Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 08:47 PM EST

PDB ID	:	8G2B
Title	:	Crystal structure of the A2503-C2,C8-dimethylated Thermus thermophilus 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNAphe, and aminoacylated P-site fMet-tRNAmet at 2.55A resolution
Authors	:	Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on	:	2023-02-03
Resolution	:	2.55 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:

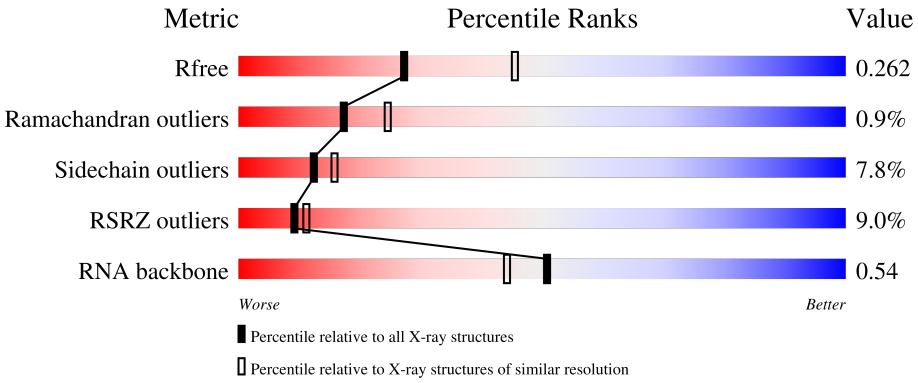
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.55 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	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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	4% 82% 16%
1	2A	2915	4% 80% 16%
2	1B	121	88% 12%

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

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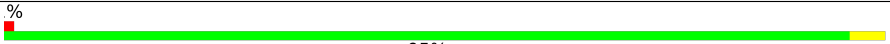
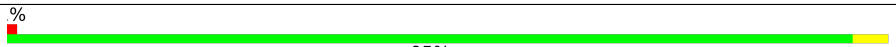
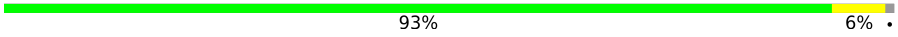
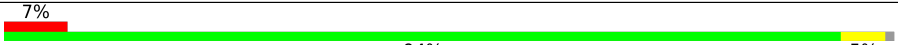
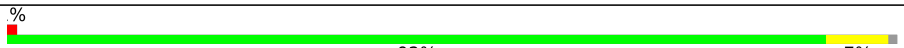
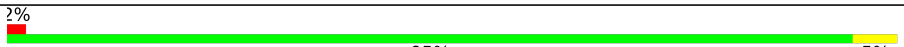
Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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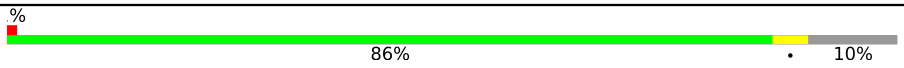
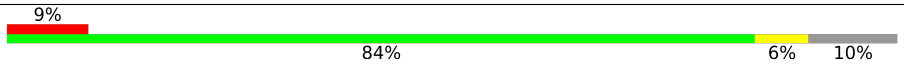
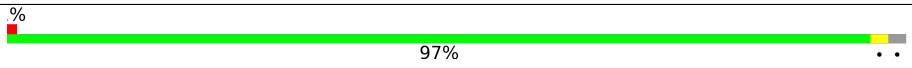
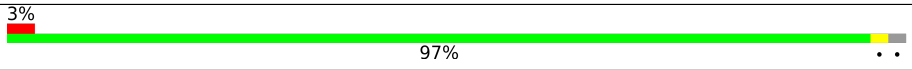
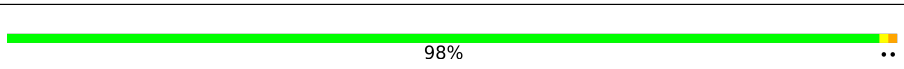
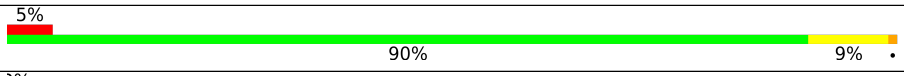
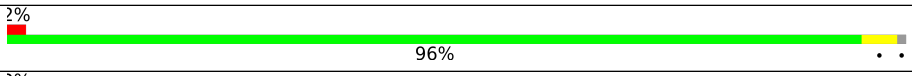
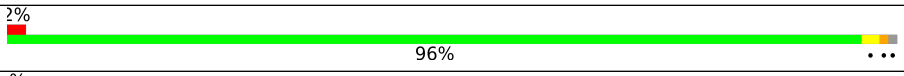
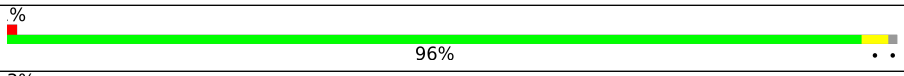
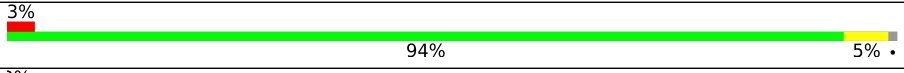
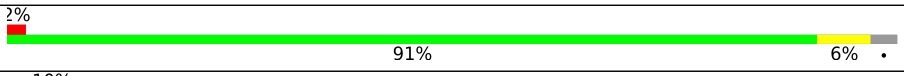
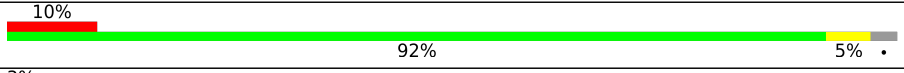
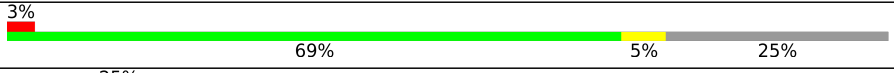
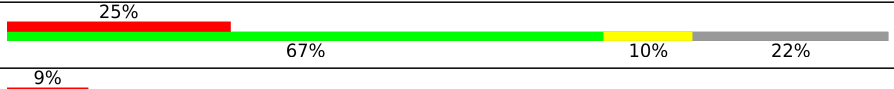
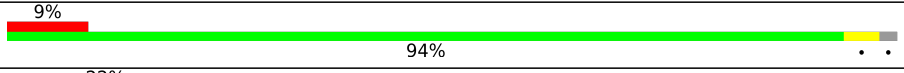
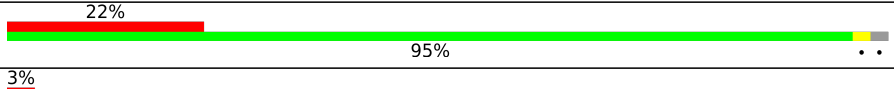
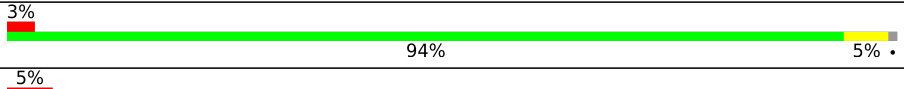
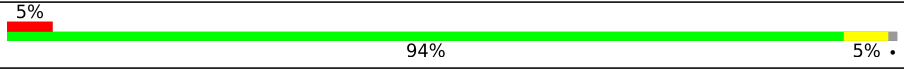
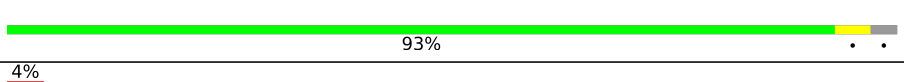
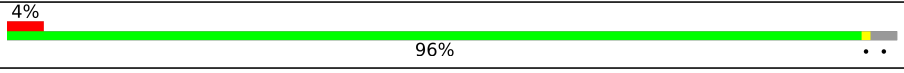
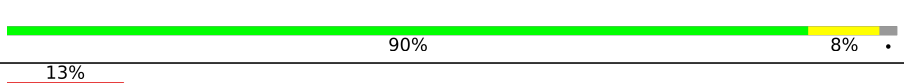
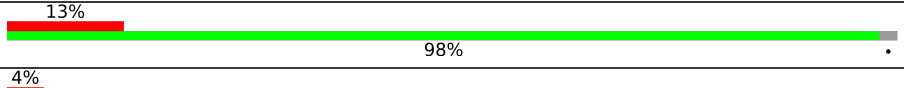
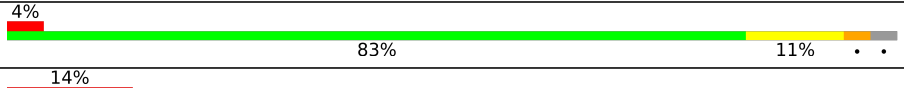
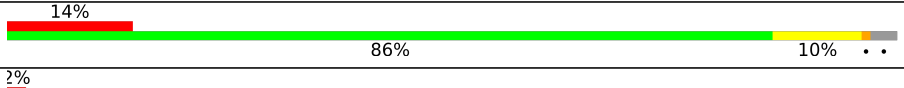
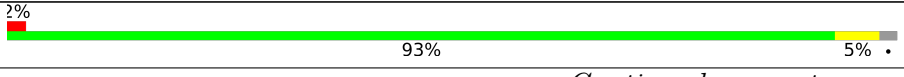
Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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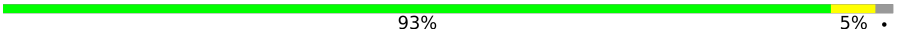
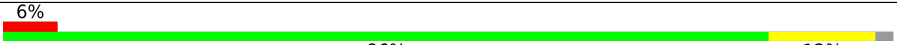
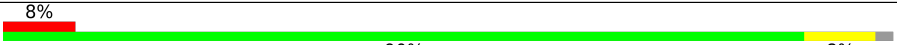
Mol	Chain	Length	Quality of chain
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
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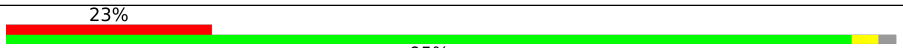
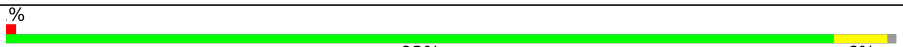
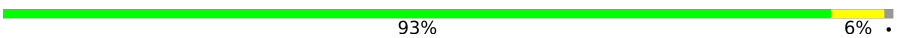
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
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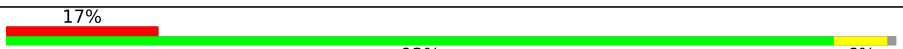
38	2g	156	
39	1h	138	
39	2h	138	

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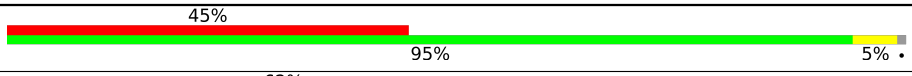
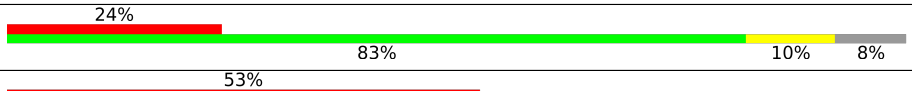
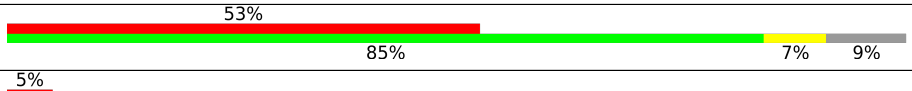
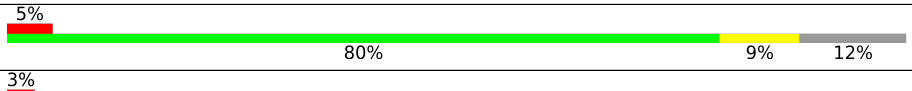
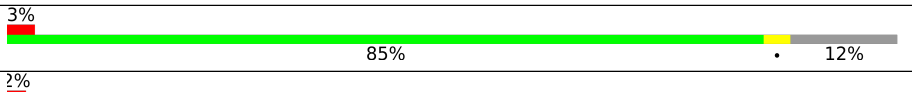
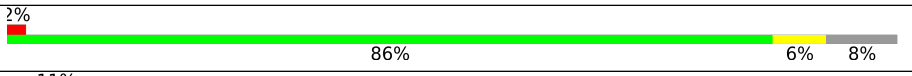
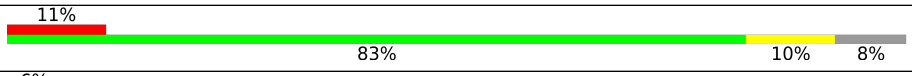
Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
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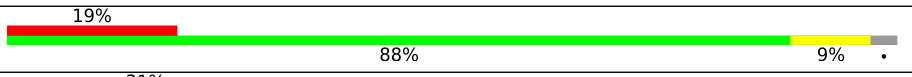
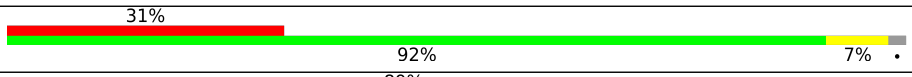
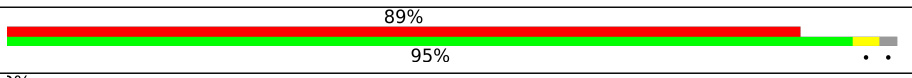
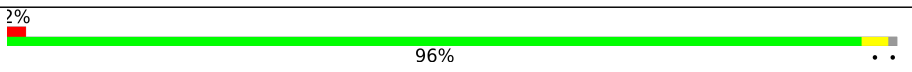
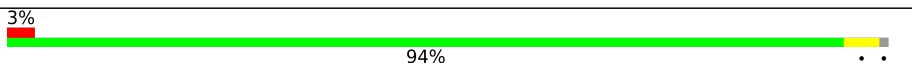
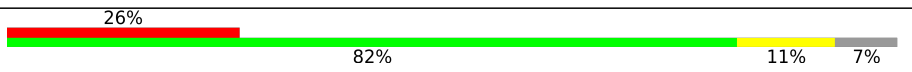
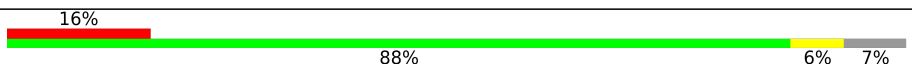
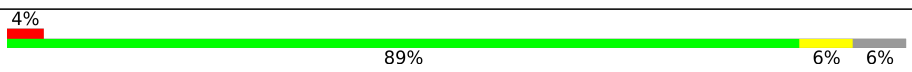
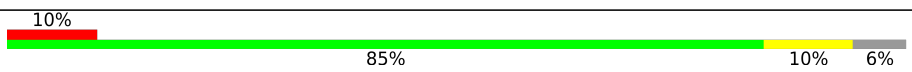
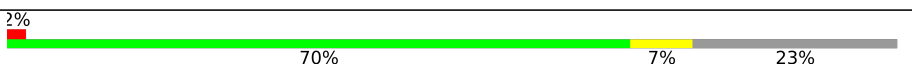
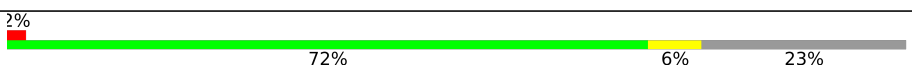
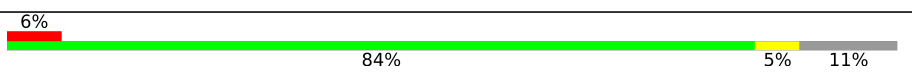
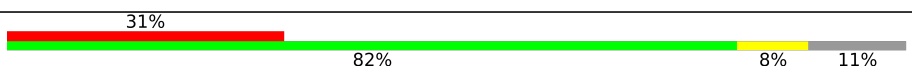
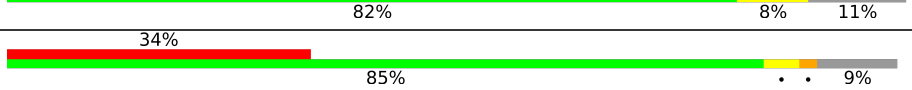
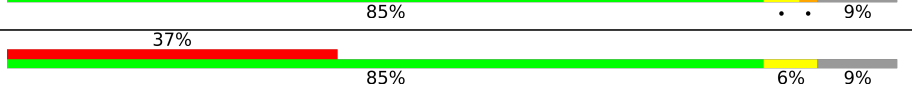
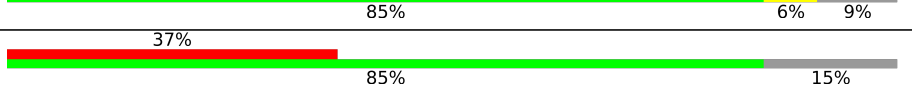
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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Mol	Chain	Length	Quality of chain
52	2u	27	56% 85% 15%
53	1v	24	12% 50% 46%
53	2v	24	25% 54% 46%
54	1w	76	13% 55% 39%
54	1y	76	12% 50% 43%
54	2w	76	11% 62% 29% 8%
54	2y	76	26% 57% 37%
55	1x	77	74% 25%
55	2x	77	% 82% 17%

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
56	MG	1A	3331	-	-	-	X
56	MG	1A	3343	-	-	-	X
56	MG	1A	3425	-	-	-	X
56	MG	1A	3546	-	-	-	X
56	MG	1A	3772	-	-	-	X
56	MG	1A	3937	-	-	-	X
56	MG	1A	3990	-	-	-	X
56	MG	1U	203	-	-	-	X
56	MG	1a	1668	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3156	-	-	-	X
56	MG	2A	3219	-	-	-	X
56	MG	2A	3224	-	-	-	X
56	MG	2A	3330	-	-	-	X
56	MG	2A	3409	-	-	-	X
56	MG	2A	3608	-	-	-	X
56	MG	2A	3829	-	-	-	X
56	MG	2B	202	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 299868 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
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	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
			1423	913	253	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 933	C 588	N 171	O 170	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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 MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1570	703	280	512	73	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	70	Total	C	N	O	P	S	0	0	0
			1502	671	270	489	70	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1083	Total	Mg	0	0
			1083	1083		
56	1B	38	Total	Mg	0	0
			38	38		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	14	Total	Mg	0	0
			14	14		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1I	1	Total Mg 1 1	0	0
56	1N	6	Total Mg 6 6	0	0
56	1O	4	Total Mg 4 4	0	0
56	1P	6	Total Mg 6 6	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	5	Total Mg 5 5	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	11	Total Mg 11 11	0	0
56	1V	7	Total Mg 7 7	0	0
56	1W	9	Total Mg 9 9	0	0
56	1X	6	Total Mg 6 6	0	0
56	1Y	4	Total Mg 4 4	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	8	Total Mg 8 8	0	0
56	11	6	Total Mg 6 6	0	0
56	12	2	Total Mg 2 2	0	0
56	13	4	Total Mg 4 4	0	0
56	14	1	Total Mg 1 1	0	0
56	15	8	Total Mg 8 8	0	0
56	16	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	17	6	Total Mg 6 6	0	0
56	18	5	Total Mg 5 5	0	0
56	19	1	Total Mg 1 1	0	0
56	1a	211	Total Mg 211 211	0	0
56	1b	1	Total Mg 1 1	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	1	Total Mg 1 1	0	0
56	1k	1	Total Mg 1 1	0	0
56	1l	2	Total Mg 2 2	0	0
56	1m	2	Total Mg 2 2	0	0
56	1n	2	Total Mg 2 2	0	0
56	1r	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	2	Total Mg 2 2	0	0
56	1w	7	Total Mg 7 7	0	0
56	1x	15	Total Mg 15 15	0	0
56	1y	1	Total Mg 1 1	0	0
56	2A	830	Total Mg 830 830	0	0
56	2B	19	Total Mg 19 19	0	0
56	2D	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2E	9	Total Mg 9 9	0	0
56	2F	7	Total Mg 7 7	0	0
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	2	Total Mg 2 2	0	0
56	2Q	4	Total Mg 4 4	0	0
56	2R	3	Total Mg 3 3	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	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	1	Total Mg 1 1	0	0
56	2Y	1	Total Mg 1 1	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	5	Total Mg 5 5	0	0
56	21	2	Total Mg 2 2	0	0
56	23	1	Total Mg 1 1	0	0
56	25	7	Total Mg 7 7	0	0
56	26	1	Total Mg 1 1	0	0
56	27	3	Total Mg 3 3	0	0

