0.95	0.15	54,54,54,54	0
56	MG	1a	1664	1/1	0.95	0.30	56,56,56,56	0
56	MG	1A	3071	1/1	0.95	0.18	27,27,27,27	0
56	MG	1A	3274	1/1	0.95	0.35	49,49,49,49	0
56	MG	1A	3146	1/1	0.95	0.20	38,38,38,38	0
56	MG	1w	3003	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3427	1/1	0.95	0.18	65,65,65,65	0
56	MG	2a	1798	1/1	0.95	0.09	43,43,43,43	0
56	MG	2a	1799	1/1	0.95	0.23	51,51,51,51	0
56	MG	2A	3673	1/1	0.95	0.30	47,47,47,47	0
56	MG	1A	3479	1/1	0.95	0.10	53,53,53,53	0
56	MG	1w	3005	1/1	0.95	0.07	65,65,65,65	0
56	MG	2A	3188	1/1	0.95	0.33	59,59,59,59	0
56	MG	1A	3276	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3149	1/1	0.95	0.62	50,50,50,50	0
56	MG	1A	3400	1/1	0.95	0.11	35,35,35,35	0
56	MG	2B	3004	1/1	0.95	0.21	50,50,50,50	0
56	MG	2l	201	1/1	0.95	0.42	77,77,77,77	0
56	MG	1A	3689	1/1	0.95	0.24	53,53,53,53	0
56	MG	1A	3401	1/1	0.95	0.15	38,38,38,38	0
56	MG	2q	203	1/1	0.95	0.05	59,59,59,59	0
56	MG	1E	305	1/1	0.95	0.17	26,26,26,26	0
56	MG	1A	3592	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3191	1/1	0.95	0.15	27,27,27,27	0
56	MG	1x	111	1/1	0.95	0.08	61,61,61,61	0
56	MG	1A	3326	1/1	0.95	0.16	44,44,44,44	0
57	4M2	1A	3894	57/57	0.95	0.27	21,37,55,60	0
56	MG	1A	3815	1/1	0.95	0.19	31,31,31,31	0
56	MG	2B	3016	1/1	0.95	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	K	2A	3242	1/1	0.95	0.18	65,65,65,65	0
56	MG	2A	3204	1/1	0.95	0.23	55,55,55,55	0
56	MG	2A	3448	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3449	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3205	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3328	1/1	0.95	0.26	61,61,61,61	0
56	MG	2D	301	1/1	0.95	0.53	46,46,46,46	0
56	MG	1A	3818	1/1	0.95	0.14	24,24,24,24	0
56	MG	2A	3209	1/1	0.95	0.10	44,44,44,44	0
56	MG	2E	301	1/1	0.95	0.10	39,39,39,39	0
56	MG	1B	215	1/1	0.96	0.08	26,26,26,26	0
56	MG	1A	3461	1/1	0.96	0.21	23,23,23,23	0
56	MG	1B	217	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3407	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3212	1/1	0.96	0.25	41,41,41,41	0
56	MG	2A	3287	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3717	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3718	1/1	0.96	0.14	23,23,23,23	0
56	MG	1a	1645	1/1	0.96	0.29	63,63,63,63	0
56	MG	2A	3098	1/1	0.96	0.12	32,32,32,32	0
56	MG	1a	1647	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3100	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	3129	1/1	0.96	0.27	41,41,41,41	0
56	MG	2A	3297	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3298	1/1	0.96	0.06	56,56,56,56	0
56	MG	1B	225	1/1	0.96	0.12	41,41,41,41	0
56	MG	2A	3517	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3824	1/1	0.96	0.17	53,53,53,53	0
56	MG	1D	303	1/1	0.96	0.32	49,49,49,49	0
56	MG	1A	3075	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3548	1/1	0.96	0.16	54,54,54,54	0
56	MG	1A	3265	1/1	0.96	0.23	41,41,41,41	0
56	MG	1A	3467	1/1	0.96	0.15	41,41,41,41	0
56	MG	1a	1807	1/1	0.96	0.20	58,58,58,58	0
56	MG	1A	3238	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3082	1/1	0.96	0.52	42,42,42,42	0
56	MG	1a	1660	1/1	0.96	0.26	56,56,56,56	0
56	MG	1A	3728	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3471	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3414	1/1	0.96	0.09	52,52,52,52	0
56	MG	1a	1817	1/1	0.96	0.16	64,64,64,64	0
56	MG	1A	3473	1/1	0.96	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3054	1/1	0.96	0.18	32,32,32,32	0
56	MG	2a	1630	1/1	0.96	0.26	62,62,62,62	0
56	MG	2a	1631	1/1	0.96	0.20	65,65,65,65	0
56	MG	1F	307	1/1	0.96	0.15	43,43,43,43	0
56	MG	1A	3736	1/1	0.96	0.28	49,49,49,49	0
56	MG	1A	3739	1/1	0.96	0.41	43,43,43,43	0
56	MG	1a	1671	1/1	0.96	0.23	48,48,48,48	0
56	MG	2A	3543	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3324	1/1	0.96	0.18	53,53,53,53	0
56	MG	1a	1825	1/1	0.96	0.12	66,66,66,66	0
56	MG	1A	3117	1/1	0.96	0.23	44,44,44,44	0
56	MG	1G	3004	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3128	1/1	0.96	0.20	33,33,33,33	0
56	MG	2a	1642	1/1	0.96	0.23	61,61,61,61	0
56	MG	2A	3549	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3742	1/1	0.96	0.17	54,54,54,54	0
56	MG	2A	3330	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3331	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3418	1/1	0.96	0.09	54,54,54,54	0
56	MG	1N	3002	1/1	0.96	0.25	45,45,45,45	0
56	MG	1N	3003	1/1	0.96	0.14	40,40,40,40	0
56	MG	2a	1652	1/1	0.96	0.11	57,57,57,57	0
56	MG	1A	3480	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3481	1/1	0.96	0.17	45,45,45,45	0
56	MG	1e	3001	1/1	0.96	0.13	71,71,71,71	0
56	MG	1A	3327	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3340	1/1	0.96	0.14	51,51,51,51	0
56	MG	1g	3001	1/1	0.96	0.17	54,54,54,54	0
56	MG	2A	3564	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3570	1/1	0.96	0.23	31,31,31,31	0
56	MG	1P	201	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3748	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3084	1/1	0.96	0.16	60,60,60,60	0
56	MG	1A	3271	1/1	0.96	0.16	33,33,33,33	0
56	MG	1A	3371	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3349	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3656	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3351	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3375	1/1	0.96	0.14	31,31,31,31	0
56	MG	2A	3353	1/1	0.96	0.18	35,35,35,35	0
56	MG	2a	1672	1/1	0.96	0.07	64,64,64,64	0
56	MG	2A	3576	1/1	0.96	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3354	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3108	1/1	0.96	0.30	36,36,36,36	0
56	MG	1A	3660	1/1	0.96	0.14	54,54,54,54	0
56	MG	2A	3359	1/1	0.96	0.07	54,54,54,54	0
56	MG	2A	3361	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3174	1/1	0.96	0.19	39,39,39,39	0
56	MG	1x	101	1/1	0.96	0.14	55,55,55,55	0
56	MG	1a	1697	1/1	0.96	0.31	51,51,51,51	0
56	MG	2A	3366	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3156	1/1	0.96	0.33	50,50,50,50	0
56	MG	2A	3370	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3427	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3864	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3373	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3428	1/1	0.96	0.16	39,39,39,39	0
56	MG	2A	3161	1/1	0.96	0.16	53,53,53,53	0
56	MG	2A	3162	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3762	1/1	0.96	0.16	68,68,68,68	0
56	MG	1A	3580	1/1	0.96	0.21	36,36,36,36	0
56	MG	1x	109	1/1	0.96	0.17	57,57,57,57	0
56	MG	1A	3023	1/1	0.96	0.20	42,42,42,42	0
56	MG	2A	3381	1/1	0.96	0.25	42,42,42,42	0
56	MG	1a	1705	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3765	1/1	0.96	0.28	66,66,66,66	0
56	MG	1A	3496	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3172	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3225	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3670	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	3382	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3201	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3391	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3876	1/1	0.96	0.51	46,46,46,46	0
56	MG	2A	3393	1/1	0.96	0.08	51,51,51,51	0
56	MG	2a	1711	1/1	0.96	0.22	69,69,69,69	0
56	MG	1A	3673	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3878	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3434	1/1	0.96	0.18	25,25,25,25	0
56	MG	10	101	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3384	1/1	0.96	0.22	41,41,41,41	0
56	MG	1A	3503	1/1	0.96	0.24	57,57,57,57	0