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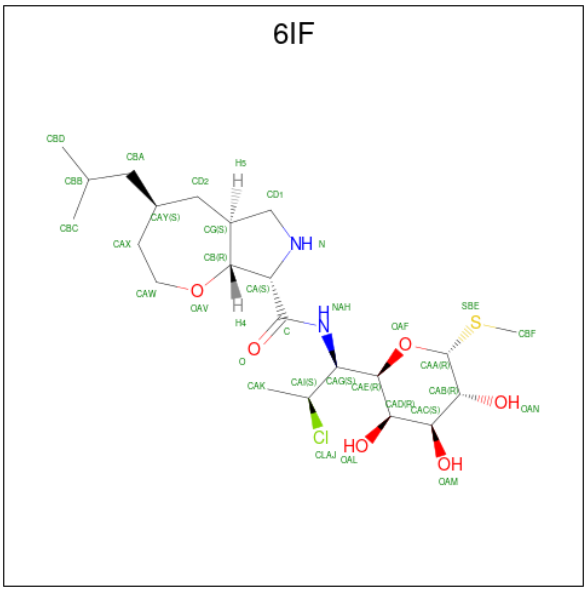
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	28	2	Total Mg 2 2	0	0
56	29	1	Total Mg 1 1	0	0
56	2a	211	Total Mg 211 211	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2l	3	Total Mg 3 3	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	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	3	Total Mg 3 3	0	0
56	2w	4	Total Mg 4 4	0	0
56	2x	7	Total Mg 7 7	0	0
56	2y	5	Total Mg 5 5	0	0

- Molecule 57 is methyl 7-chloro-6,7,8-trideoxy-6-{[(4S,5aS,8S,8aR)-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carbonyl]amino}-1-thio-L-threo-alpha-D-galacto-octopyranoside (three-letter code: 6IF) (formula: $C_{22}H_{39}ClN_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C Cl N O S 32 22 1 2 6 1	0	0
57	2A	1	Total C Cl N O S 32 22 1 2 6 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0

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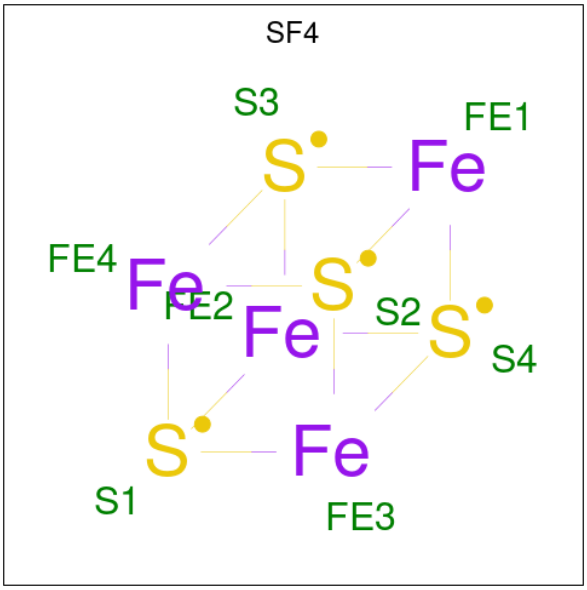
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1d	1	Total Fe S 8 4 4	0	0
59	2d	1	Total Fe S 8 4 4	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1x	1	Total K 1 1	0	0
60	2x	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1971	Total O 1971 1971	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1B	60	Total O 60 60	0	0
61	1D	28	Total O 28 28	0	0
61	1E	30	Total O 30 30	0	0
61	1F	16	Total O 16 16	0	0
61	1G	2	Total O 2 2	0	0
61	1H	3	Total O 3 3	0	0
61	1N	9	Total O 9 9	0	0
61	1O	4	Total O 4 4	0	0
61	1P	15	Total O 15 15	0	0
61	1Q	10	Total O 10 10	0	0
61	1R	12	Total O 12 12	0	0
61	1S	5	Total O 5 5	0	0
61	1T	8	Total O 8 8	0	0
61	1U	14	Total O 14 14	0	0
61	1V	8	Total O 8 8	0	0
61	1W	4	Total O 4 4	0	0
61	1X	6	Total O 6 6	0	0
61	1Y	2	Total O 2 2	0	0
61	1Z	1	Total O 1 1	0	0
61	10	13	Total O 13 13	0	0
61	11	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	12	4	Total O 4 4	0	0
61	13	3	Total O 3 3	0	0
61	14	1	Total O 1 1	0	0
61	15	4	Total O 4 4	0	0
61	16	2	Total O 2 2	0	0
61	17	9	Total O 9 9	0	0
61	18	13	Total O 13 13	0	0
61	1a	357	Total O 357 357	0	0
61	1b	1	Total O 1 1	0	0
61	1e	1	Total O 1 1	0	0
61	1i	2	Total O 2 2	0	0
61	1l	4	Total O 4 4	0	0
61	1m	2	Total O 2 2	0	0
61	1o	1	Total O 1 1	0	0
61	1p	1	Total O 1 1	0	0
61	1q	2	Total O 2 2	0	0
61	1t	1	Total O 1 1	0	0
61	1u	1	Total O 1 1	0	0
61	1v	4	Total O 4 4	0	0
61	1w	10	Total O 10 10	0	0
61	1x	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1y	1	Total O 1 1	0	0
61	2A	1109	Total O 1109 1109	0	0
61	2B	20	Total O 20 20	0	0
61	2D	21	Total O 21 21	0	0
61	2E	13	Total O 13 13	0	0
61	2F	11	Total O 11 11	0	0
61	2O	3	Total O 3 3	0	0
61	2P	8	Total O 8 8	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	3	Total O 3 3	0	0
61	2T	6	Total O 6 6	0	0
61	2U	4	Total O 4 4	0	0
61	2W	1	Total O 1 1	0	0
61	2X	1	Total O 1 1	0	0
61	2Y	1	Total O 1 1	0	0
61	20	4	Total O 4 4	0	0
61	21	6	Total O 6 6	0	0
61	23	2	Total O 2 2	0	0
61	25	2	Total O 2 2	0	0
61	27	1	Total O 1 1	0	0
61	28	6	Total O 6 6	0	0

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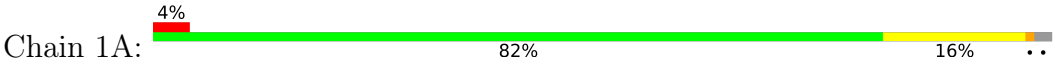
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	29	1	Total O 1 1	0	0
61	2a	221	Total O 221 221	0	0
61	2d	2	Total O 2 2	0	0
61	2j	3	Total O 3 3	0	0
61	2l	1	Total O 1 1	0	0
61	2o	1	Total O 1 1	0	0
61	2p	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2x	4	Total O 4 4	0	0
61	2y	7	Total O 7 7	0	0

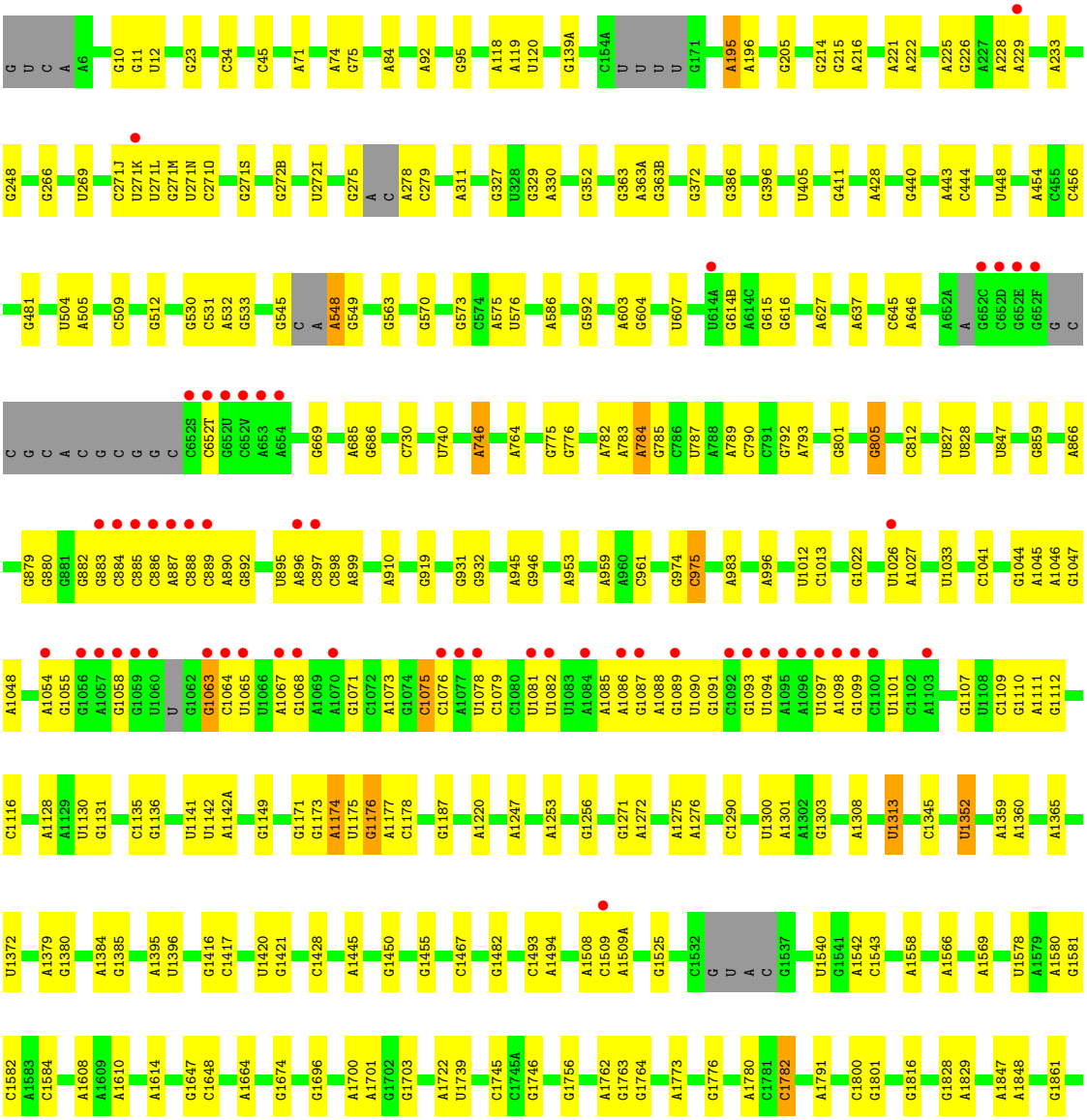
3 Residue-property plots (i)

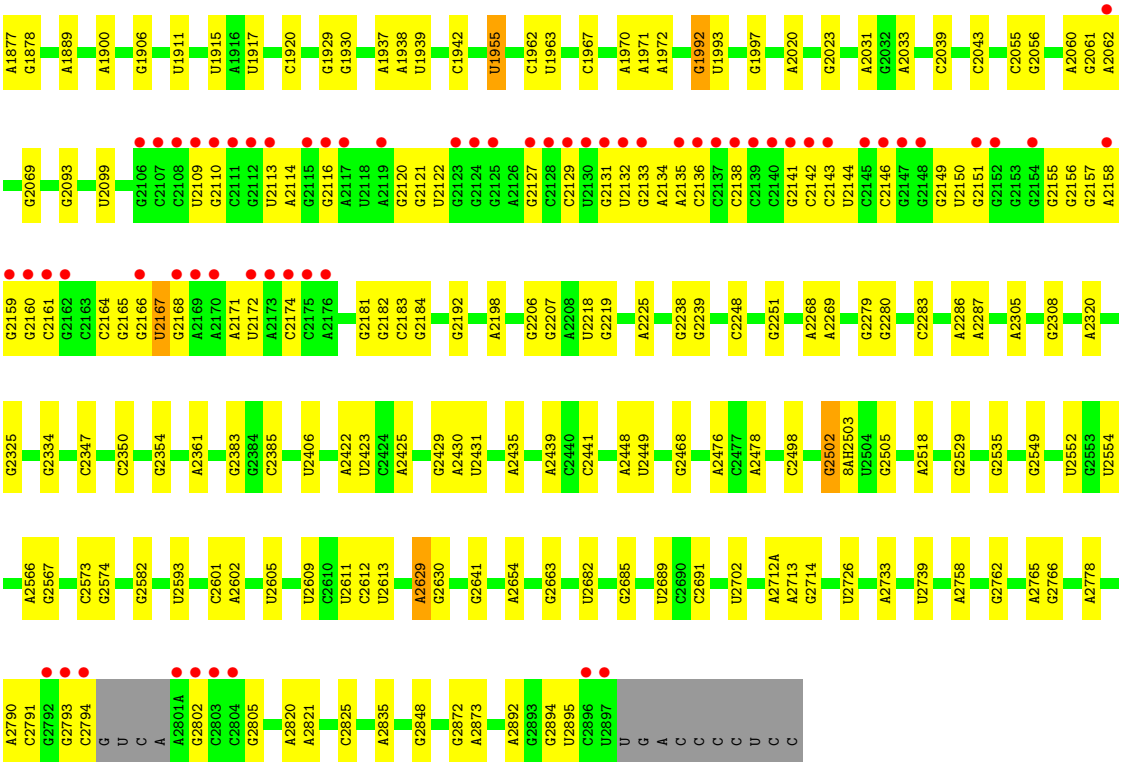
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

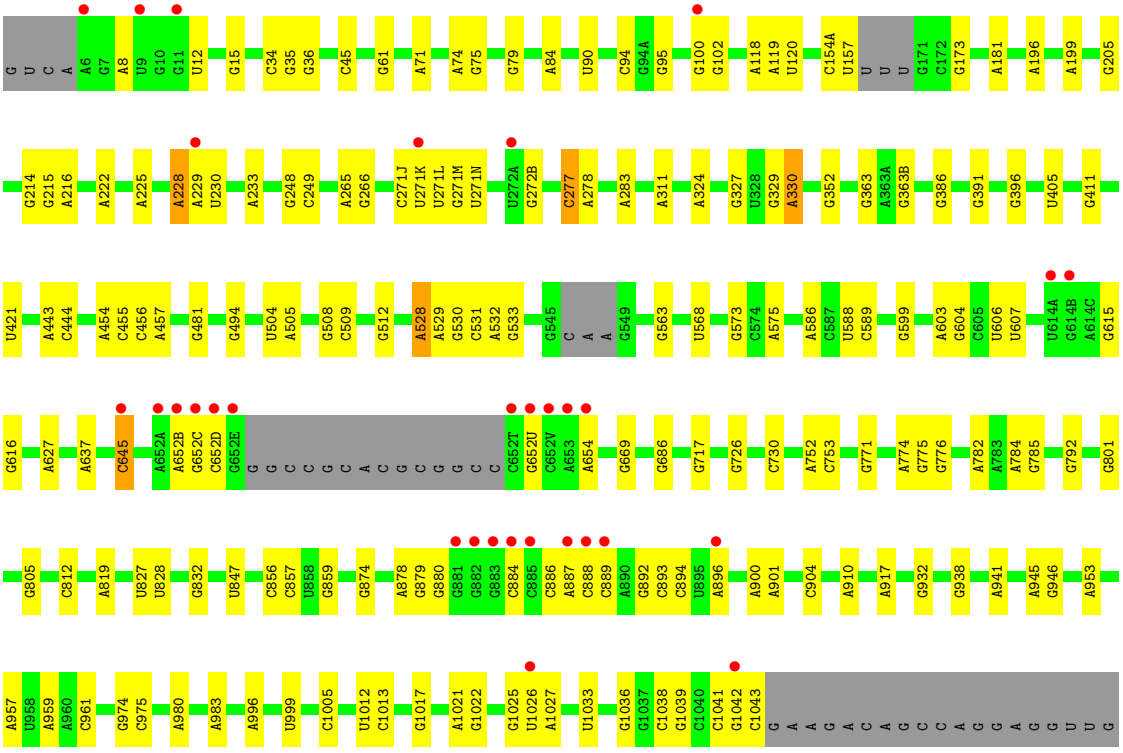


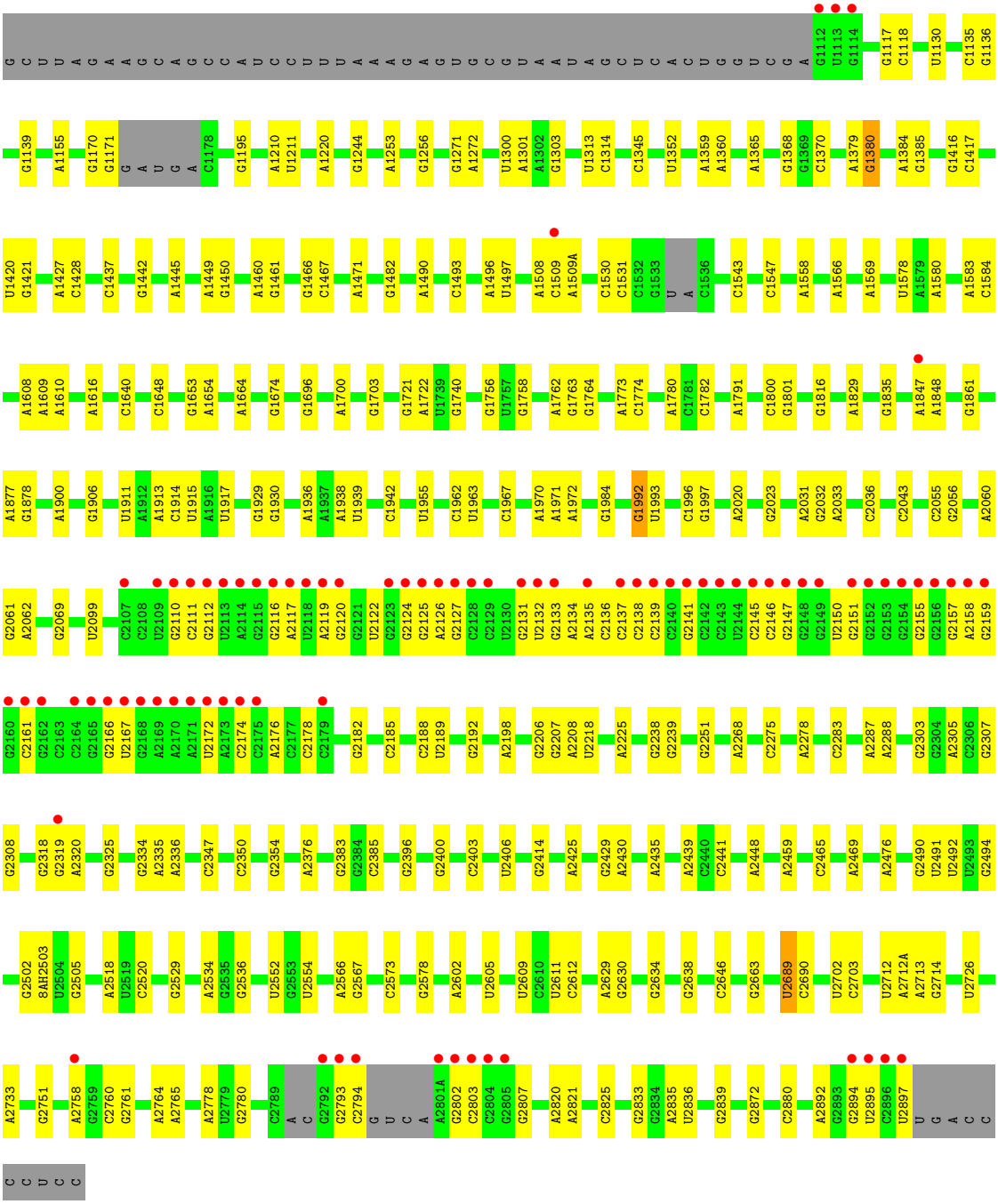




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



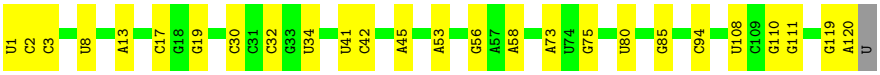


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

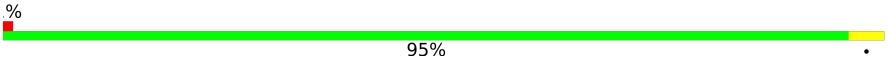
• Molecule 2: 5S Ribosomal RNA

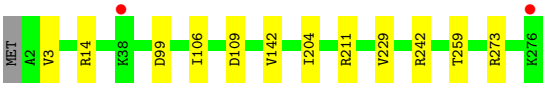
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