56	MG	10	104	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3008	1/1	0.96	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3009	1/1	0.96	0.13	45,45,45,45	0
56	MG	2A	3010	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3011	1/1	0.96	0.13	35,35,35,35	0
56	MG	2a	1723	1/1	0.96	0.15	56,56,56,56	0
56	MG	2A	3627	1/1	0.96	0.05	49,49,49,49	0
56	MG	1A	3436	1/1	0.96	0.19	40,40,40,40	0
56	MG	1A	3122	1/1	0.96	0.21	51,51,51,51	0
56	MG	2A	3015	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3179	1/1	0.96	0.24	26,26,26,26	0
56	MG	1A	3308	1/1	0.96	0.27	39,39,39,39	0
56	MG	1A	3065	1/1	0.96	0.19	29,29,29,29	0
56	MG	1A	3389	1/1	0.96	0.17	23,23,23,23	0
56	MG	2A	3202	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3390	1/1	0.96	0.09	64,64,64,64	0
56	MG	1a	1730	1/1	0.96	0.12	63,63,63,63	0
56	MG	2A	3640	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3253	1/1	0.96	0.23	33,33,33,33	0
56	MG	1A	3445	1/1	0.96	0.12	26,26,26,26	0
56	MG	2A	3207	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3898	1/1	0.96	0.35	31,31,31,31	0
56	MG	2A	3026	1/1	0.96	0.44	41,41,41,41	0
56	MG	1a	1734	1/1	0.96	0.07	53,53,53,53	0
56	MG	2A	3647	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3786	1/1	0.96	0.12	59,59,59,59	0
56	MG	16	103	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3424	1/1	0.96	0.17	54,54,54,54	0
56	MG	17	101	1/1	0.96	0.13	55,55,55,55	0
56	MG	2A	3032	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3605	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3519	1/1	0.96	0.10	51,51,51,51	0
56	MG	2a	1754	1/1	0.96	0.16	73,73,73,73	0
56	MG	1A	3903	1/1	0.96	0.31	39,39,39,39	0
56	MG	1A	3789	1/1	0.96	0.16	56,56,56,56	0
56	MG	2a	1757	1/1	0.96	0.14	71,71,71,71	0
56	MG	2a	1758	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3659	1/1	0.96	0.16	31,31,31,31	0
56	MG	1A	3906	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3907	1/1	0.96	0.20	34,34,34,34	0
56	MG	2A	3042	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3393	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3910	1/1	0.96	0.57	38,38,38,38	0
56	MG	1A	3911	1/1	0.96	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3522	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3227	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3125	1/1	0.96	0.17	34,34,34,34	0
56	MG	2a	1770	1/1	0.96	0.12	67,67,67,67	0
56	MG	2A	3442	1/1	0.96	0.12	29,29,29,29	0
56	MG	1A	3692	1/1	0.96	0.22	52,52,52,52	0
56	MG	2A	3444	1/1	0.96	0.05	57,57,57,57	0
56	MG	2A	3445	1/1	0.96	0.12	53,53,53,53	0
56	MG	2a	1775	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3920	1/1	0.96	0.45	34,34,34,34	0
56	MG	2B	3001	1/1	0.96	0.13	59,59,59,59	0
56	MG	1A	3126	1/1	0.96	0.12	36,36,36,36	0
56	MG	2A	3053	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3526	1/1	0.96	0.17	52,52,52,52	0
56	MG	1a	1755	1/1	0.96	0.19	44,44,44,44	0
56	MG	2B	3006	1/1	0.96	0.13	59,59,59,59	0
56	MG	1a	1756	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3527	1/1	0.96	0.08	69,69,69,69	0
56	MG	2A	3240	1/1	0.96	0.30	45,45,45,45	0
56	MG	1a	1759	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3060	1/1	0.96	0.14	49,49,49,49	0
56	MG	1a	1614	1/1	0.96	0.16	59,59,59,59	0
56	MG	2B	3013	1/1	0.96	0.13	54,54,54,54	0
56	MG	2B	3014	1/1	0.96	0.12	68,68,68,68	0
56	MG	1A	3800	1/1	0.96	0.34	46,46,46,46	0
56	MG	2A	3063	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3247	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3528	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3928	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3250	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3345	1/1	0.96	0.17	45,45,45,45	0
56	MG	2A	3252	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3253	1/1	0.96	0.14	57,57,57,57	0
56	MG	2D	303	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3452	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3346	1/1	0.96	0.06	56,56,56,56	0
56	MG	2A	3256	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3019	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3533	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3475	1/1	0.96	0.04	53,53,53,53	0
56	MG	1A	3703	1/1	0.96	0.15	60,60,60,60	0
56	MG	1A	3705	1/1	0.96	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2F	303	1/1	0.96	0.34	51,51,51,51	0
56	MG	2A	3261	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3257	1/1	0.96	0.57	48,48,48,48	0
56	MG	1A	3188	1/1	0.96	0.24	28,28,28,28	0
56	MG	1a	1777	1/1	0.96	0.08	57,57,57,57	0
56	MG	2v	3001	1/1	0.96	0.17	60,60,60,60	0
56	MG	1A	3352	1/1	0.96	0.09	56,56,56,56	0
56	MG	1a	1780	1/1	0.96	0.15	74,74,74,74	0
56	MG	2w	3003	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3267	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3268	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3487	1/1	0.96	0.16	53,53,53,53	0
56	MG	1a	1781	1/1	0.96	0.08	76,76,76,76	0
56	MG	2U	201	1/1	0.96	0.16	35,35,35,35	0
59	ZN	1Y	501	1/1	0.96	0.18	71,71,71,71	0
56	MG	1a	1782	1/1	0.96	0.14	60,60,60,60	0
56	MG	1a	1631	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3272	1/1	0.96	0.08	47,47,47,47	0
56	MG	1B	207	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3083	1/1	0.96	0.36	41,41,41,41	0
56	MG	2X	102	1/1	0.96	0.28	63,63,63,63	0
56	MG	1B	209	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3353	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3074	1/1	0.96	0.19	40,40,40,40	0
56	MG	2A	3280	1/1	0.97	0.13	25,25,25,25	0
56	MG	2A	3281	1/1	0.97	0.28	52,52,52,52	0
56	MG	2A	3441	1/1	0.97	0.16	48,48,48,48	0
56	MG	1A	3039	1/1	0.97	0.20	49,49,49,49	0
56	MG	1y	3005	1/1	0.97	0.07	78,78,78,78	0
56	MG	1A	3136	1/1	0.97	0.45	36,36,36,36	0
56	MG	1A	3283	1/1	0.97	0.37	44,44,44,44	0
56	MG	1A	3049	1/1	0.97	0.19	42,42,42,42	0
56	MG	1A	3501	1/1	0.97	0.33	62,62,62,62	0
56	MG	1a	1634	1/1	0.97	0.23	45,45,45,45	0
56	MG	2A	3289	1/1	0.97	0.08	37,37,37,37	0
56	MG	1F	302	1/1	0.97	0.28	32,32,32,32	0
56	MG	2A	3291	1/1	0.97	0.16	28,28,28,28	0
56	MG	1F	303	1/1	0.97	0.33	41,41,41,41	0
56	MG	2A	3007	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3193	1/1	0.97	0.48	40,40,40,40	0
56	MG	1A	3103	1/1	0.97	0.48	44,44,44,44	0
56	MG	2A	3628	1/1	0.97	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3629	1/1	0.97	0.07	53,53,53,53	0
56	MG	1A	3029	1/1	0.97	0.41	40,40,40,40	0
56	MG	1A	3288	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3458	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3459	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3121	1/1	0.97	0.16	38,38,38,38	0
56	MG	1A	3708	1/1	0.97	0.21	55,55,55,55	0
56	MG	2A	3150	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	3021	1/1	0.97	0.16	17,17,17,17	0
56	MG	1A	3641	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3511	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3154	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3156	1/1	0.97	0.07	50,50,50,50	0
56	MG	1I	3001	1/1	0.97	0.22	65,65,65,65	0
56	MG	1A	3106	1/1	0.97	0.32	47,47,47,47	0
56	MG	2A	3020	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3325	1/1	0.97	0.25	43,43,43,43	0
56	MG	1a	1652	1/1	0.97	0.18	63,63,63,63	0
56	MG	1A	3791	1/1	0.97	0.41	34,34,34,34	0
56	MG	2a	1687	1/1	0.97	0.28	50,50,50,50	0
56	MG	2A	3648	1/1	0.97	0.09	43,43,43,43	0
56	MG	1a	1771	1/1	0.97	0.15	40,40,40,40	0
56	MG	1N	3005	1/1	0.97	0.16	40,40,40,40	0
56	MG	1A	3792	1/1	0.97	0.35	34,34,34,34	0
56	MG	1A	3124	1/1	0.97	0.43	46,46,46,46	0
56	MG	1A	3716	1/1	0.97	0.11	60,60,60,60	0
56	MG	2A	3320	1/1	0.97	0.20	51,51,51,51	0