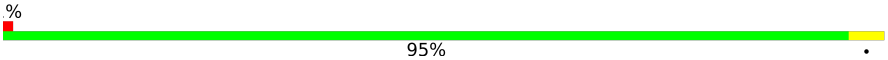
Chain 1D:





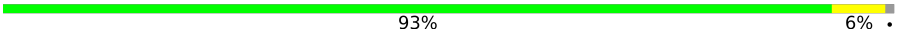
• Molecule 3: 50S ribosomal protein L2

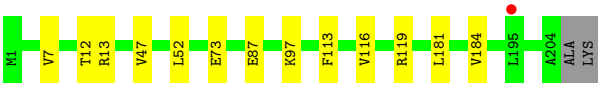
Chain 2D:



• Molecule 4: 50S ribosomal protein L3

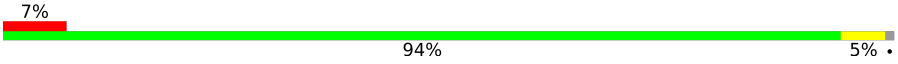
Chain 1E:

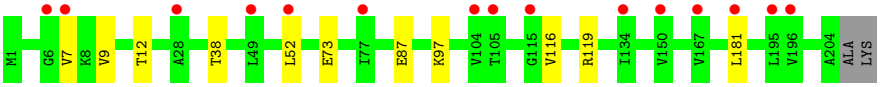




• Molecule 4: 50S ribosomal protein L3

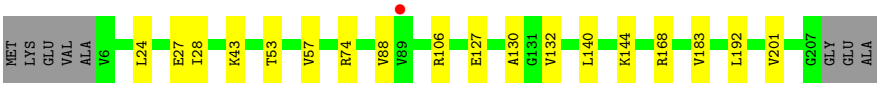
Chain 2E:





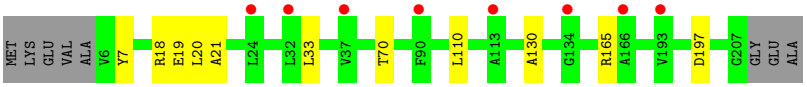
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



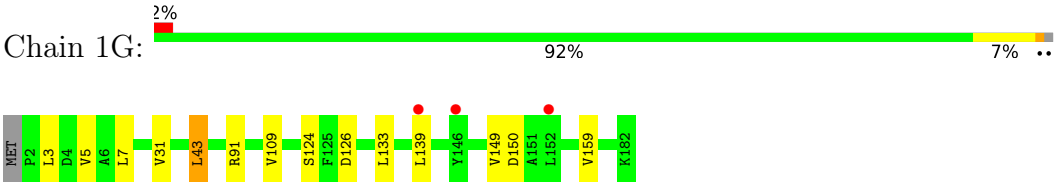
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



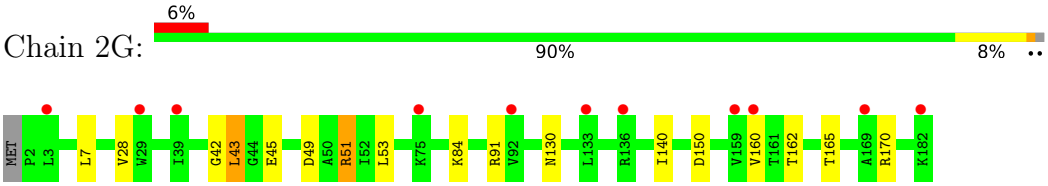
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



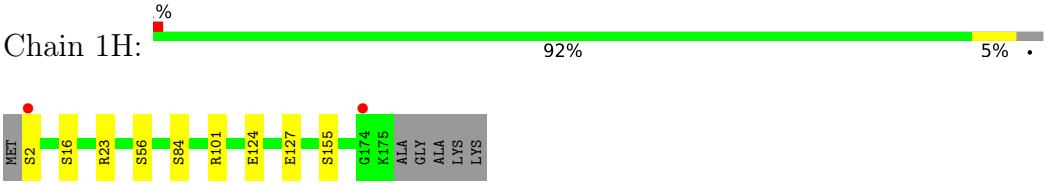
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



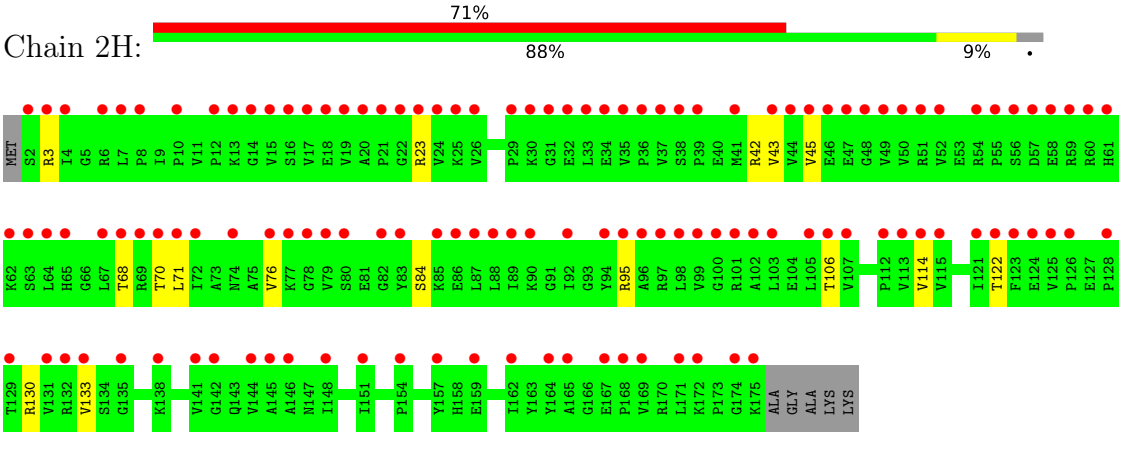
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



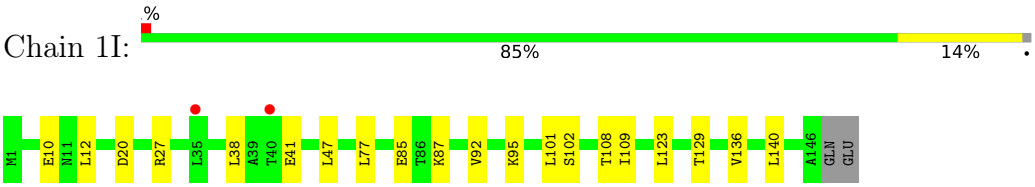
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



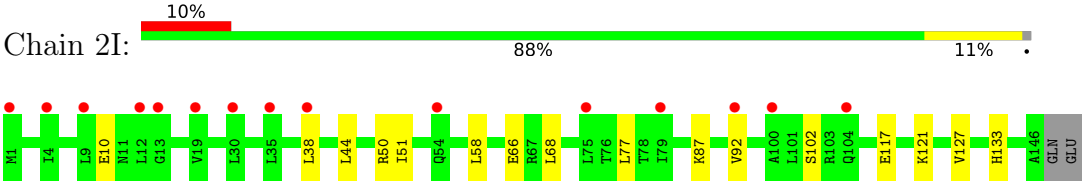
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



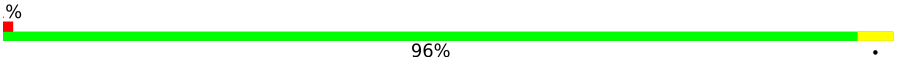
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



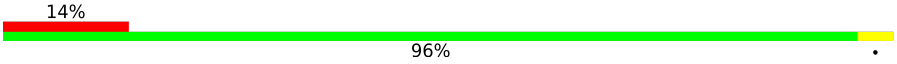
• Molecule 9: 50S ribosomal protein L13

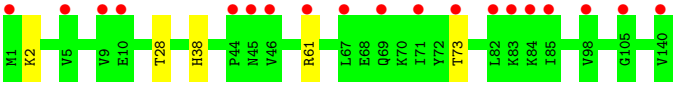
Chain 1N:



• Molecule 9: 50S ribosomal protein L13

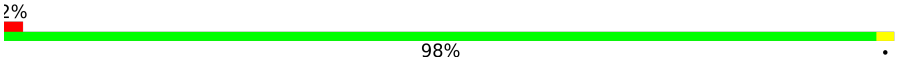
Chain 2N:

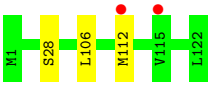




• Molecule 10: 50S ribosomal protein L14

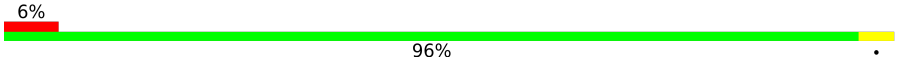
Chain 1O:

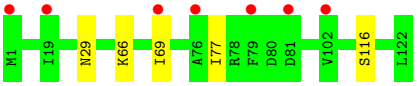




• Molecule 10: 50S ribosomal protein L14

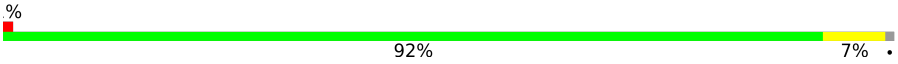
Chain 2O:

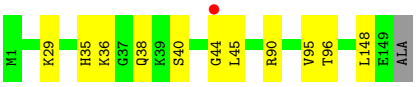




• Molecule 11: 50S ribosomal protein L15

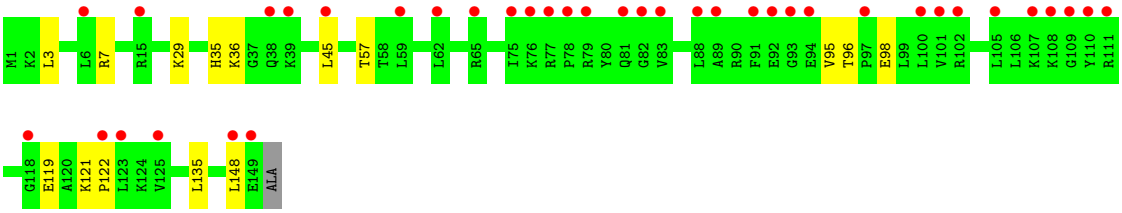
Chain 1P:





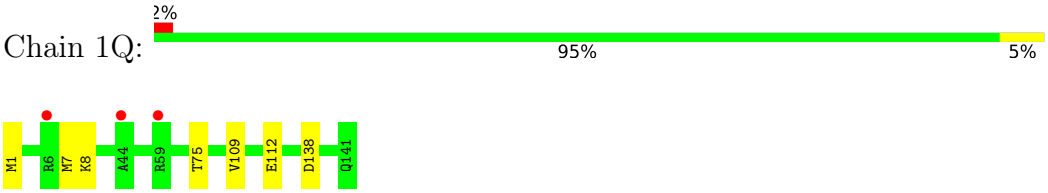
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



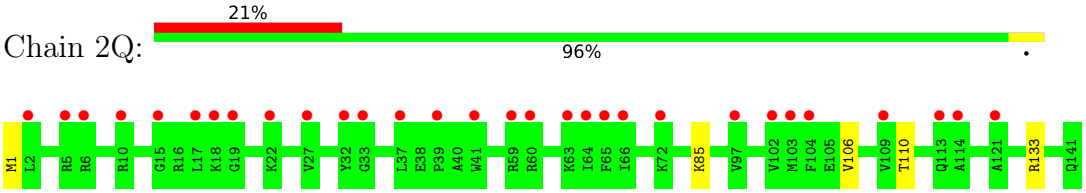
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



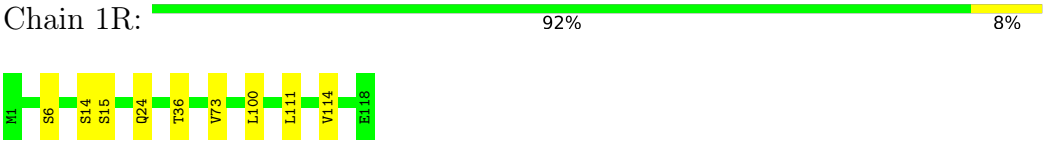
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



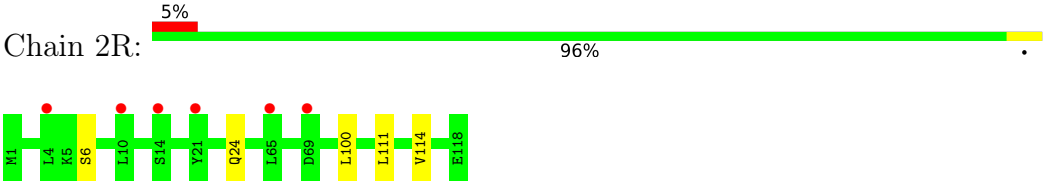
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



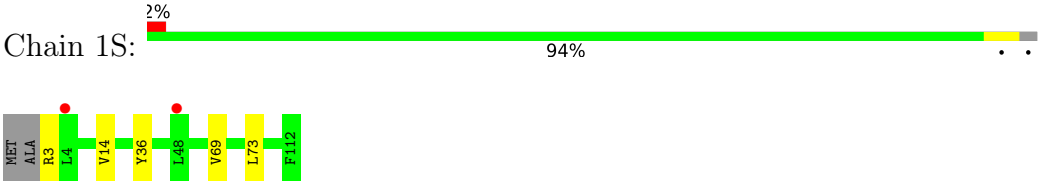
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



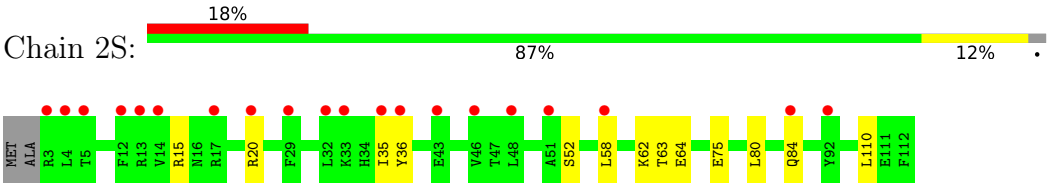
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



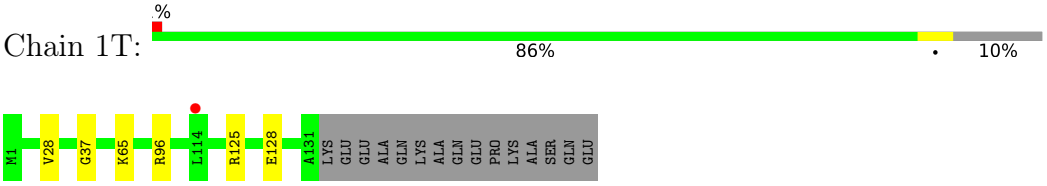
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



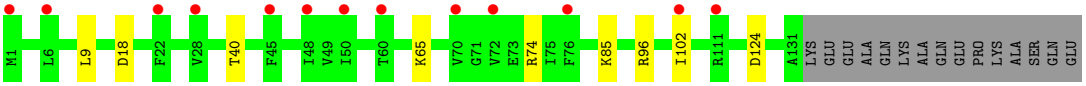
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



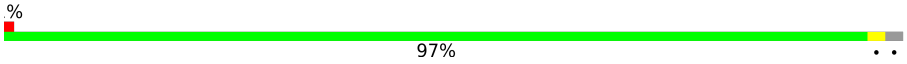
• Molecule 15: 50S ribosomal protein L19

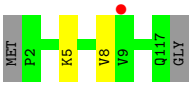
Chain 2T:



• Molecule 16: 50S ribosomal protein L20

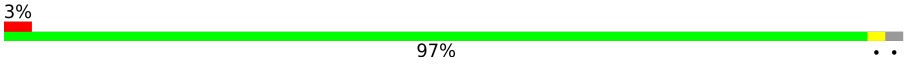
Chain 1U:

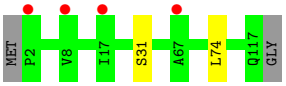




• Molecule 16: 50S ribosomal protein L20

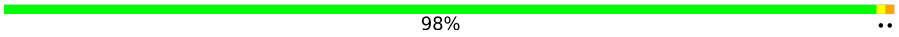
Chain 2U:

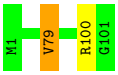




• Molecule 17: 50S ribosomal protein L21

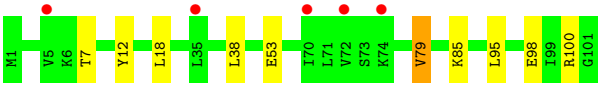
Chain 1V:





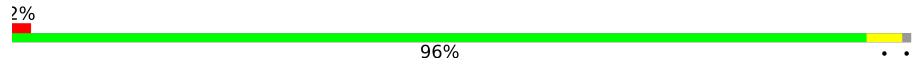
• Molecule 17: 50S ribosomal protein L21

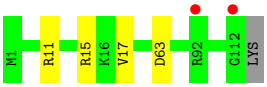
Chain 2V:



• Molecule 18: 50S ribosomal protein L22

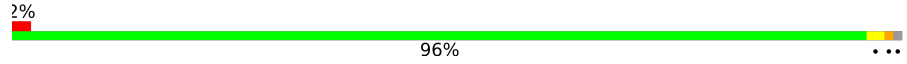
Chain 1W:

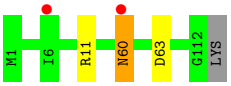




• Molecule 18: 50S ribosomal protein L22

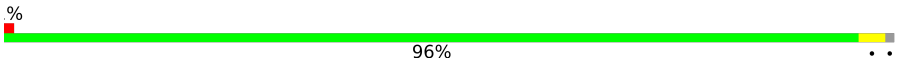
Chain 2W:

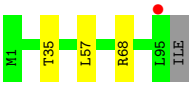




• Molecule 19: 50S ribosomal protein L23

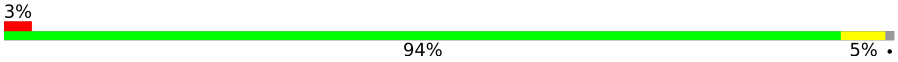
Chain 1X:

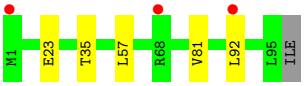




• Molecule 19: 50S ribosomal protein L23

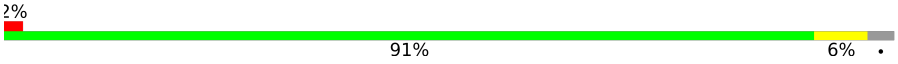
Chain 2X:

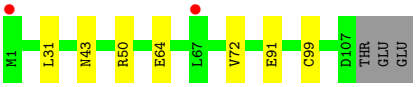




• Molecule 20: 50S ribosomal protein L24

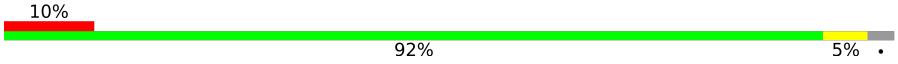
Chain 1Y:

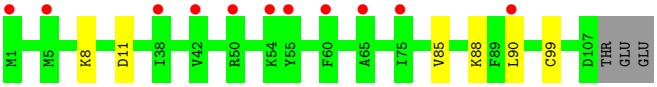




• Molecule 20: 50S ribosomal protein L24

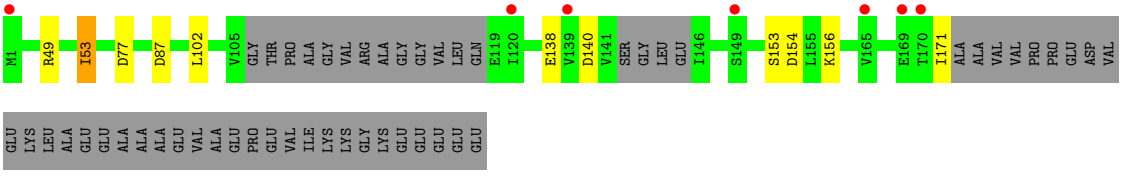
Chain 2Y:





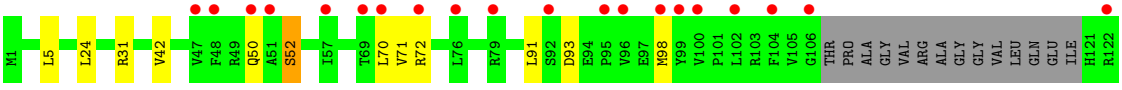
• Molecule 21: 50S ribosomal protein L25

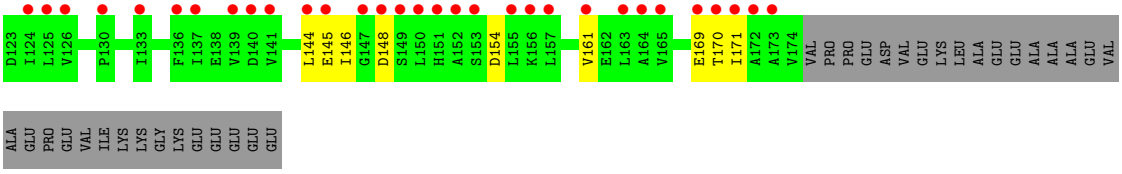
Chain 1Z:



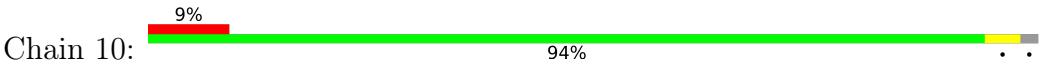
• Molecule 21: 50S ribosomal protein L25

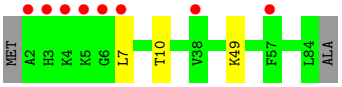
Chain 2Z:



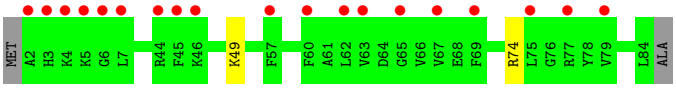


• Molecule 22: 50S ribosomal protein L27

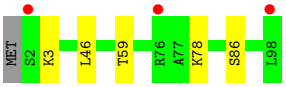




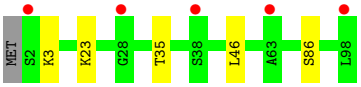
• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28

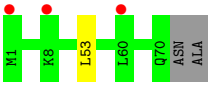


• Molecule 23: 50S ribosomal protein L28



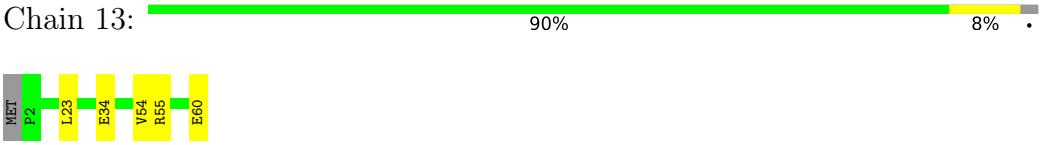
• Molecule 24: 50S ribosomal protein L29

• Molecule 24: 50S ribosomal protein L29



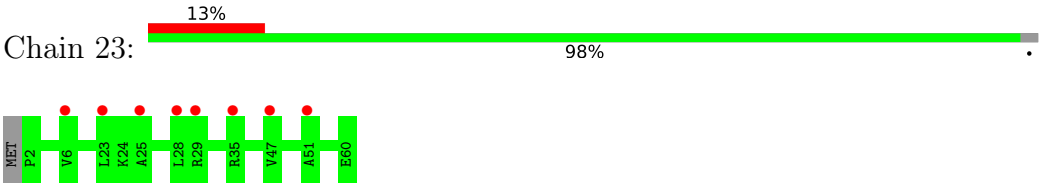
• Molecule 25: 50S ribosomal protein L30

Chain 13:



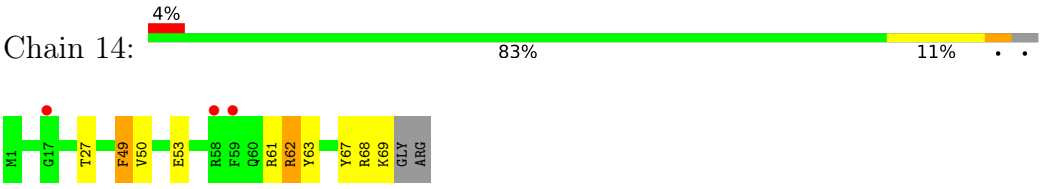
• Molecule 25: 50S ribosomal protein L30

Chain 23:



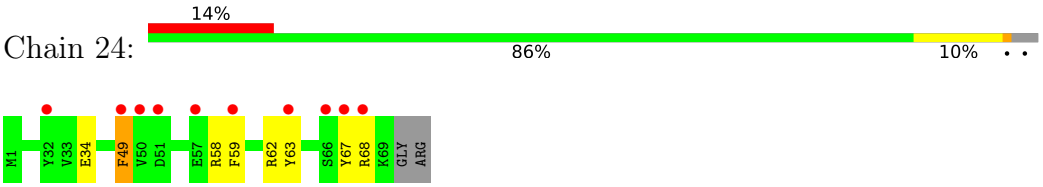
• Molecule 26: 50S ribosomal protein L31

Chain 14:



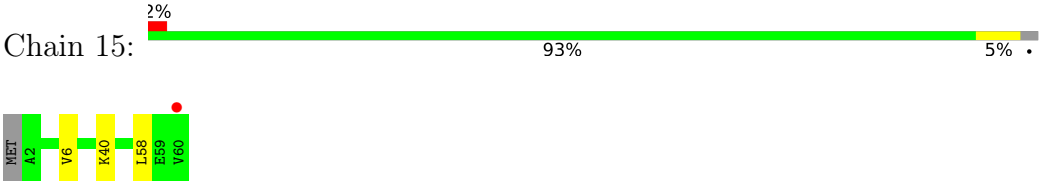
• Molecule 26: 50S ribosomal protein L31

Chain 24:



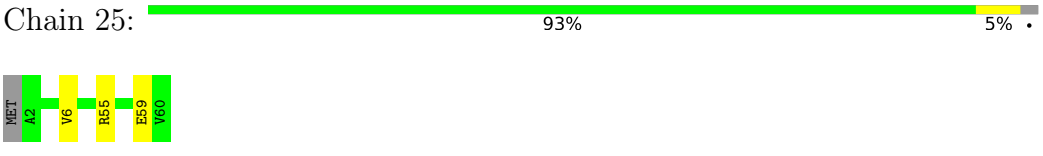
• Molecule 27: 50S ribosomal protein L32

Chain 15:



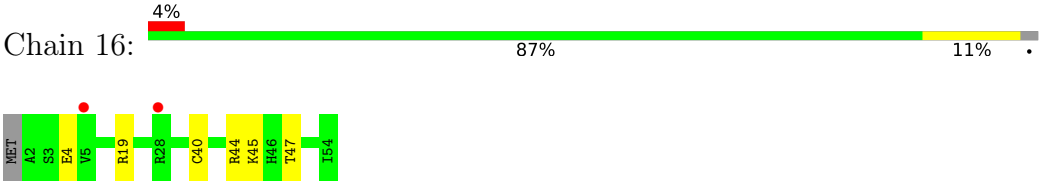
• Molecule 27: 50S ribosomal protein L32

Chain 25:



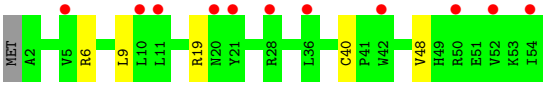
• Molecule 28: 50S ribosomal protein L33

Chain 16:



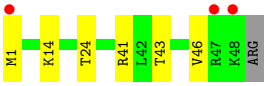
• Molecule 28: 50S ribosomal protein L33

Chain 26:



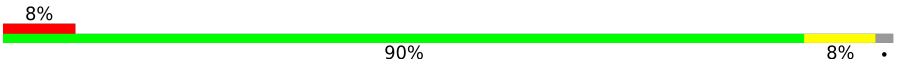
• Molecule 29: 50S ribosomal protein L34

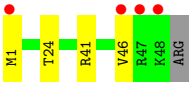
Chain 17:



• Molecule 29: 50S ribosomal protein L34

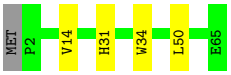
Chain 27:





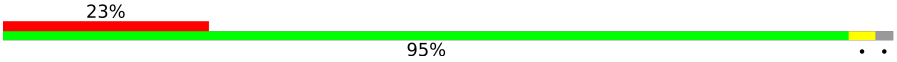
• Molecule 30: 50S ribosomal protein L35

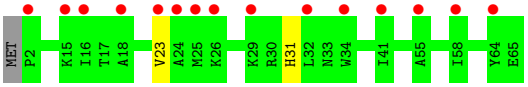
Chain 18:



• Molecule 30: 50S ribosomal protein L35

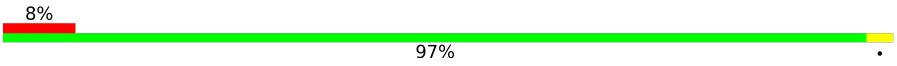
Chain 28:

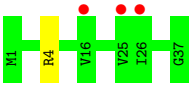




• Molecule 31: 50S ribosomal protein L36

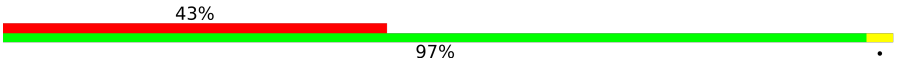
Chain 19:

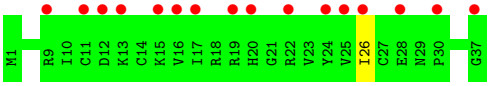




• Molecule 31: 50S ribosomal protein L36

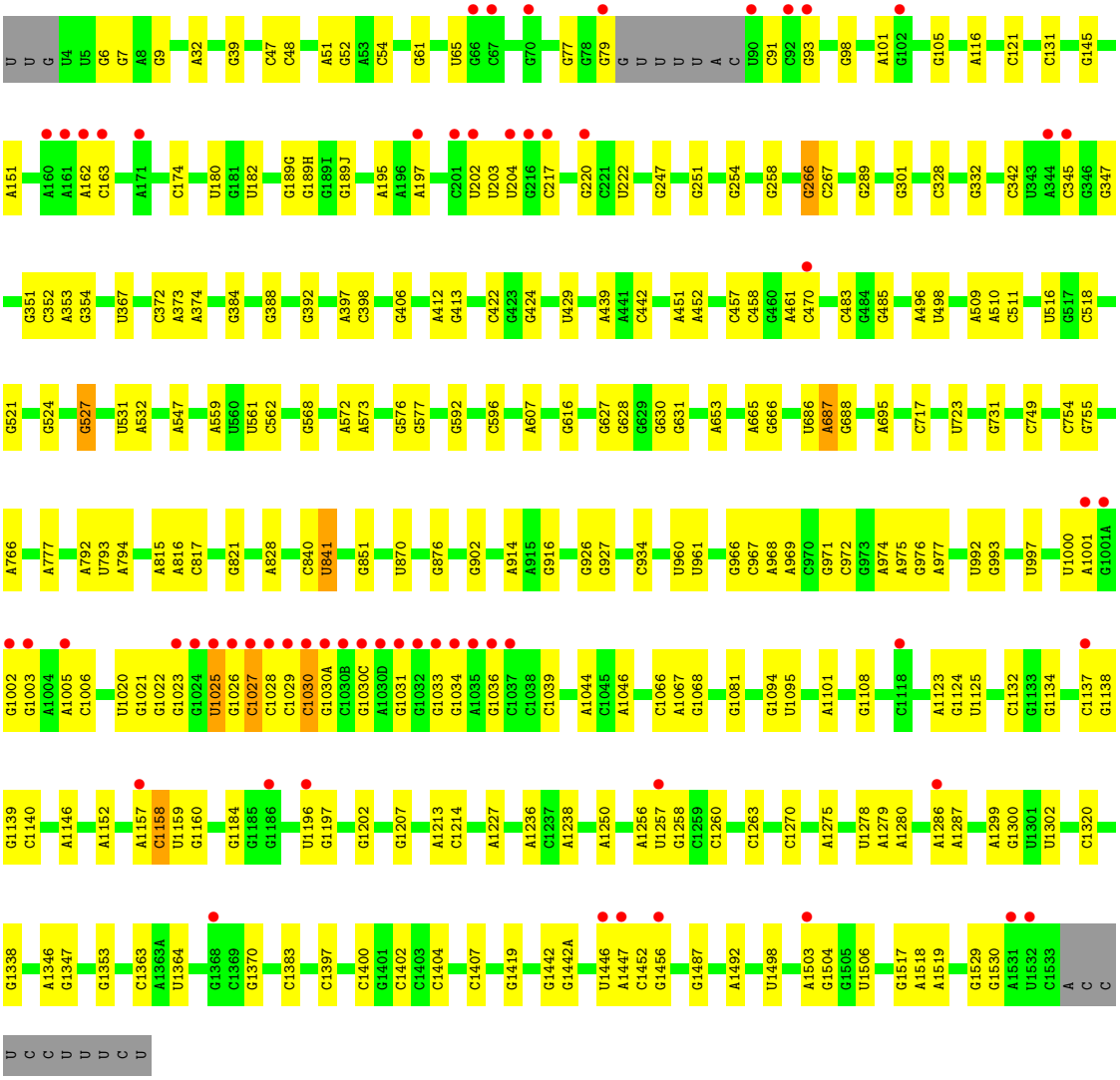
Chain 29:





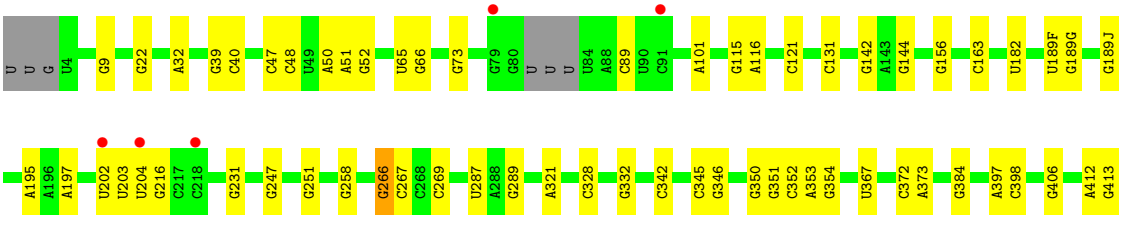
• Molecule 32: 16S Ribosomal RNA

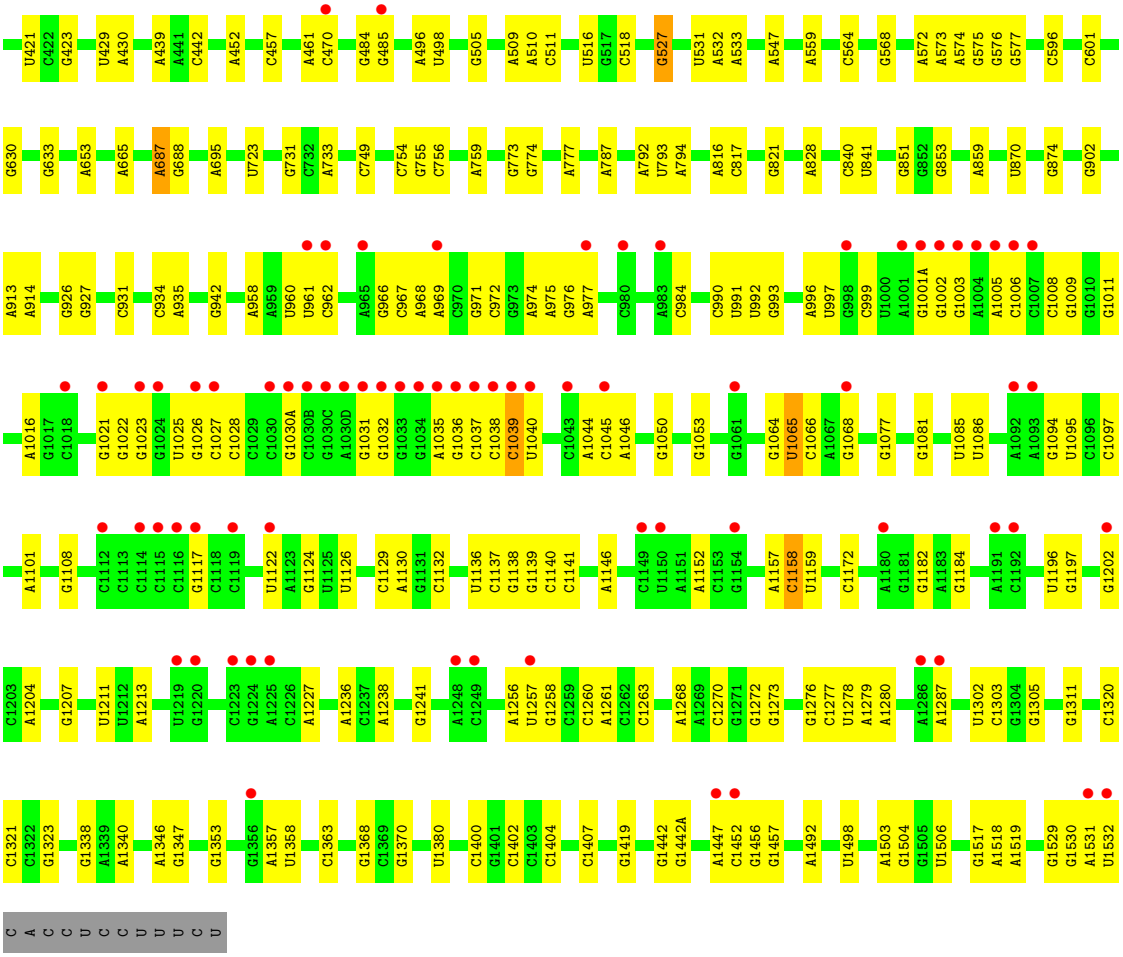
Chain 1a:



• Molecule 32: 16S Ribosomal RNA

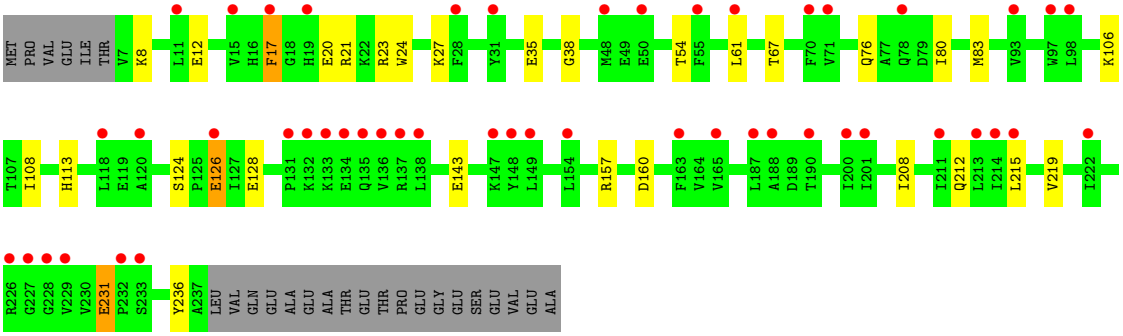
Chain 2a:





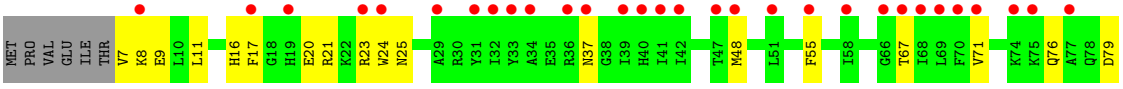
• Molecule 33: 30S ribosomal protein S2

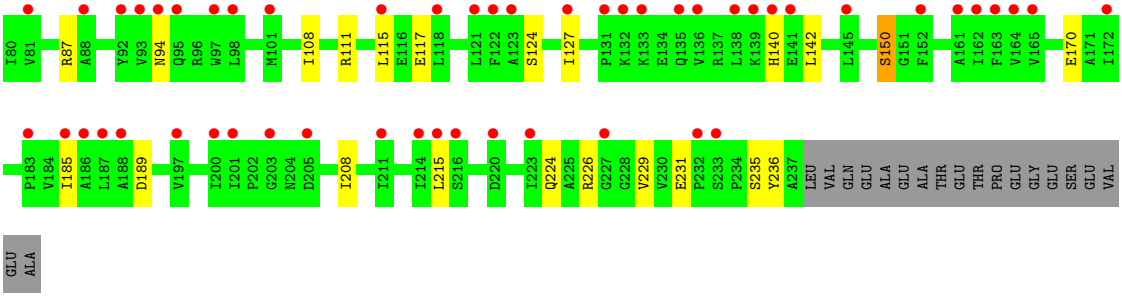
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

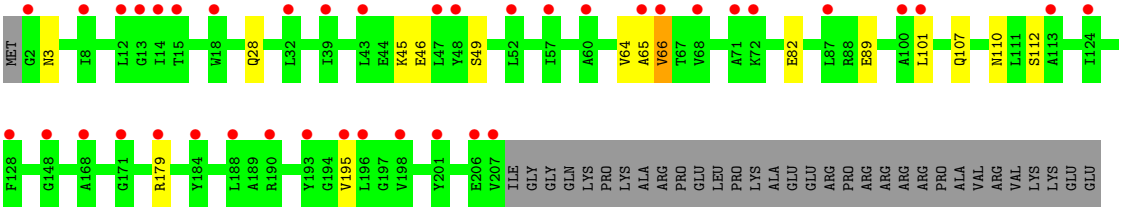
Chain 2b:





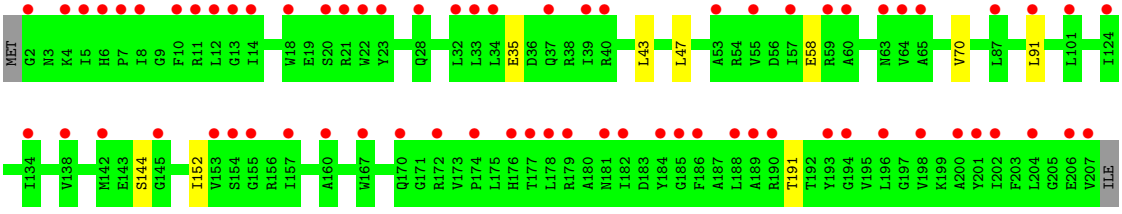
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



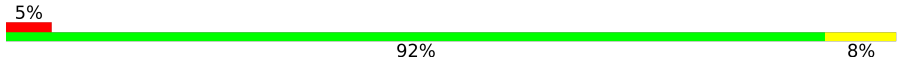
• Molecule 34: 30S ribosomal protein S3

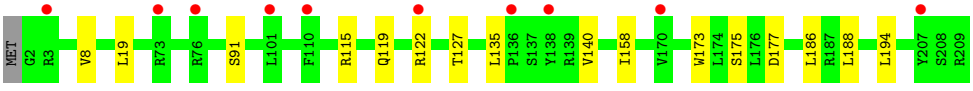
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

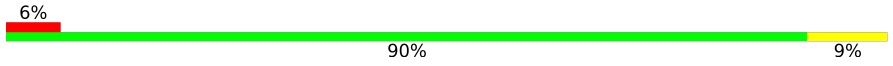
Chain 1d:

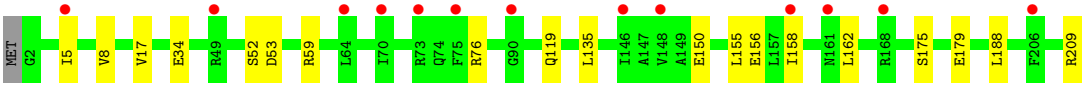




• Molecule 35: 30S ribosomal protein S4

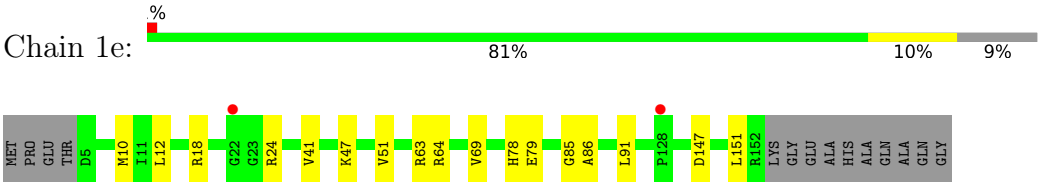
Chain 2d:





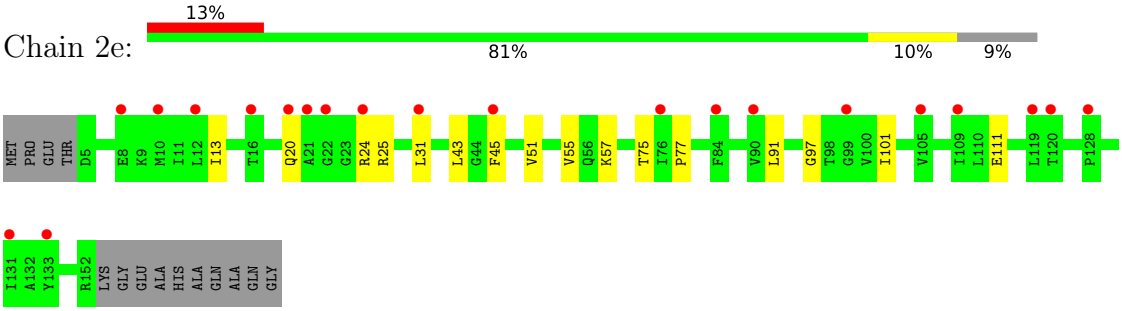
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



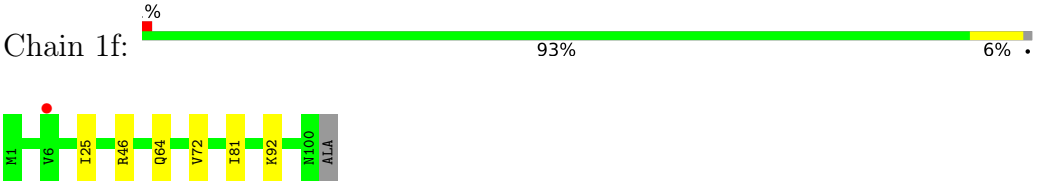
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



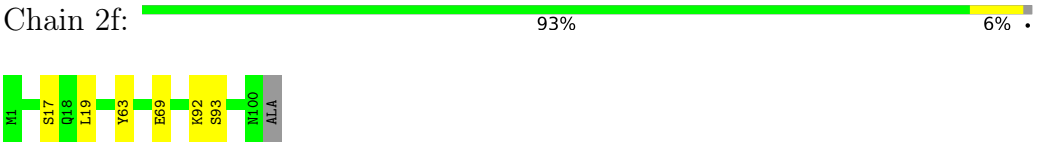
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



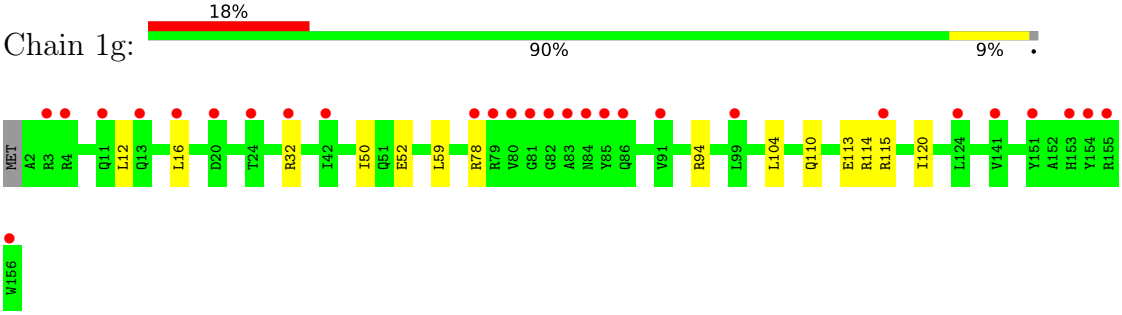
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



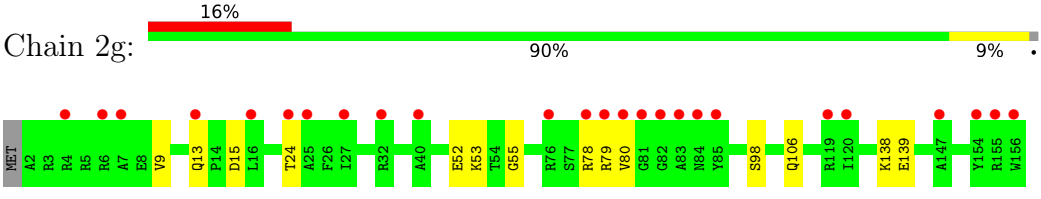
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



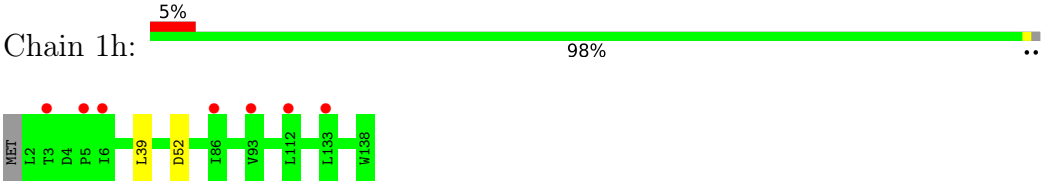
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



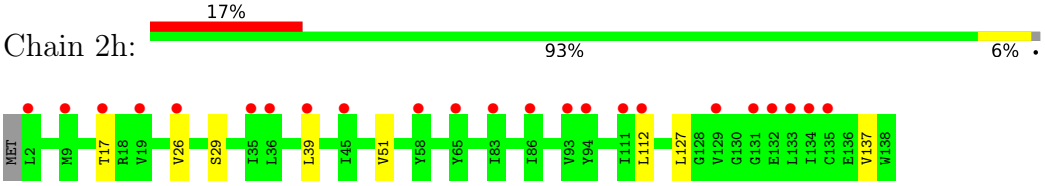
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



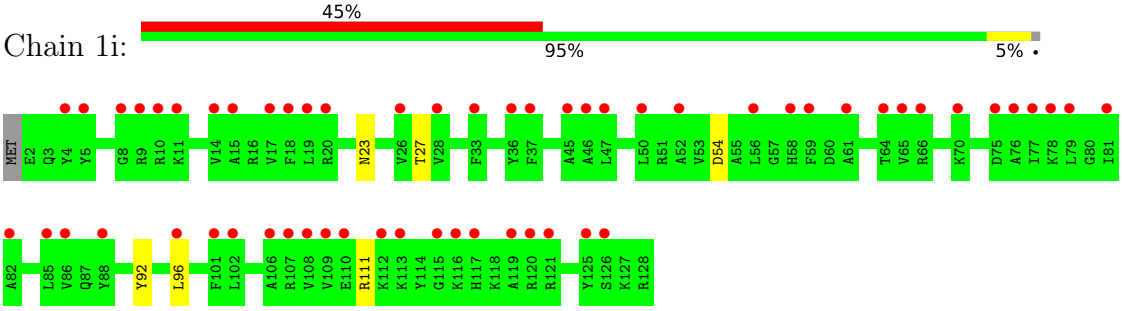
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



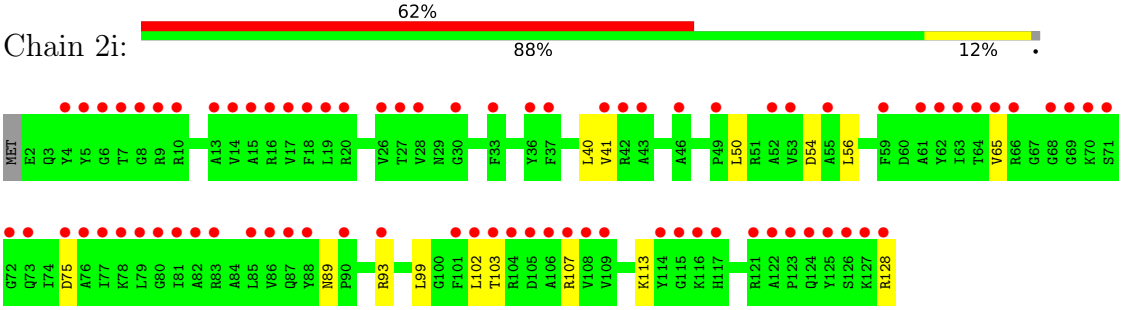
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



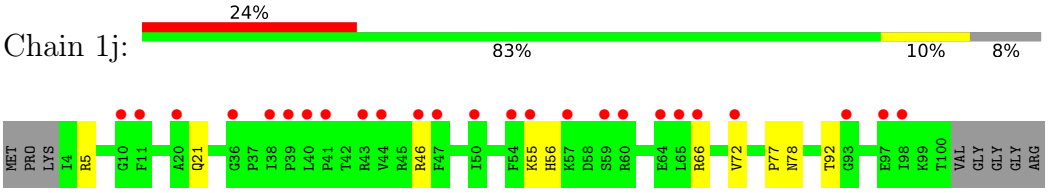
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



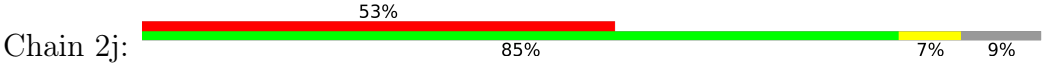
• Molecule 41: 30S ribosomal protein S10

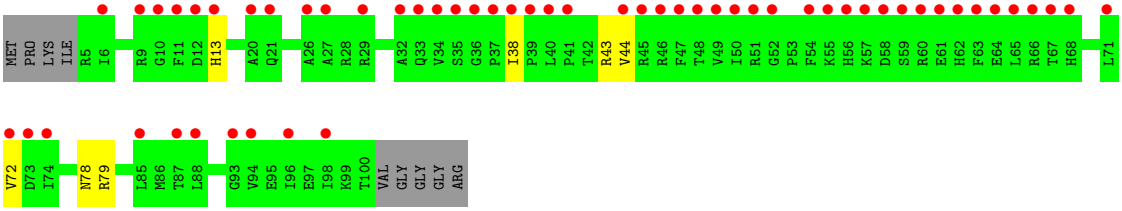
Chain 1j:



• Molecule 41: 30S ribosomal protein S10

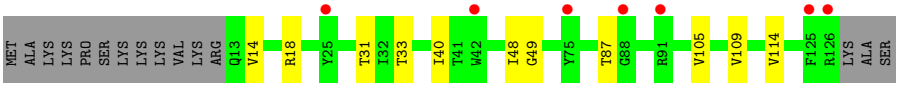
Chain 2j:





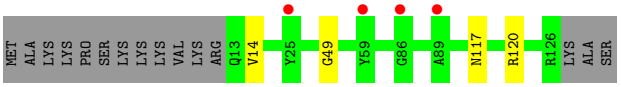
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



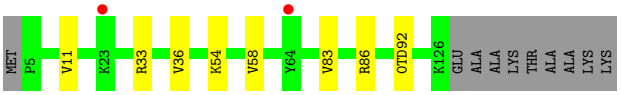
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



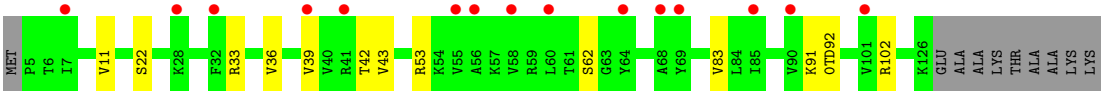
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



• Molecule 43: 30S ribosomal protein S12

Chain 2l:

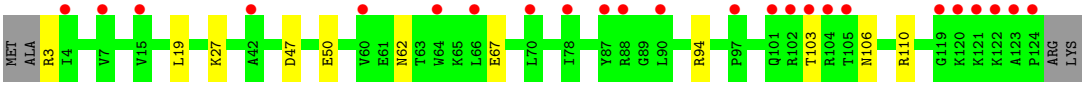


• Molecule 44: 30S ribosomal protein S13

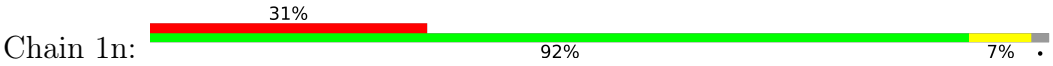
Chain 1m:

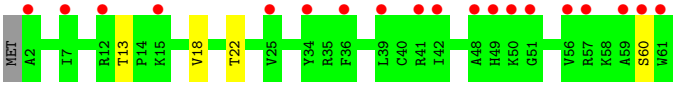
• Molecule 44: 30S ribosomal protein S13

Chain 2m:

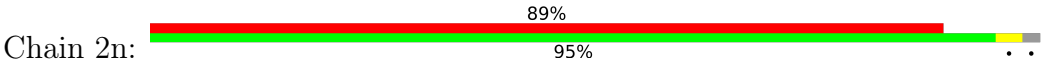


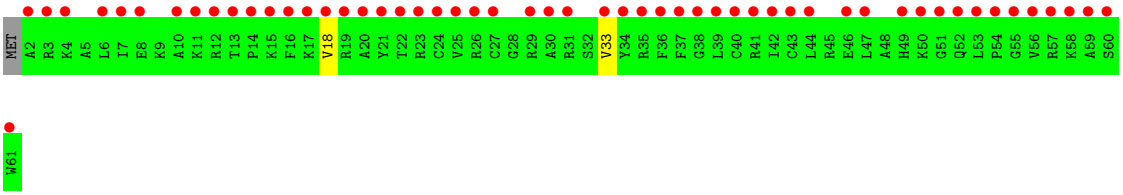
• Molecule 45: 30S ribosomal protein S14 type Z



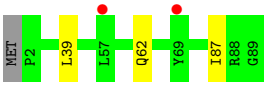


• Molecule 45: 30S ribosomal protein S14 type Z

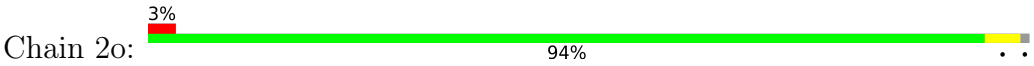


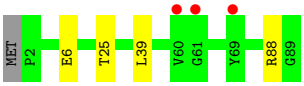


• Molecule 46: 30S ribosomal protein S15

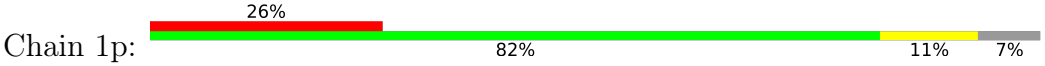


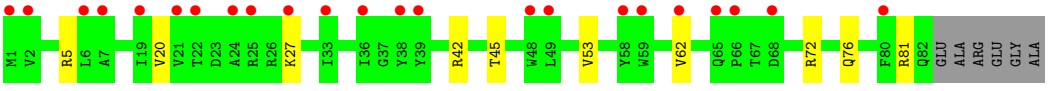
• Molecule 46: 30S ribosomal protein S15