56	MG	1A	3260	1/1	0.97	0.54	37,37,37,37	0
56	MG	1A	3884	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3484	1/1	0.97	0.06	44,44,44,44	0
56	MG	2A	3658	1/1	0.97	0.12	44,44,44,44	0
56	MG	1a	1779	1/1	0.97	0.18	52,52,52,52	0
56	MG	2A	3660	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3261	1/1	0.97	0.22	36,36,36,36	0
56	MG	2A	3662	1/1	0.97	0.44	37,37,37,37	0
56	MG	1A	3011	1/1	0.97	0.41	32,32,32,32	0
56	MG	1a	1662	1/1	0.97	0.12	25,25,25,25	0
56	MG	1a	1783	1/1	0.97	0.13	58,58,58,58	0
56	MG	2a	1708	1/1	0.97	0.10	61,61,61,61	0
56	MG	2A	3177	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3650	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	3373	1/1	0.97	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3493	1/1	0.97	0.12	39,39,39,39	0
56	MG	2A	3040	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3330	1/1	0.97	0.21	39,39,39,39	0
56	MG	2A	3675	1/1	0.97	0.30	57,57,57,57	0
56	MG	2A	3333	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3145	1/1	0.97	0.25	37,37,37,37	0
56	MG	1a	1788	1/1	0.97	0.14	50,50,50,50	0
56	MG	2A	3679	1/1	0.97	0.45	46,46,46,46	0
56	MG	2A	3185	1/1	0.97	0.30	50,50,50,50	0
56	MG	1R	201	1/1	0.97	0.09	45,45,45,45	0
56	MG	1A	3012	1/1	0.97	0.27	33,33,33,33	0
56	MG	2A	3503	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3147	1/1	0.97	0.29	36,36,36,36	0
56	MG	1A	3727	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3586	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3729	1/1	0.97	0.10	47,47,47,47	0
56	MG	2A	3052	1/1	0.97	0.28	58,58,58,58	0
56	MG	1A	3657	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3510	1/1	0.97	0.11	46,46,46,46	0
56	MG	1A	3731	1/1	0.97	0.32	52,52,52,52	0
56	MG	2A	3195	1/1	0.97	0.22	32,32,32,32	0
56	MG	1a	1676	1/1	0.97	0.29	53,53,53,53	0
56	MG	2a	1736	1/1	0.97	0.11	66,66,66,66	0
56	MG	2A	3197	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3056	1/1	0.97	0.11	23,23,23,23	0
56	MG	2a	1739	1/1	0.97	0.17	64,64,64,64	0
56	MG	1a	1677	1/1	0.97	0.19	51,51,51,51	0
56	MG	1A	3148	1/1	0.97	0.36	35,35,35,35	0
56	MG	1A	3904	1/1	0.97	0.19	27,27,27,27	0
56	MG	1A	3380	1/1	0.97	0.17	26,26,26,26	0
56	MG	1A	3591	1/1	0.97	0.04	69,69,69,69	0
56	MG	1A	3735	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	3027	1/1	0.97	0.21	35,35,35,35	0
56	MG	2A	3360	1/1	0.97	0.12	19,19,19,19	0
56	MG	2A	3524	1/1	0.97	0.15	24,24,24,24	0
56	MG	1A	3909	1/1	0.97	0.27	42,42,42,42	0
56	MG	1A	3816	1/1	0.97	0.15	25,25,25,25	0
56	MG	1A	3474	1/1	0.97	0.17	26,26,26,26	0
56	MG	2E	303	1/1	0.97	0.06	40,40,40,40	0
56	MG	2A	3210	1/1	0.97	0.12	58,58,58,58	0
56	MG	1A	3594	1/1	0.97	0.13	52,52,52,52	0
56	MG	2A	3530	1/1	0.97	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3367	1/1	0.97	0.10	44,44,44,44	0
56	MG	2A	3532	1/1	0.97	0.14	57,57,57,57	0
56	MG	2A	3533	1/1	0.97	0.08	73,73,73,73	0
56	MG	2F	304	1/1	0.97	0.26	49,49,49,49	0
56	MG	1a	1809	1/1	0.97	0.07	60,60,60,60	0
56	MG	1A	3055	1/1	0.97	0.16	45,45,45,45	0
56	MG	2a	1762	1/1	0.97	0.21	64,64,64,64	0
56	MG	1Y	503	1/1	0.97	0.10	56,56,56,56	0
56	MG	1Z	301	1/1	0.97	0.37	46,46,46,46	0
56	MG	1a	1813	1/1	0.97	0.23	50,50,50,50	0
56	MG	1A	3820	1/1	0.97	0.10	52,52,52,52	0
56	MG	1a	1815	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3177	1/1	0.97	0.61	52,52,52,52	0
56	MG	1A	3477	1/1	0.97	0.15	18,18,18,18	0
56	MG	1A	3028	1/1	0.97	0.30	19,19,19,19	0
56	MG	1A	3096	1/1	0.97	0.40	52,52,52,52	0
56	MG	1A	3098	1/1	0.97	0.22	24,24,24,24	0
56	MG	1A	3132	1/1	0.97	0.17	17,17,17,17	0
56	MG	1A	3927	1/1	0.97	0.36	40,40,40,40	0
56	MG	1A	3539	1/1	0.97	0.17	17,17,17,17	0
56	MG	1A	3057	1/1	0.97	0.20	43,43,43,43	0
56	MG	2A	3385	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3228	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3229	1/1	0.97	0.21	41,41,41,41	0
56	MG	1A	3831	1/1	0.97	0.18	23,23,23,23	0
56	MG	1A	3832	1/1	0.97	0.09	23,23,23,23	0
56	MG	1a	1828	1/1	0.97	0.07	83,83,83,83	0
56	MG	1A	3833	1/1	0.97	0.07	66,66,66,66	0
56	MG	2A	3234	1/1	0.97	0.16	56,56,56,56	0
56	MG	1a	1830	1/1	0.97	0.16	61,61,61,61	0
56	MG	2A	3090	1/1	0.97	0.30	37,37,37,37	0
56	MG	1A	3343	1/1	0.97	0.16	34,34,34,34	0
56	MG	1A	3751	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3046	1/1	0.97	0.18	28,28,28,28	0
56	MG	1A	3187	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3392	1/1	0.97	0.09	31,31,31,31	0
56	MG	2A	3097	1/1	0.97	0.31	42,42,42,42	0
56	MG	1A	3246	1/1	0.97	0.34	40,40,40,40	0
56	MG	1A	3841	1/1	0.97	0.14	33,33,33,33	0
56	MG	1a	1713	1/1	0.97	0.13	34,34,34,34	0
56	MG	2a	1610	1/1	0.97	0.32	53,53,53,53	0
56	MG	1A	3547	1/1	0.97	0.25	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3159	1/1	0.97	0.18	29,29,29,29	0
56	MG	1B	211	1/1	0.97	0.13	43,43,43,43	0
56	MG	1B	212	1/1	0.97	0.14	50,50,50,50	0
56	MG	1n	502	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3549	1/1	0.97	0.13	40,40,40,40	0
56	MG	1B	214	1/1	0.97	0.16	41,41,41,41	0
56	MG	2f	3001	1/1	0.97	0.15	47,47,47,47	0
56	MG	2A	3580	1/1	0.97	0.11	50,50,50,50	0
56	MG	2a	1619	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3218	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3551	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3553	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3160	1/1	0.97	0.19	24,24,24,24	0
56	MG	1A	3619	1/1	0.97	0.16	44,44,44,44	0
56	MG	2q	201	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	3397	1/1	0.97	0.14	17,17,17,17	0
56	MG	1A	3766	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	3493	1/1	0.97	0.12	53,53,53,53	0
56	MG	1B	224	1/1	0.97	0.09	63,63,63,63	0
56	MG	2v	3002	1/1	0.97	0.14	60,60,60,60	0
56	MG	1A	3494	1/1	0.97	0.16	34,34,34,34	0
56	MG	1A	3559	1/1	0.97	0.19	40,40,40,40	0
56	MG	2A	3594	1/1	0.97	0.14	52,52,52,52	0
56	MG	2x	3001	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	3350	1/1	0.97	0.20	40,40,40,40	0
56	MG	1D	304	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3561	1/1	0.97	0.18	43,43,43,43	0
56	MG	1D	306	1/1	0.97	0.30	36,36,36,36	0
56	MG	1a	1738	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3857	1/1	0.97	0.10	25,25,25,25	0
56	MG	2A	3125	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3351	1/1	0.97	0.14	55,55,55,55	0
56	MG	1D	309	1/1	0.97	0.46	28,28,28,28	0
56	MG	2A	3274	1/1	0.97	0.08	43,43,43,43	0
56	MG	1a	1624	1/1	0.97	0.08	45,45,45,45	0
59	ZN	26	501	1/1	0.97	0.18	63,63,63,63	0
56	MG	2A	3276	1/1	0.97	0.21	51,51,51,51	0
56	MG	1E	301	1/1	0.97	0.24	43,43,43,43	0
60	SF4	2d	501	8/8	0.97	0.14	58,71,79,93	0
56	MG	1A	3628	1/1	0.97	0.08	46,46,46,46	0
56	MG	1E	303	1/1	0.97	0.34	48,48,48,48	0
56	MG	1A	3932	1/1	0.98	0.36	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3598	1/1	0.98	0.17	52,52,52,52	0
56	MG	1A	3933	1/1	0.98	0.16	44,44,44,44	0
56	MG	1A	3517	1/1	0.98	0.10	51,51,51,51	0
56	MG	2A	3365	1/1	0.98	0.16	52,52,52,52	0
56	MG	1a	1826	1/1	0.98	0.14	60,60,60,60	0
56	MG	1A	3180	1/1	0.98	0.14	40,40,40,40	0
56	MG	2A	3368	1/1	0.98	0.09	41,41,41,41	0
56	MG	1a	1736	1/1	0.98	0.17	58,58,58,58	0
56	MG	1a	1646	1/1	0.98	0.08	52,52,52,52	0
56	MG	1A	3558	1/1	0.98	0.19	43,43,43,43	0
56	MG	2A	3155	1/1	0.98	0.49	46,46,46,46	0
56	MG	1A	3068	1/1	0.98	0.15	17,17,17,17	0
56	MG	1A	3372	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3521	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3695	1/1	0.98	0.19	45,45,45,45	0
56	MG	1B	204	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3062	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3649	1/1	0.98	0.07	67,67,67,67	0