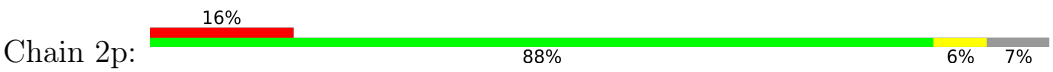


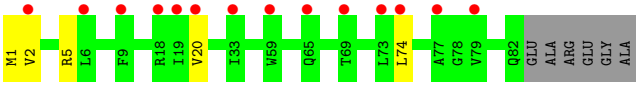
• Molecule 47: 30S ribosomal protein S16





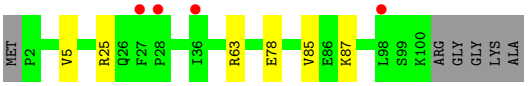
• Molecule 47: 30S ribosomal protein S16





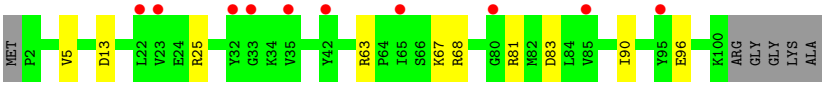
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



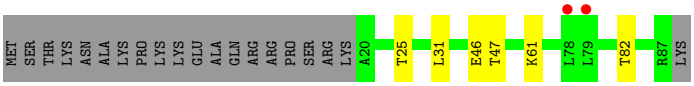
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



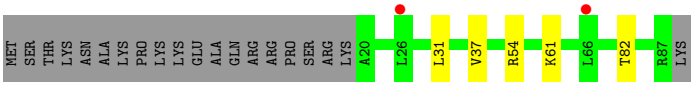
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



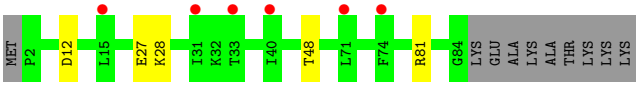
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



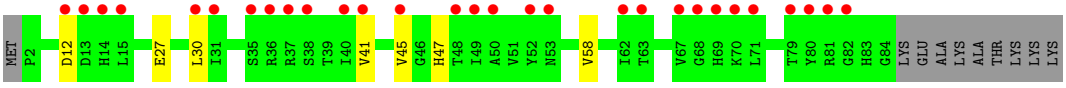
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



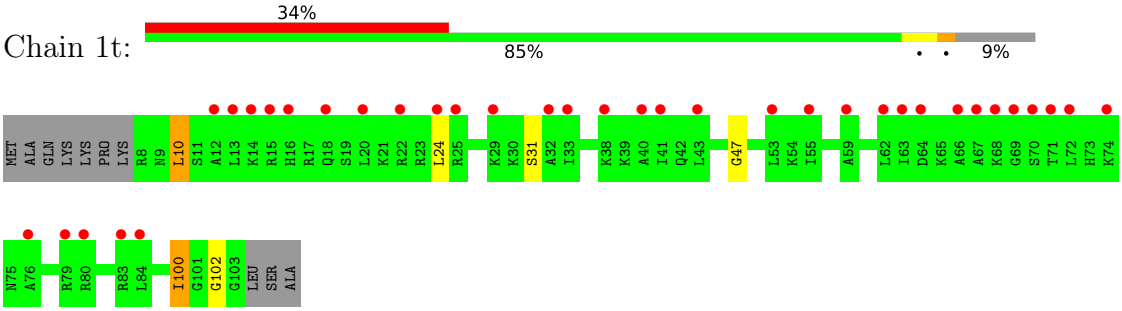
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



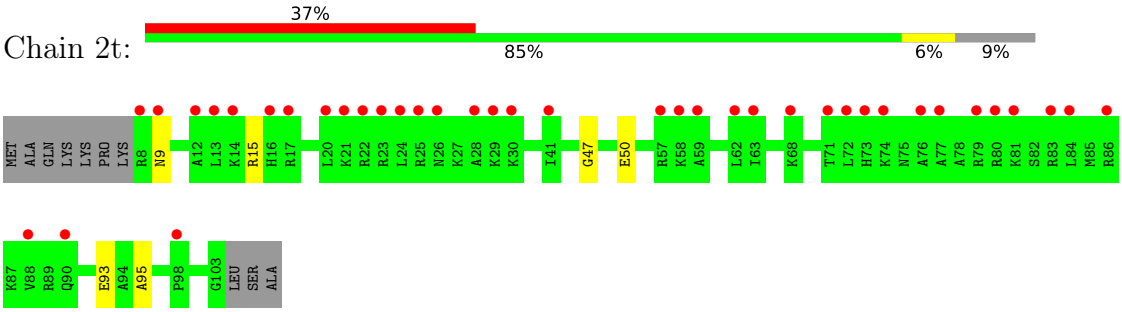
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



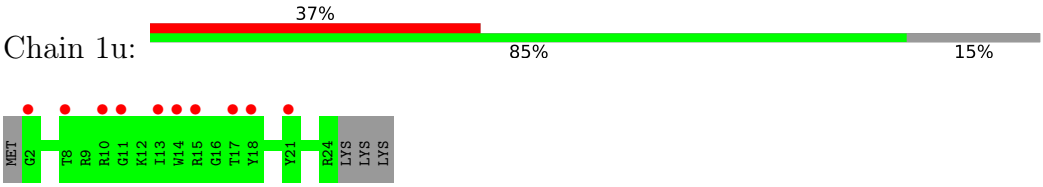
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



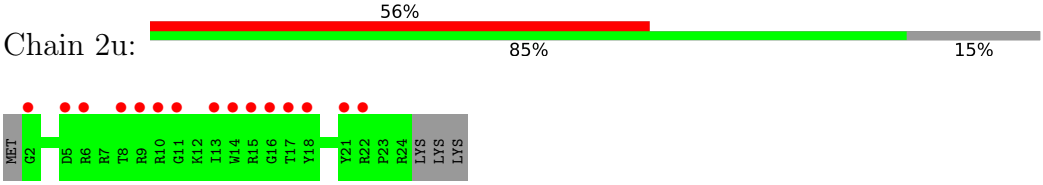
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



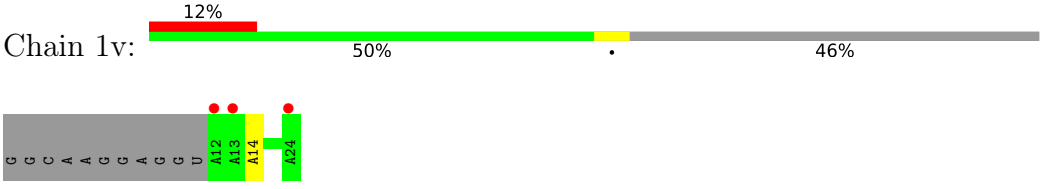
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



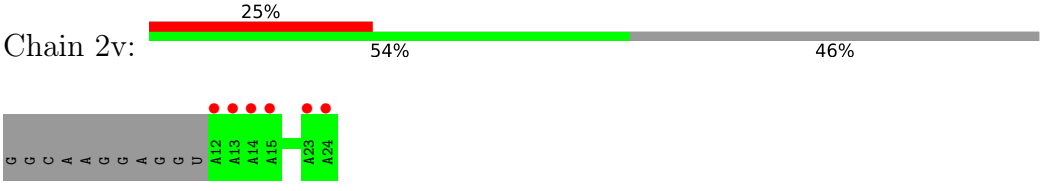
• Molecule 53: MF-mRNA

Chain 1v:



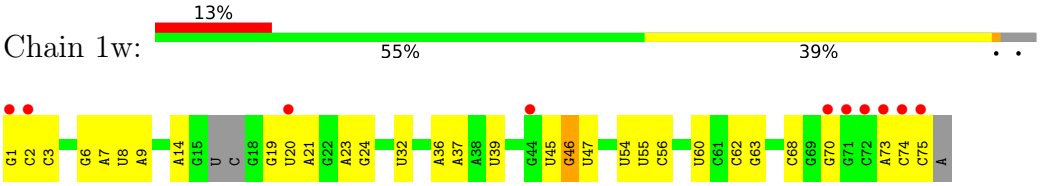
• Molecule 53: MF-mRNA

Chain 2v:



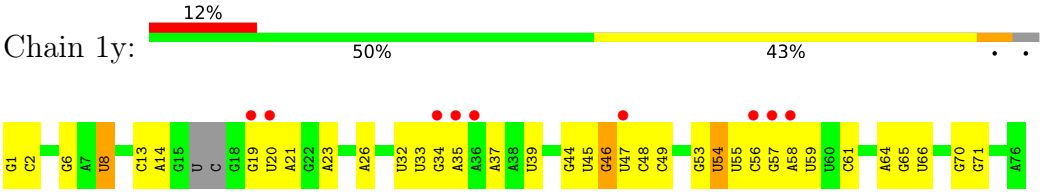
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 1w:



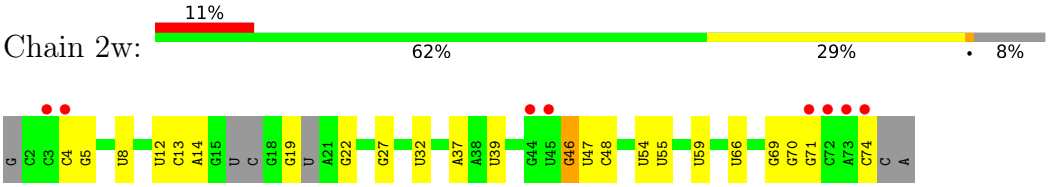
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 1y:



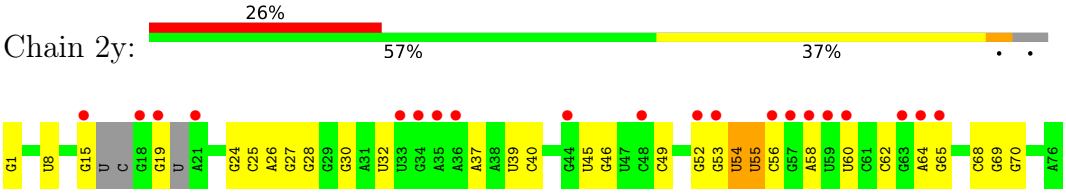
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 2w:



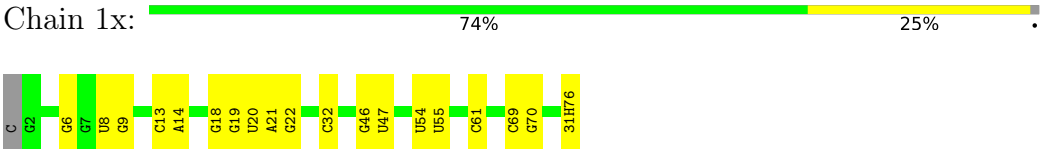
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 2y:



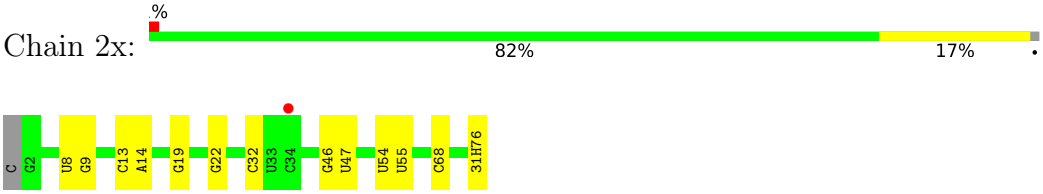
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

Chain 1x:



• Molecule 55: P-site Aminoacylated fMet-tRNAmet

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.64Å 449.56Å 621.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.21 – 2.55 181.69 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.2 (123.21-2.55) 98.2 (181.69-2.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.262 0.218 , 0.262	Depositor DCC
R_{free} test set	92600 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	299868	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

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

[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: MIA, UR3, 4SU, SF4, K, 8AH, OMG, OMC, MA6, MG, 2MG, PSU, 5MC, 4OC, 2MU, ZN, 5MU, 31H, M2G, 6IF, G7M, 0TD

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	0.48	0/69010	0.93	60/107716 (0.1%)
1	2A	0.37	0/67294	0.84	21/105038 (0.0%)
2	1B	0.42	1/2882 (0.0%)	0.83	1/4494 (0.0%)
2	2B	0.38	1/2879 (0.0%)	0.81	1/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.33	0/1592	0.54	0/2149
4	2E	0.30	0/1592	0.49	0/2149
5	1F	0.33	0/1618	0.54	0/2191
5	2F	0.29	0/1614	0.50	0/2186
6	1G	0.31	0/1448	0.51	0/1957
6	2G	0.29	0/1453	0.48	0/1963
7	1H	0.31	0/1356	0.52	0/1834
7	2H	0.28	0/1356	0.45	0/1834
8	1I	0.29	0/1112	0.48	0/1514
8	2I	0.28	0/1079	0.51	0/1475
9	1N	0.34	0/1144	0.51	0/1543
9	2N	0.28	0/1144	0.45	0/1543
10	1O	0.34	0/943	0.53	0/1269
10	2O	0.30	0/943	0.51	0/1269
11	1P	0.33	0/1152	0.59	0/1533
11	2P	0.30	0/1152	0.53	0/1533
12	1Q	0.34	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.47	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/883	0.52	0/1176
14	2S	0.30	0/880	0.50	0/1172
15	1T	0.30	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.48	0/1468
16	1U	0.35	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.42	0/1301
17	1V	0.35	0/782	0.54	0/1049
17	2V	0.29	0/782	0.49	0/1049
18	1W	0.35	0/897	0.52	0/1205
18	2W	0.30	0/897	0.48	0/1205
19	1X	0.36	0/764	0.57	0/1025
19	2X	0.29	0/764	0.50	0/1025
20	1Y	0.32	0/819	0.52	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.30	0/1267	0.50	0/1717
21	2Z	0.28	0/1299	0.49	0/1763
22	10	0.35	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.32	0/762	0.50	0/1014
23	21	0.31	0/762	0.51	0/1014
24	12	0.32	0/590	0.47	0/781
24	22	0.26	0/590	0.41	0/781
25	13	0.34	0/474	0.55	0/635
25	23	0.30	0/469	0.45	0/630
26	14	0.33	0/565	0.62	1/761 (0.1%)
26	24	0.31	0/545	0.48	0/737
27	15	0.34	0/469	0.53	0/635
27	25	0.31	0/469	0.49	0/635
28	16	0.33	0/460	0.51	0/613
28	26	0.28	0/456	0.48	0/608
29	17	0.35	0/426	0.52	0/561
29	27	0.30	0/426	0.46	0/561
30	18	0.31	0/525	0.54	0/691
30	28	0.29	0/525	0.49	0/691
31	19	0.35	0/310	0.54	0/407
31	29	0.27	0/310	0.52	0/407
32	1a	0.36	0/35795	0.86	17/55864 (0.0%)
32	2a	0.34	4/35886 (0.0%)	0.87	30/56005 (0.1%)
33	1b	0.29	0/1881	0.49	0/2542
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.48	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.28	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.45	0/2284
36	1e	0.29	0/1145	0.51	0/1543
36	2e	0.29	0/1149	0.48	0/1548
37	1f	0.29	0/823	0.47	0/1115
37	2f	0.30	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.27	0/1250	0.44	0/1679
38	2g	0.26	0/1254	0.43	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.50	0/1346
40	2i	0.29	0/997	0.50	0/1343
41	1j	0.28	0/722	0.49	0/982
41	2j	0.27	0/727	0.48	0/988
42	1k	0.28	0/844	0.51	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.28	0/937	0.50	0/1260
44	1m	0.29	0/969	0.47	0/1302
44	2m	0.27	0/961	0.49	0/1291
45	1n	0.30	0/501	0.47	0/664
45	2n	0.29	0/501	0.47	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.27	0/697	0.49	0/939
47	2p	0.27	0/693	0.51	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.28	0/836	0.48	0/1117
49	1r	0.28	0/560	0.50	0/746
49	2r	0.28	0/560	0.45	0/746
50	1s	0.26	0/667	0.50	0/900
50	2s	0.29	0/661	0.55	0/893
51	1t	0.27	0/730	0.45	0/965
51	2t	0.27	0/729	0.41	0/965
52	1u	0.27	0/203	0.47	0/266
52	2u	0.31	0/203	0.50	0/266
53	1v	0.38	0/310	0.89	0/480
53	2v	0.32	0/310	0.81	0/480
54	1w	0.49	1/1581 (0.1%)	1.02	0/2458
54	1y	0.50	1/1606 (0.1%)	1.04	2/2497 (0.1%)
54	2w	0.44	0/1509	0.97	1/2345 (0.0%)
54	2y	0.49	1/1583 (0.1%)	0.97	2/2459 (0.1%)
55	1x	0.54	3/1700 (0.2%)	1.13	20/2650 (0.8%)
55	2x	0.48	1/1700 (0.1%)	1.09	17/2650 (0.6%)
All	All	0.38	13/316564 (0.0%)	0.80	173/473927 (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
11	1P	0	1
11	2P	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	1	G	OP3-P	-10.28	1.48	1.61
2	2B	1	U	OP3-P	-10.11	1.49	1.61
54	2y	1	G	OP3-P	-10.04	1.49	1.61
2	1B	1	U	OP3-P	-10.03	1.49	1.61
54	1w	1	G	OP3-P	-10.00	1.49	1.61
32	2a	1272	G	N1-C2	-9.04	1.30	1.37
32	2a	1272	G	C6-N1	-8.74	1.33	1.39
32	2a	1263	C	N3-C4	-5.81	1.29	1.33
55	1x	22	G	N7-C5	5.59	1.42	1.39
55	1x	22	G	C8-N7	5.29	1.34	1.30
32	2a	1263	C	N1-C2	5.22	1.45	1.40
55	2x	22	G	N7-C5	5.01	1.42	1.39
55	1x	14	A	N7-C5	-5.00	1.36	1.39