56	MG	1A	3374	1/1	0.98	0.18	32,32,32,32	0
56	MG	2A	3064	1/1	0.98	0.10	50,50,50,50	0
56	MG	2A	3165	1/1	0.98	0.27	31,31,31,31	0
56	MG	1B	208	1/1	0.98	0.13	56,56,56,56	0
56	MG	1A	3183	1/1	0.98	0.40	36,36,36,36	0
56	MG	1A	3809	1/1	0.98	0.14	50,50,50,50	0
56	MG	2a	1735	1/1	0.98	0.12	56,56,56,56	0
56	MG	1A	3034	1/1	0.98	0.53	44,44,44,44	0
56	MG	1A	3157	1/1	0.98	0.16	41,41,41,41	0
56	MG	2A	3502	1/1	0.98	0.11	51,51,51,51	0
56	MG	2A	3171	1/1	0.98	0.22	47,47,47,47	0
56	MG	1A	3609	1/1	0.98	0.17	31,31,31,31	0
56	MG	1s	3001	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3460	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3704	1/1	0.98	0.20	26,26,26,26	0
56	MG	1A	3202	1/1	0.98	0.14	46,46,46,46	0
56	MG	2A	3394	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3186	1/1	0.98	0.51	36,36,36,36	0
56	MG	1A	3760	1/1	0.98	0.11	19,19,19,19	0
56	MG	1B	219	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	3406	1/1	0.98	0.17	27,27,27,27	0
56	MG	1a	1670	1/1	0.98	0.06	56,56,56,56	0
56	MG	2A	3182	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3222	1/1	0.98	0.45	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1763	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	3880	1/1	0.98	0.19	23,23,23,23	0
56	MG	1A	3097	1/1	0.98	0.19	26,26,26,26	0
56	MG	1A	3882	1/1	0.98	0.17	41,41,41,41	0
56	MG	1a	1767	1/1	0.98	0.10	50,50,50,50	0
56	MG	12	102	1/1	0.98	0.16	49,49,49,49	0
56	MG	1A	3710	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3822	1/1	0.98	0.18	56,56,56,56	0
56	MG	1A	3109	1/1	0.98	0.19	28,28,28,28	0
56	MG	1A	3358	1/1	0.98	0.10	45,45,45,45	0
56	MG	1a	1773	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3092	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3468	1/1	0.98	0.12	30,30,30,30	0
56	MG	2A	3302	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3537	1/1	0.98	0.19	28,28,28,28	0
56	MG	1A	3038	1/1	0.98	0.26	33,33,33,33	0
56	MG	1A	3088	1/1	0.98	0.20	22,22,22,22	0
56	MG	1A	3829	1/1	0.98	0.11	40,40,40,40	0
56	MG	2A	3201	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3892	1/1	0.98	0.28	34,34,34,34	0
56	MG	1A	3010	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3668	1/1	0.98	0.17	45,45,45,45	0
56	MG	2a	1645	1/1	0.98	0.17	47,47,47,47	0
56	MG	1A	3896	1/1	0.98	0.70	41,41,41,41	0
56	MG	2A	3540	1/1	0.98	0.06	53,53,53,53	0
56	MG	2A	3312	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3897	1/1	0.98	0.31	30,30,30,30	0
56	MG	2A	3665	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3073	1/1	0.98	0.56	51,51,51,51	0
56	MG	1A	3504	1/1	0.98	0.08	13,13,13,13	0
56	MG	2A	3316	1/1	0.98	0.11	31,31,31,31	0
56	MG	1A	3625	1/1	0.98	0.35	55,55,55,55	0
56	MG	1A	3835	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	3902	1/1	0.98	0.12	40,40,40,40	0
56	MG	1A	3091	1/1	0.98	0.21	42,42,42,42	0
56	MG	1A	3723	1/1	0.98	0.07	58,58,58,58	0
56	MG	1F	306	1/1	0.98	0.09	46,46,46,46	0
56	MG	2a	1660	1/1	0.98	0.20	52,52,52,52	0
56	MG	1A	3506	1/1	0.98	0.15	53,53,53,53	0
56	MG	2A	3013	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3211	1/1	0.98	0.30	44,44,44,44	0
56	MG	2A	3680	1/1	0.98	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3066	1/1	0.98	0.20	17,17,17,17	0
56	MG	2A	3440	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	3446	1/1	0.98	0.14	26,26,26,26	0
56	MG	1A	3033	1/1	0.98	0.18	20,20,20,20	0
56	MG	2A	3559	1/1	0.98	0.12	52,52,52,52	0
56	MG	1A	3588	1/1	0.98	0.14	55,55,55,55	0
56	MG	1A	3367	1/1	0.98	0.18	13,13,13,13	0
56	MG	1A	3590	1/1	0.98	0.17	24,24,24,24	0
56	MG	1a	1620	1/1	0.98	0.14	37,37,37,37	0
56	MG	1A	3914	1/1	0.98	0.19	37,37,37,37	0
56	MG	1A	3513	1/1	0.98	0.13	25,25,25,25	0
56	MG	1A	3916	1/1	0.98	0.21	41,41,41,41	0
56	MG	1N	3004	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3917	1/1	0.98	0.29	32,32,32,32	0