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	28.12	135.77	118.90
32	2a	1272	G	N3-C2-N2	22.07	135.35	119.90
32	2a	1272	G	C5-C6-O6	20.40	140.84	128.60
32	2a	1272	G	N1-C2-N2	-19.28	98.85	116.20
32	2a	1263	C	N3-C2-O2	-16.52	110.34	121.90
32	2a	1263	C	C2-N3-C4	14.92	127.36	119.90
55	1x	46	G	C6-N1-C2	-12.71	117.47	125.10
32	2a	1272	G	C6-N1-C2	12.10	132.36	125.10
32	2a	1272	G	N1-C6-O6	-11.72	112.87	119.90
55	2x	46	G	C6-N1-C2	-11.40	118.26	125.10
32	2a	1263	C	C5-C6-N1	11.21	126.61	121.00
32	2a	1272	G	C5-C6-N1	-10.51	106.25	111.50
55	1x	22	G	C5-N7-C8	-10.20	99.20	104.30
32	2a	1263	C	C2-N1-C1'	9.64	129.40	118.80
1	1A	975	C	N1-C2-O2	-9.48	113.21	118.90
32	2a	1272	G	C2-N3-C4	-9.27	107.27	111.90
55	1x	14	A	C4-C5-C6	9.13	121.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1063	G	C5-C6-O6	9.12	134.07	128.60
1	1A	2682	U	O5'-P-OP2	-8.96	97.64	105.70
55	2x	22	G	C5-N7-C8	-8.83	99.89	104.30
32	1a	1034	G	C6-N1-C2	8.80	130.38	125.10
1	1A	1075	C	C2-N3-C4	8.78	124.29	119.90
1	1A	1075	C	N1-C2-O2	8.69	124.11	118.90
32	2a	1263	C	C4-C5-C6	-8.62	113.09	117.40
55	1x	14	A	C5-N7-C8	8.32	108.06	103.90
1	1A	2167	U	C2-N1-C1'	8.16	127.50	117.70
55	2x	46	G	N3-C2-N2	-8.11	114.22	119.90
32	2a	1263	C	C6-N1-C2	-8.07	117.07	120.30
55	1x	46	G	N3-C2-N2	-7.88	114.38	119.90
55	2x	14	A	C5-N7-C8	7.86	107.83	103.90
32	2a	1263	C	N3-C4-N4	-7.83	112.52	118.00
32	2a	1263	C	C5-C4-N4	7.75	125.63	120.20
1	1A	576	U	O5'-P-OP1	-7.75	98.72	105.70
32	1a	1025	U	N1-C2-O2	7.66	128.16	122.80
32	2a	1263	C	N1-C2-N3	-7.59	113.89	119.20
1	1A	1086	A	N1-C6-N6	-7.59	114.05	118.60
1	1A	570	G	C5-C6-O6	-7.50	124.10	128.60
1	2A	2136	C	N1-C2-O2	7.47	123.38	118.90
55	2x	14	A	C4-C5-C6	7.45	120.72	117.00
1	1A	512	G	O4'-C1'-N9	7.45	114.16	108.20
55	1x	22	G	C4-C5-C6	-7.37	114.38	118.80
1	1A	2167	U	N3-C2-O2	-7.35	117.05	122.20
55	1x	46	G	C5-C6-N1	7.35	115.17	111.50
2	2B	80	U	O4'-C1'-N1	7.26	114.00	108.20
1	1A	2167	U	N1-C2-O2	7.11	127.78	122.80
1	1A	1063	G	C6-N1-C2	7.03	129.31	125.10
1	2A	512	G	O4'-C1'-N9	6.97	113.78	108.20
55	2x	22	G	C4-C5-C6	-6.96	114.62	118.80
54	1y	33	U	C2-N1-C1'	6.95	126.04	117.70
55	1x	22	G	N7-C8-N9	6.90	116.55	113.10
32	2a	1272	G	C8-N9-C1'	-6.88	118.05	127.00
55	2x	46	G	N1-C2-N3	6.87	128.02	123.90
1	1A	1614	A	O5'-P-OP1	-6.86	99.53	105.70
55	1x	46	G	N1-C2-N3	6.79	127.97	123.90
55	1x	14	A	C5-C6-N1	-6.78	114.31	117.70
1	1A	975	C	C2-N1-C1'	-6.73	111.40	118.80
32	2a	1272	G	C4-N9-C1'	6.64	135.13	126.50
1	1A	1352	U	O5'-P-OP1	-6.62	99.74	105.70
1	2A	2155	G	C6-N1-C2	6.59	129.05	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1782	C	O5'-P-OP1	-6.50	99.85	105.70
55	2x	22	G	N1-C6-O6	-6.47	116.02	119.90
32	1a	754	C	C2-N1-C1'	6.45	125.90	118.80
1	1A	226	G	O4'-C1'-N9	6.44	113.35	108.20
1	1A	1075	C	C5-C4-N4	6.44	124.71	120.20
55	2x	46	G	N9-C4-C5	6.39	107.96	105.40
1	2A	801	G	O5'-P-OP2	-6.39	99.95	105.70
55	2x	22	G	N7-C8-N9	6.32	116.26	113.10
55	1x	22	G	C5-C6-N1	6.30	114.65	111.50
54	2y	26	A	N1-C6-N6	6.23	122.34	118.60
1	2A	1313	U	C2-N1-C1'	6.22	125.17	117.70
55	2x	46	G	C4-C5-N7	-6.21	108.32	110.80
1	2A	645	C	C2-N1-C1'	6.16	125.57	118.80
32	2a	1263	C	C6-N1-C1'	-6.14	113.43	120.80
1	1A	2248	C	O5'-P-OP2	-6.12	100.19	105.70
1	1A	2582	G	O5'-P-OP1	-6.11	100.21	105.70
55	2x	14	A	C5-C6-N1	-6.08	114.66	117.70
1	1A	847	U	C2-N1-C1'	6.07	124.98	117.70
1	1A	1776	G	O5'-P-OP2	-6.06	100.25	105.70
1	1A	1992	G	P-O3'-C3'	5.96	126.86	119.70
32	2a	754	C	C2-N1-C1'	5.96	125.36	118.80
55	2x	46	G	C5-C6-N1	5.91	114.45	111.50
32	1a	754	C	N1-C2-O2	5.89	122.44	118.90
32	1a	266	G	P-O3'-C3'	5.89	126.77	119.70
55	1x	46	G	N9-C4-C5	5.88	107.75	105.40
32	1a	254	G	O5'-P-OP1	-5.87	100.42	105.70
26	14	27	THR	C-N-CA	5.87	136.36	121.70
1	1A	801	G	O5'-P-OP2	-5.85	100.43	105.70
55	1x	22	G	C8-N9-C1'	5.85	134.61	127.00
32	1a	841	U	C5-C6-N1	5.85	125.62	122.70
1	2A	2155	G	C5-C6-O6	5.84	132.10	128.60
32	1a	1158	C	C2-N1-C1'	5.82	125.20	118.80
1	1A	2685	G	N1-C6-O6	-5.82	116.41	119.90
1	1A	2629	A	P-O3'-C3'	5.81	126.67	119.70
1	2A	2492	U	O5'-P-OP1	-5.80	100.48	105.70
1	1A	975	C	C5-C6-N1	-5.79	118.11	121.00
55	1x	22	G	N1-C6-O6	-5.78	116.43	119.90
32	1a	1030	C	N1-C2-O2	5.78	122.37	118.90
1	1A	2129	C	C2-N1-C1'	5.78	125.16	118.80
1	1A	975	C	C2-N3-C4	-5.74	117.03	119.90
1	1A	746	A	O4'-C1'-N9	5.68	112.75	108.20
1	1A	2502	G	O5'-P-OP2	-5.66	100.61	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	46	G	C5-C6-O6	-5.64	125.22	128.60
1	1A	784	A	OP1-P-O3'	5.61	117.54	105.20
54	1y	33	U	N1-C2-O2	5.61	126.73	122.80
1	1A	1174	A	P-O3'-C3'	5.59	126.41	119.70
55	1x	22	G	N3-C4-N9	-5.59	122.64	126.00
1	1A	805	G	N9-C4-C5	-5.59	103.17	105.40
55	1x	22	G	C4-C5-N7	5.59	113.03	110.80
1	1A	1075	C	N3-C4-C5	-5.57	119.67	121.90
1	1A	1174	A	OP1-P-O3'	5.56	117.44	105.20
32	1a	1027	C	C6-N1-C1'	5.56	127.47	120.80
1	1A	1828	G	O5'-P-OP2	-5.56	100.70	105.70
1	2A	2689	U	P-O3'-C3'	5.55	126.36	119.70
1	1A	1176	G	OP1-P-O3'	5.55	117.41	105.20
55	1x	46	G	C4-C5-N7	-5.55	108.58	110.80
55	2x	22	G	C8-N9-C1'	5.54	134.20	127.00
32	1a	1034	G	C5-C6-O6	5.53	131.92	128.60
1	1A	1187	G	N1-C6-O6	-5.53	116.58	119.90
1	1A	1313	U	C2-N1-C1'	5.51	124.31	117.70
1	1A	793	A	O5'-P-OP2	-5.50	100.75	105.70
32	1a	1034	G	C5-C6-N1	-5.49	108.76	111.50
1	2A	847	U	C2-N1-C1'	5.48	124.28	117.70
32	1a	1067	A	P-O3'-C3'	5.46	126.25	119.70
1	2A	528	A	P-O3'-C3'	5.46	126.25	119.70
1	1A	1063	G	N1-C6-O6	-5.45	116.63	119.90
1	1A	787	U	O5'-P-OP1	-5.44	100.80	105.70
1	1A	2593	U	N3-C4-O4	-5.43	115.60	119.40
2	1B	41	U	C5-C6-N1	-5.42	119.99	122.70
32	2a	754	C	N1-C2-O2	5.42	122.15	118.90
1	1A	1075	C	N3-C2-O2	-5.41	118.11	121.90
1	2A	1992	G	P-O3'-C3'	5.40	126.18	119.70
54	2w	13	C	P-O3'-C3'	5.39	126.17	119.70
55	2x	14	A	C4-C5-N7	-5.33	108.04	110.70
54	2y	26	A	C5-C6-N6	-5.32	119.44	123.70
1	1A	1372	U	C5-C4-O4	-5.29	122.73	125.90
32	2a	1065	U	P-O3'-C3'	5.29	126.04	119.70
1	1A	1313	U	N1-C2-O2	5.27	126.49	122.80
1	1A	195	A	P-O3'-C3'	5.26	126.01	119.70
32	2a	687	A	P-O3'-C3'	5.26	126.01	119.70
32	1a	687	A	P-O3'-C3'	5.25	126.00	119.70
1	1A	2848	G	O4'-C1'-N9	5.25	112.40	108.20
55	1x	14	A	C8-N9-C1'	-5.23	118.28	127.70
55	1x	14	A	C4-N9-C1'	5.22	135.71	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1158	C	N1-C2-O2	5.22	122.03	118.90
1	2A	2318	G	N3-C4-C5	-5.22	125.99	128.60
32	1a	1036	G	N1-C6-O6	-5.20	116.78	119.90
1	1A	1372	U	N3-C4-O4	5.20	123.04	119.40
1	2A	330	A	C2-N3-C4	-5.19	108.00	110.60
1	2A	645	C	N1-C2-O2	5.18	122.01	118.90
32	1a	1027	C	C2-N1-C1'	-5.17	113.11	118.80
1	1A	2167	U	C6-N1-C2	-5.16	117.91	121.00
1	1A	372	G	O4'-C1'-N9	5.15	112.32	108.20
1	1A	975	C	N3-C2-O2	5.15	125.50	121.90
1	2A	1313	U	O4'-C1'-N1	5.15	112.32	108.20
1	1A	784	A	O4'-C1'-N9	5.15	112.32	108.20
32	2a	1039	C	N1-C2-O2	5.14	121.99	118.90
1	2A	277	C	OP2-P-O3'	5.14	116.50	105.20
32	2a	266	G	P-O3'-C3'	5.14	125.86	119.70
1	1A	548	A	P-O3'-C3'	5.13	125.86	119.70
55	2x	22	G	N3-C4-N9	-5.12	122.93	126.00
1	2A	2712	U	O4'-C1'-N1	5.12	112.30	108.20
1	1A	2167	U	C5-C6-N1	5.12	125.26	122.70
32	2a	65	U	P-O3'-C3'	5.12	125.84	119.70
32	2a	913	A	P-O3'-C3'	5.10	125.82	119.70
1	1A	1955	U	C2-N1-C1'	-5.09	111.59	117.70
32	2a	1158	C	C2-N1-C1'	5.09	124.40	118.80
55	2x	14	A	C4-N9-C1'	5.07	135.42	126.30
1	2A	2335	A	O4'-C1'-N9	5.06	112.25	108.20
32	2a	115	G	P-O3'-C3'	5.06	125.77	119.70
1	2A	228	A	P-O3'-C3'	5.04	125.75	119.70
1	2A	1380	G	O5'-P-OP2	-5.03	101.18	105.70
1	1A	1131	G	O4'-C1'-N9	5.02	112.21	108.20
1	1A	784	A	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	259 (95%)	14 (5%)	0	100 100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100 100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29 40
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29 40
5	1F	200/210 (95%)	192 (96%)	7 (4%)	1 (0%)	29 40
5	2F	200/210 (95%)	189 (94%)	9 (4%)	2 (1%)	15 22
6	1G	179/182 (98%)	165 (92%)	12 (7%)	2 (1%)	14 19
6	2G	179/182 (98%)	154 (86%)	21 (12%)	4 (2%)	6 7
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100 100
7	2H	172/180 (96%)	156 (91%)	16 (9%)	0	100 100
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100 100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	22 30
9	1N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22 30
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22 30
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19 27
11	1P	147/150 (98%)	136 (92%)	7 (5%)	4 (3%)	5 4
11	2P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	5 4
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100 100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100 100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100 100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	8 9
15	1T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	19 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100 100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15 22
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7 8
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	17 24
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100 100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
21	1Z	148/206 (72%)	125 (84%)	20 (14%)	3 (2%)	7 8
21	2Z	156/206 (76%)	122 (78%)	29 (19%)	5 (3%)	4 3
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	75 (93%)	6 (7%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14 19
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14 19
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	53 (79%)	12 (18%)	2 (3%)	4 3
26	24	67/71 (94%)	51 (76%)	15 (22%)	1 (2%)	10 14
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3 2
33	2b	229/256 (90%)	185 (81%)	38 (17%)	6 (3%)	5 5
34	1c	204/239 (85%)	186 (91%)	15 (7%)	3 (2%)	10 14
34	2c	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	15 22
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	29 40
35	2d	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	15 22
36	1e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	7 7
36	2e	146/162 (90%)	135 (92%)	9 (6%)	2 (1%)	11 15
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100 100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
38	1g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	22 30
38	2g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	12 16
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100 100
39	2h	135/138 (98%)	121 (90%)	14 (10%)	0	100 100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	19 27
40	2i	125/128 (98%)	108 (86%)	17 (14%)	0	100 100
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	3 1
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	4 3
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8 10
42	2k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	17 24
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100 100
44	1m	121/126 (96%)	110 (91%)	10 (8%)	1 (1%)	19 27
44	2m	120/126 (95%)	102 (85%)	17 (14%)	1 (1%)	19 27
45	1n	58/61 (95%)	56 (97%)	1 (2%)	1 (2%)	9 11
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13 17
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
47	1p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	12 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100 100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
48	2q	97/105 (92%)	89 (92%)	5 (5%)	3 (3%)	4 3
49	1r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	10 14
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
50	1s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	5 5
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100 100
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2 1
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	7 7
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
All	All	11368/12128 (94%)	10445 (92%)	822 (7%)	101 (1%)	17 24

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
33	1b	17	PHE
34	1c	66	VAL
40	1i	54	ASP
41	1j	55	LYS
41	1j	56	HIS
44	1m	67	GLU
5	2F	130	ALA
6	2G	51	ARG
8	2I	10	GLU
11	2P	29	LYS
21	2Z	144	LEU
33	2b	17	PHE
42	2k	49	GLY
44	2m	67	GLU
11	1P	44	GLY
15	1T	37	GLY
17	1V	79	VAL
26	14	49	PHE
26	14	62	ARG
33	1b	106	LYS

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Mol	Chain	Res	Type
34	1c	107	GLN
38	1g	52	GLU
50	1s	81	ARG
51	1t	47	GLY
6	2G	42	GLY
6	2G	43	LEU
17	2V	79	VAL
26	24	49	PHE
33	2b	21	ARG
38	2g	55	GLY
38	2g	80	VAL
41	2j	79	ARG
48	2q	68	ARG
21	1Z	153	SER
23	11	3	LYS
33	1b	126	GLU
35	1d	173	TRP
36	1e	86	ALA
41	1j	78	ASN
42	1k	49	GLY
51	1t	100	ILE
4	2E	52	LEU
9	2N	2	LYS
14	2S	84	GLN
21	2Z	52	SER
21	2Z	145	GLU
33	2b	20	GLU
33	2b	226	ARG
36	2e	77	PRO
36	2e	97	GLY
4	1E	52	LEU
6	1G	43	LEU
9	1N	2	LYS
11	1P	38	GLN
33	1b	20	GLU
33	1b	124	SER
34	1c	65	ALA
47	1p	81	ARG
51	1t	10	LEU
6	2G	84	LYS
11	2P	36	LYS
23	21	3	LYS

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Mol	Chain	Res	Type
41	2j	43	ARG
41	2j	78	ASN
48	2q	67	LYS
48	2q	81	ARG
51	2t	95	ALA
6	1G	124	SER
11	1P	45	LEU
21	1Z	156	LYS
33	1b	8	LYS
45	1n	60	SER
50	1s	27	GLU
5	2F	21	ALA
10	2O	29	ASN
11	2P	45	LEU
17	2V	53	GLU
18	2W	60	ASN
21	2Z	93	ASP
33	2b	150	SER
34	2c	91	LEU
34	2c	144	SER
35	2d	179	GLU
11	1P	29	LYS
36	1e	85	GLY
42	1k	105	VAL
49	1r	25	THR
14	2S	35	ILE
33	1b	231	GLU
46	1o	87	ILE
41	1j	77	PRO
33	2b	231	GLU
35	2d	5	ILE
36	1e	69	VAL
33	1b	38	GLY
51	1t	102	GLY
21	2Z	146	ILE
51	2t	47	GLY
11	2P	122	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%)	203 (94%)	12 (6%)	21 28
3	2D	215/218 (99%)	203 (94%)	12 (6%)	21 28
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14 18
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18 24
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6 7
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20 27
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9 11
6	2G	143/156 (92%)	128 (90%)	15 (10%)	7 7
7	1H	144/148 (97%)	135 (94%)	9 (6%)	18 23
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6 6
8	1I	113/124 (91%)	93 (82%)	20 (18%)	2 2
8	2I	105/124 (85%)	90 (86%)	15 (14%)	3 3
9	1N	118/119 (99%)	113 (96%)	5 (4%)	30 40
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37 50
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41 55
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31 43
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23 30
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10 12
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18 23
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27 37
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9 12
13	2R	101/101 (100%)	96 (95%)	5 (5%)	24 33
14	1S	86/88 (98%)	81 (94%)	5 (6%)	20 26
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4 3
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29 39
15	2T	113/127 (89%)	104 (92%)	9 (8%)	12 15
16	1U	93/94 (99%)	91 (98%)	2 (2%)	52 66
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52 66
17	1V	80/82 (98%)	78 (98%)	2 (2%)	47 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6 5
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28 38
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38 51
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32 44
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17 23
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	11 14
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14 19
21	1Z	135/179 (75%)	126 (93%)	9 (7%)	16 21
21	2Z	137/179 (76%)	120 (88%)	17 (12%)	4 4
22	10	65/67 (97%)	62 (95%)	3 (5%)	27 36
22	20	65/67 (97%)	63 (97%)	2 (3%)	40 54
23	11	80/83 (96%)	76 (95%)	4 (5%)	24 33
23	21	80/83 (96%)	76 (95%)	4 (5%)	24 33
24	12	65/67 (97%)	62 (95%)	3 (5%)	27 36
24	22	65/67 (97%)	64 (98%)	1 (2%)	65 77
25	13	51/52 (98%)	46 (90%)	5 (10%)	8 9
25	23	50/52 (96%)	50 (100%)	0	100 100
26	14	59/63 (94%)	50 (85%)	9 (15%)	2 2
26	24	53/63 (84%)	45 (85%)	8 (15%)	3 2
27	15	50/52 (96%)	47 (94%)	3 (6%)	19 25
27	25	50/52 (96%)	47 (94%)	3 (6%)	19 25
28	16	51/52 (98%)	45 (88%)	6 (12%)	5 5
28	26	50/52 (96%)	45 (90%)	5 (10%)	7 8
29	17	41/42 (98%)	35 (85%)	6 (15%)	3 2
29	27	41/42 (98%)	37 (90%)	4 (10%)	8 9
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 18
30	28	54/55 (98%)	52 (96%)	2 (4%)	34 46
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 57
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 57
33	1b	192/220 (87%)	166 (86%)	26 (14%)	4 3
33	2b	187/220 (85%)	152 (81%)	35 (19%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	1c	142/188 (76%)	128 (90%)	14 (10%)	8 9
34	2c	140/188 (74%)	133 (95%)	7 (5%)	24 33
35	1d	169/181 (93%)	154 (91%)	15 (9%)	9 12
35	2d	173/181 (96%)	156 (90%)	17 (10%)	8 9
36	1e	113/123 (92%)	99 (88%)	14 (12%)	4 4
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4 4
37	1f	84/90 (93%)	78 (93%)	6 (7%)	14 19
37	2f	85/90 (94%)	79 (93%)	6 (7%)	14 19
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6 6
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7 8
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59 74
39	2h	114/119 (96%)	106 (93%)	8 (7%)	15 19
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21 28
40	2i	89/99 (90%)	74 (83%)	15 (17%)	2 2
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9 11
41	2j	69/92 (75%)	65 (94%)	4 (6%)	20 26
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6 6
42	2k	83/99 (84%)	80 (96%)	3 (4%)	35 47
43	1l	96/108 (89%)	89 (93%)	7 (7%)	14 18
43	2l	96/108 (89%)	84 (88%)	12 (12%)	4 4
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5 5
44	2m	92/101 (91%)	82 (89%)	10 (11%)	6 6
45	1n	49/50 (98%)	46 (94%)	3 (6%)	18 24
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30 41
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46 61
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24 32
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4 3
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 18
48	1q	94/97 (97%)	88 (94%)	6 (6%)	17 23
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13 18
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10 13
50	1s	69/80 (86%)	66 (96%)	3 (4%)	29 39
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7 7
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20 27
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20 27
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8575 (92%)	728 (8%)	12 16