56	MG	1A	3918	1/1	0.98	0.29	39,39,39,39	0
56	MG	1A	3552	1/1	0.98	0.15	20,20,20,20	0
56	MG	1A	3683	1/1	0.98	0.09	53,53,53,53	0
56	MG	1a	1717	1/1	0.98	0.08	60,60,60,60	0
56	MG	2q	202	1/1	0.98	0.49	80,80,80,80	0
56	MG	1A	3368	1/1	0.98	0.21	37,37,37,37	0
56	MG	1a	1630	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3922	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	3638	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3578	1/1	0.98	0.09	51,51,51,51	0
56	MG	2A	3460	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3737	1/1	0.98	0.20	40,40,40,40	0
56	MG	2A	3581	1/1	0.98	0.12	34,34,34,34	0
56	MG	2A	3462	1/1	0.98	0.08	37,37,37,37	0
56	MG	1Q	3001	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3738	1/1	0.98	0.27	39,39,39,39	0
56	MG	2A	3039	1/1	0.98	0.09	37,37,37,37	0
56	MG	2a	1695	1/1	0.98	0.15	66,66,66,66	0
56	MG	1A	3794	1/1	0.98	0.12	21,21,21,21	0
56	MG	2E	306	1/1	0.98	0.16	47,47,47,47	0
56	MG	2A	3041	1/1	0.98	0.19	29,29,29,29	0
56	MG	2A	3140	1/1	0.98	0.24	37,37,37,37	0
56	MG	2A	3589	1/1	0.98	0.09	49,49,49,49	0
56	MG	2a	1701	1/1	0.98	0.05	55,55,55,55	0
56	MG	2A	3141	1/1	0.98	0.10	49,49,49,49	0
56	MG	2A	3355	1/1	0.98	0.09	22,22,22,22	0
56	MG	1A	3450	1/1	0.98	0.13	36,36,36,36	0
56	MG	1A	3595	1/1	0.98	0.14	48,48,48,48	0

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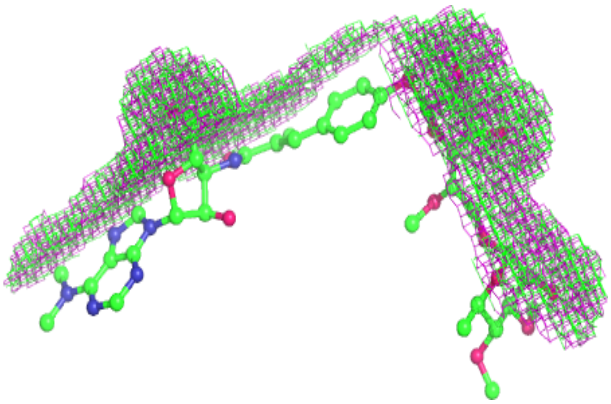
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	SF4	1d	501	8/8	0.98	0.18	51,62,75,79	0
56	MG	1a	1639	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3369	1/1	0.98	0.21	37,37,37,37	0
56	MG	1A	3930	1/1	0.98	0.30	41,41,41,41	0
56	MG	1a	1689	1/1	0.99	0.18	39,39,39,39	0
56	MG	1A	3030	1/1	0.99	0.17	36,36,36,36	0
56	MG	1E	304	1/1	0.99	0.17	23,23,23,23	0
56	MG	1A	3602	1/1	0.99	0.18	33,33,33,33	0
56	MG	1W	3003	1/1	0.99	0.26	34,34,34,34	0
56	MG	1A	3155	1/1	0.99	0.26	36,36,36,36	0
56	MG	1a	1695	1/1	0.99	0.22	42,42,42,42	0
56	MG	1a	1758	1/1	0.99	0.13	29,29,29,29	0
56	MG	2A	3347	1/1	0.99	0.07	54,54,54,54	0
56	MG	2A	3049	1/1	0.99	0.04	41,41,41,41	0
56	MG	1A	3525	1/1	0.99	0.18	23,23,23,23	0
56	MG	2A	3674	1/1	0.99	0.07	39,39,39,39	0
56	MG	1A	3544	1/1	0.99	0.22	35,35,35,35	0
56	MG	1D	302	1/1	0.99	0.20	32,32,32,32	0
56	MG	1A	3509	1/1	0.99	0.17	48,48,48,48	0
56	MG	2A	3002	1/1	0.99	0.12	29,29,29,29	0
56	MG	1A	3772	1/1	0.99	0.13	33,33,33,33	0
56	MG	2A	3029	1/1	0.99	0.10	26,26,26,26	0
56	MG	1a	1721	1/1	0.99	0.18	47,47,47,47	0
56	MG	2a	1728	1/1	0.99	0.10	75,75,75,75	0
56	MG	2A	3357	1/1	0.99	0.08	35,35,35,35	0
56	MG	2A	3561	1/1	0.99	0.14	34,34,34,34	0
56	MG	1a	1831	1/1	0.99	0.09	37,37,37,37	0
56	MG	1a	1832	1/1	0.99	0.28	57,57,57,57	0
59	ZN	19	501	1/1	0.99	0.20	42,42,42,42	0
59	ZN	1n	501	1/1	0.99	0.16	56,56,56,56	0
56	MG	1A	3047	1/1	0.99	0.16	28,28,28,28	0
56	MG	1A	3403	1/1	0.99	0.13	15,15,15,15	0
59	ZN	25	501	1/1	0.99	0.18	54,54,54,54	0
56	MG	1A	3490	1/1	0.99	0.10	9,9,9,9	0
56	MG	1A	3912	1/1	0.99	0.32	37,37,37,37	0
56	MG	1a	1649	1/1	0.99	0.33	58,58,58,58	0
56	MG	1A	3432	1/1	0.99	0.14	29,29,29,29	0
56	MG	1A	3873	1/1	0.99	0.14	13,13,13,13	0
56	MG	1A	3443	1/1	0.99	0.19	31,31,31,31	0
56	MG	2a	1644	1/1	0.99	0.11	61,61,61,61	0

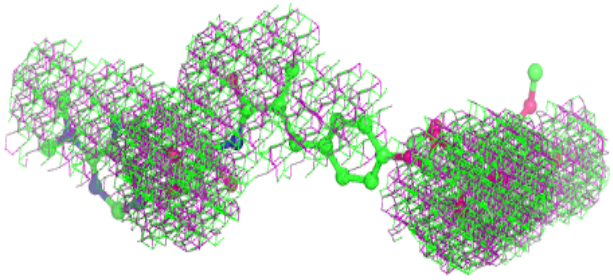
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

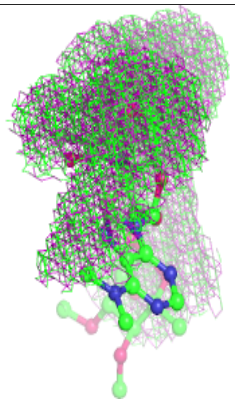
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4M2 2A 3670:

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

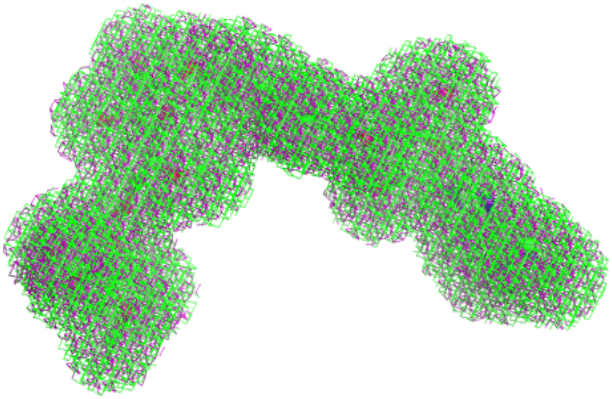


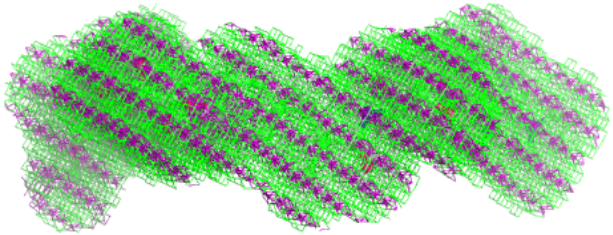


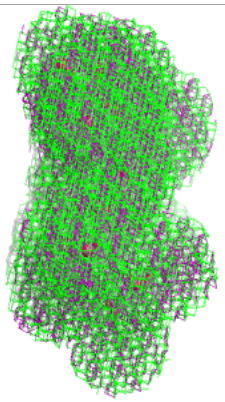


Electron density around 4M2 1A 3894:

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







6.5 Other polymers (i)

There are no such residues in this entry.