All (728) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	99	ASP
3	1D	106	ILE
3	1D	109	ASP
3	1D	142	VAL
3	1D	204	ILE
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	7	VAL
4	1E	12	THR
4	1E	13	ARG
4	1E	47	VAL
4	1E	73	GLU
4	1E	87	GLU
4	1E	97	LYS
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	181	LEU
4	1E	184	VAL
5	1F	24	LEU
5	1F	27	GLU
5	1F	28	ILE
5	1F	43	LYS

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Mol	Chain	Res	Type
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	127	GLU
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	91	ARG
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	139	LEU
6	1G	149	VAL
6	1G	150	ASP
6	1G	159	VAL
7	1H	2	SER
7	1H	16	SER
7	1H	23	ARG
7	1H	56	SER
7	1H	84	SER
7	1H	101	ARG
7	1H	124	GLU
7	1H	127	GLU
7	1H	155	SER
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	27	ARG
8	1I	38	LEU
8	1I	41	GLU
8	1I	47	LEU

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Mol	Chain	Res	Type
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	95	LYS
8	1I	101	LEU
8	1I	102	SER
8	1I	108	THR
8	1I	109	ILE
8	1I	123	LEU
8	1I	129	THR
8	1I	136	VAL
8	1I	140	LEU
9	1N	1	MET
9	1N	28	THR
9	1N	46	VAL
9	1N	48	MET
9	1N	83	LYS
10	1O	28	SER
10	1O	106	LEU
10	1O	112	MET
11	1P	36	LYS
11	1P	40	SER
11	1P	90	ARG
11	1P	95	VAL
11	1P	96	THR
11	1P	148	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
12	1Q	138	ASP
13	1R	6	SER
13	1R	14	SER
13	1R	15	SER
13	1R	24	GLN
13	1R	36	THR
13	1R	73	VAL
13	1R	100	LEU
13	1R	111	LEU

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Mol	Chain	Res	Type
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	36	TYR
14	1S	69	VAL
14	1S	73	LEU
15	1T	28	VAL
15	1T	65	LYS
15	1T	96	ARG
15	1T	125	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	8	VAL
17	1V	79	VAL
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	63	ASP
19	1X	35	THR
19	1X	57	LEU
19	1X	68	ARG
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	49	ARG
21	1Z	53	ILE
21	1Z	77	ASP
21	1Z	87	ASP
21	1Z	102	LEU
21	1Z	138	GLU
21	1Z	140	ASP
21	1Z	154	ASP
21	1Z	171	ILE
22	10	7	LEU
22	10	10	THR
22	10	49	LYS
23	11	46	LEU

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Mol	Chain	Res	Type
23	11	59	THR
23	11	78	LYS
23	11	86	SER
24	12	3	LEU
24	12	65	ASN
24	12	66	GLU
25	13	23	LEU
25	13	34	GLU
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	49	PHE
26	14	50	VAL
26	14	53	GLU
26	14	61	ARG
26	14	62	ARG
26	14	63	TYR
26	14	67	TYR
26	14	68	ARG
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
27	15	58	LEU
28	16	4	GLU
28	16	19	ARG
28	16	40	CYS
28	16	44	ARG
28	16	45	LYS
28	16	47	THR
29	17	1	MET
29	17	14	LYS
29	17	24	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	31	HIS
30	18	34	TRP
30	18	50	LEU
31	19	4	ARG
33	1b	12	GLU
33	1b	17	PHE

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Mol	Chain	Res	Type
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	27	LYS
33	1b	35	GLU
33	1b	54	THR
33	1b	61	LEU
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	83	MET
33	1b	108	ILE
33	1b	113	HIS
33	1b	126	GLU
33	1b	128	GLU
33	1b	143	GLU
33	1b	157	ARG
33	1b	160	ASP
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	219	VAL
33	1b	231	GLU
33	1b	236	TYR
34	1c	3	ASN
34	1c	28	GLN
34	1c	45	LYS
34	1c	46	GLU
34	1c	49	SER
34	1c	64	VAL
34	1c	66	VAL
34	1c	82	GLU
34	1c	89	GLU
34	1c	101	LEU
34	1c	110	ASN
34	1c	112	SER
34	1c	179	ARG
34	1c	195	VAL
35	1d	8	VAL
35	1d	19	LEU
35	1d	91	SER
35	1d	115	ARG

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Mol	Chain	Res	Type
35	1d	119	GLN
35	1d	122	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	158	ILE
35	1d	175	SER
35	1d	177	ASP
35	1d	186	LEU
35	1d	188	LEU
35	1d	194	LEU
36	1e	10	MET
36	1e	12	LEU
36	1e	18	ARG
36	1e	24	ARG
36	1e	41	VAL
36	1e	47	LYS
36	1e	51	VAL
36	1e	63	ARG
36	1e	64	ARG
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	147	ASP
36	1e	151	LEU
37	1f	25	ILE
37	1f	46	ARG
37	1f	64	GLN
37	1f	72	VAL
37	1f	81	ILE
37	1f	92	LYS
38	1g	12	LEU
38	1g	16	LEU
38	1g	32	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	78	ARG
38	1g	94	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	114	ARG

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Mol	Chain	Res	Type
38	1g	115	ARG
38	1g	120	ILE
39	1h	39	LEU
39	1h	52	ASP
40	1i	23	ASN
40	1i	27	THR
40	1i	92	TYR
40	1i	96	LEU
40	1i	111	ARG
41	1j	5	ARG
41	1j	21	GLN
41	1j	46	ARG
41	1j	66	ARG
41	1j	72	VAL
41	1j	92	THR
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	33	THR
42	1k	40	ILE
42	1k	48	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
43	1l	11	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	54	LYS
43	1l	58	VAL
43	1l	83	VAL
43	1l	86	ARG
44	1m	4	ILE
44	1m	9	ILE
44	1m	11	ARG
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	94	ARG
44	1m	109	THR
44	1m	110	ARG

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Mol	Chain	Res	Type
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
46	1o	39	LEU
46	1o	62	GLN
47	1p	5	ARG
47	1p	20	VAL
47	1p	27	LYS
47	1p	42	ARG
47	1p	45	THR
47	1p	53	VAL
47	1p	62	VAL
47	1p	72	ARG
47	1p	76	GLN
48	1q	5	VAL
48	1q	25	ARG
48	1q	63	ARG
48	1q	78	GLU
48	1q	85	VAL
48	1q	87	LYS
49	1r	31	LEU
49	1r	46	GLU
49	1r	47	THR
49	1r	61	LYS
49	1r	82	THR
50	1s	12	ASP
50	1s	28	LYS
50	1s	48	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	31	SER
51	1t	100	ILE
3	2D	3	VAL
3	2D	20	ASP
3	2D	37	LEU
3	2D	88	ARG
3	2D	142	VAL
3	2D	173	VAL
3	2D	211	ARG
3	2D	242	ARG
3	2D	259	THR
3	2D	260	ARG

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Mol	Chain	Res	Type
3	2D	275	LYS
3	2D	276	LYS
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR
4	2E	38	THR
4	2E	73	GLU
4	2E	87	GLU
4	2E	97	LYS
4	2E	116	VAL
4	2E	119	ARG
4	2E	181	LEU
5	2F	7	TYR
5	2F	18	ARG
5	2F	19	GLU
5	2F	20	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	110	LEU
5	2F	165	ARG
5	2F	197	ASP
6	2G	7	LEU
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	51	ARG
6	2G	53	LEU
6	2G	91	ARG
6	2G	130	ASN
6	2G	140	ILE
6	2G	150	ASP
6	2G	160	VAL
6	2G	162	THR
6	2G	165	THR
6	2G	170	ARG
7	2H	3	ARG
7	2H	23	ARG
7	2H	42	ARG
7	2H	43	VAL
7	2H	45	VAL
7	2H	68	THR

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Mol	Chain	Res	Type
7	2H	70	THR
7	2H	71	LEU
7	2H	76	VAL
7	2H	84	SER
7	2H	95	ARG
7	2H	106	THR
7	2H	114	VAL
7	2H	122	THR
7	2H	130	ARG
7	2H	133	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	50	ARG
8	2I	51	ILE
8	2I	58	LEU
8	2I	66	GLU
8	2I	68	LEU
8	2I	77	LEU
8	2I	87	LYS
8	2I	92	VAL
8	2I	102	SER
8	2I	117	GLU
8	2I	121	LYS
8	2I	127	VAL
8	2I	133	HIS
9	2N	28	THR
9	2N	38	HIS
9	2N	61	ARG
9	2N	73	THR
10	2O	66	LYS
10	2O	69	ILE
10	2O	77	ILE
10	2O	116	SER
11	2P	3	LEU
11	2P	7	ARG
11	2P	57	THR
11	2P	95	VAL
11	2P	96	THR
11	2P	98	GLU
11	2P	119	GLU
11	2P	121	LYS
11	2P	135	LEU

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Mol	Chain	Res	Type
11	2P	148	LEU
12	2Q	1	MET
12	2Q	85	LYS
12	2Q	106	VAL
12	2Q	110	THR
12	2Q	133	ARG
13	2R	6	SER
13	2R	24	GLN
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	15	ARG
14	2S	20	ARG
14	2S	36	TYR
14	2S	52	SER
14	2S	58	LEU
14	2S	62	LYS
14	2S	63	THR
14	2S	64	GLU
14	2S	75	GLU
14	2S	80	LEU
14	2S	110	LEU
15	2T	9	LEU
15	2T	18	ASP
15	2T	40	THR
15	2T	65	LYS
15	2T	74	ARG
15	2T	85	LYS
15	2T	96	ARG
15	2T	102	ILE
15	2T	124	ASP
16	2U	31	SER
16	2U	74	LEU
17	2V	7	THR
17	2V	12	TYR
17	2V	18	LEU
17	2V	38	LEU
17	2V	79	VAL
17	2V	85	LYS
17	2V	95	LEU
17	2V	98	GLU
17	2V	100	ARG

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Mol	Chain	Res	Type
18	2W	11	ARG
18	2W	60	ASN
18	2W	63	ASP
19	2X	23	GLU
19	2X	35	THR
19	2X	57	LEU
19	2X	81	VAL
19	2X	92	LEU
20	2Y	8	LYS
20	2Y	11	ASP
20	2Y	85	VAL
20	2Y	88	LYS
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	24	LEU
21	2Z	31	ARG
21	2Z	42	VAL
21	2Z	50	GLN
21	2Z	52	SER
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	91	LEU
21	2Z	98	MET
21	2Z	148	ASP
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	169	GLU
21	2Z	170	THR
21	2Z	171	ILE
22	20	49	LYS
22	20	74	ARG
23	21	23	LYS
23	21	35	THR
23	21	46	LEU
23	21	86	SER
24	22	53	LEU
26	24	34	GLU
26	24	49	PHE
26	24	58	ARG
26	24	59	PHE

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Mol	Chain	Res	Type
26	24	62	ARG
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	55	ARG
27	25	59	GLU
28	26	6	ARG
28	26	9	LEU
28	26	19	ARG
28	26	40	CYS
28	26	48	VAL
29	27	1	MET
29	27	24	THR
29	27	41	ARG
29	27	46	VAL
30	28	23	VAL
30	28	31	HIS
31	29	26	ILE
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	23	ARG
33	2b	24	TRP
33	2b	25	ASN
33	2b	37	ASN
33	2b	48	MET
33	2b	55	PHE
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	79	ASP
33	2b	87	ARG
33	2b	94	ASN
33	2b	108	ILE
33	2b	111	ARG
33	2b	115	LEU
33	2b	117	GLU
33	2b	124	SER
33	2b	127	ILE

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Mol	Chain	Res	Type
33	2b	140	HIS
33	2b	142	LEU
33	2b	150	SER
33	2b	170	GLU
33	2b	185	ILE
33	2b	189	ASP
33	2b	208	ILE
33	2b	215	LEU
33	2b	224	GLN
33	2b	229	VAL
33	2b	235	SER
33	2b	236	TYR
34	2c	35	GLU
34	2c	43	LEU
34	2c	47	LEU
34	2c	58	GLU
34	2c	70	VAL
34	2c	152	ILE
34	2c	191	THR
35	2d	8	VAL
35	2d	17	VAL
35	2d	34	GLU
35	2d	52	SER
35	2d	53	ASP
35	2d	59	ARG
35	2d	76	ARG
35	2d	119	GLN
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	162	LEU
35	2d	175	SER
35	2d	188	LEU
35	2d	209	ARG
36	2e	13	ILE
36	2e	20	GLN
36	2e	24	ARG
36	2e	25	ARG
36	2e	31	LEU
36	2e	43	LEU

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Mol	Chain	Res	Type
36	2e	45	PHE
36	2e	51	VAL
36	2e	55	VAL
36	2e	57	LYS
36	2e	75	THR
36	2e	91	LEU
36	2e	101	ILE
36	2e	111	GLU
37	2f	17	SER
37	2f	19	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	92	LYS
37	2f	93	SER
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	24	THR
38	2g	52	GLU
38	2g	53	LYS
38	2g	78	ARG
38	2g	79	ARG
38	2g	98	SER
38	2g	106	GLN
38	2g	138	LYS
38	2g	139	GLU
39	2h	17	THR
39	2h	26	VAL
39	2h	29	SER
39	2h	39	LEU
39	2h	51	VAL
39	2h	112	LEU
39	2h	127	LEU
39	2h	137	VAL
40	2i	40	LEU
40	2i	41	VAL
40	2i	50	LEU
40	2i	54	ASP
40	2i	56	LEU
40	2i	65	VAL
40	2i	75	ASP
40	2i	89	ASN

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Mol	Chain	Res	Type
40	2i	93	ARG
40	2i	99	LEU
40	2i	102	LEU
40	2i	103	THR
40	2i	107	ARG
40	2i	113	LYS
40	2i	128	ARG
41	2j	13	HIS
41	2j	38	ILE
41	2j	44	VAL
41	2j	72	VAL
42	2k	14	VAL
42	2k	117	ASN
42	2k	120	ARG
43	2l	11	VAL
43	2l	22	SER
43	2l	33	ARG
43	2l	36	VAL
43	2l	39	VAL
43	2l	42	THR
43	2l	43	VAL
43	2l	53	ARG
43	2l	62	SER
43	2l	83	VAL
43	2l	91	LYS
43	2l	102	ARG
44	2m	3	ARG
44	2m	19	LEU
44	2m	27	LYS
44	2m	47	ASP
44	2m	50	GLU
44	2m	62	ASN
44	2m	94	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
45	2n	18	VAL
45	2n	33	VAL
46	2o	6	GLU
46	2o	25	THR
46	2o	39	LEU
46	2o	88	ARG

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Mol	Chain	Res	Type
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	20	VAL
47	2p	74	LEU
48	2q	5	VAL
48	2q	13	ASP
48	2q	25	ARG
48	2q	63	ARG
48	2q	83	ASP
48	2q	90	ILE
48	2q	96	GLU
49	2r	31	LEU
49	2r	37	VAL
49	2r	54	ARG
49	2r	61	LYS
49	2r	82	THR
50	2s	12	ASP
50	2s	27	GLU
50	2s	30	LEU
50	2s	41	VAL
50	2s	45	VAL
50	2s	47	HIS
50	2s	58	VAL
51	2t	9	ASN
51	2t	15	ARG
51	2t	50	GLU
51	2t	93	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
6	1G	26	GLN
8	1I	133	HIS
10	1O	3	GLN
12	1Q	12	GLN
12	1Q	123	HIS
14	1S	38	GLN

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Mol	Chain	Res	Type
15	1T	58	ASN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
21	1Z	73	GLN
22	10	35	ASN
25	13	32	GLN
26	14	47	GLN
33	1b	40	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	170	GLN
35	1d	45	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
41	1j	69	ASN
43	1l	99	HIS
44	1m	77	ASN
47	1p	13	HIS
47	1p	76	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
3	2D	87	ASN

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Mol	Chain	Res	Type
3	2D	126	GLN
4	2E	48	GLN
6	2G	58	GLN
6	2G	66	GLN
6	2G	121	ASN
6	2G	132	ASN
8	2I	139	GLN
9	2N	56	ASN
10	2O	3	GLN
10	2O	5	GLN
10	2O	90	GLN
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	61	HIS
14	2S	38	GLN
14	2S	84	GLN
15	2T	43	GLN
16	2U	81	HIS
16	2U	94	ASN
19	2X	31	HIS
20	2Y	43	ASN
21	2Z	55	HIS
21	2Z	73	GLN
24	22	43	GLN
26	24	46	GLN
33	2b	40	HIS
33	2b	76	GLN
33	2b	78	GLN
33	2b	95	GLN
33	2b	135	GLN
33	2b	224	GLN
34	2c	98	ASN
34	2c	162	GLN
35	2d	116	GLN
35	2d	119	GLN
35	2d	160	GLN
36	2e	73	ASN
36	2e	141	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN

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Mol	Chain	Res	Type
38	2g	56	GLN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	89	ASN
40	2i	117	HIS
42	2k	78	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	62	GLN
48	2q	16	GLN
50	2s	83	HIS
51	2t	16	HIS
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	440 (15%)	30 (1%)
1	2A	2789/2915 (95%)	451 (16%)	26 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1494/1521 (98%)	250 (16%)	0
32	2a	1498/1521 (98%)	277 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	0	0
54	1w	70/76 (92%)	24 (34%)	0
54	1y	71/76 (93%)	30 (42%)	0
54	2w	66/76 (86%)	16 (24%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	74/77 (96%)	11 (14%)	0
55	2x	74/77 (96%)	5 (6%)	0
All	All	9328/9620 (96%)	1564 (16%)	56 (0%)

All (1564) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G

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Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	23	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	92	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	139(A)	G
1	1A	196	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(J)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	327	G
1	1A	329	G

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Mol	Chain	Res	Type
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	440	G
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(T)	C

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Mol	Chain	Res	Type
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	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	899	A
1	1A	910	A
1	1A	919	G
1	1A	931	G
1	1A	932	G
1	1A	945	A

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Mol	Chain	Res	Type
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
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	1063	G
1	1A	1064	C
1	1A	1065	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1082	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G

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Mol	Chain	Res	Type
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1107	G
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1142	U
1	1A	1149	G
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	1220	A
1	1A	1247	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1276	A
1	1A	1290	C
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1313	U
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A

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Mol	Chain	Res	Type
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
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	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1540	U
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G

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Mol	Chain	Res	Type
1	1A	1722	A
1	1A	1739	U
1	1A	1745	C
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
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
1	1A	1847	A
1	1A	1848	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
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	2033	A
1	1A	2039	C

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Mol	Chain	Res	Type
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2093	G
1	1A	2099	U
1	1A	2109	U
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2120	G
1	1A	2121	G
1	1A	2122	U
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	2141	G
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2161	C
1	1A	2164	C
1	1A	2165	G

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Mol	Chain	Res	Type
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2174	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	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2601	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2613	U
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2691	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2739	U
1	1A	2758	A

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Mol	Chain	Res	Type
1	1A	2762	G
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2825	C
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	12	C
2	1B	13	A
2	1B	15	A
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	6	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	52	G
32	1a	54	C
32	1a	61	G

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Mol	Chain	Res	Type
32	1a	65	U
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	93	G
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	151	A
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(G)	G
32	1a	189(H)	G
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	217	C
32	1a	220	G
32	1a	222	U
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	328	C
32	1a	332	G
32	1a	342	C
32	1a	345	C
32	1a	347	G
32	1a	351	G

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Mol	Chain	Res	Type
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	374	A
32	1a	384	G
32	1a	388	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U

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Mol	Chain	Res	Type
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	607	A
32	1a	616	G
32	1a	627	G
32	1a	628	G
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	686	U
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	876	G
32	1a	902	G

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Mol	Chain	Res	Type
32	1a	914	A
32	1a	916	G
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
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
32	1a	1046	A
32	1a	1066	C

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Mol	Chain	Res	Type
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
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
32	1a	1158	C
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1263	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A

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Mol	Chain	Res	Type
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1383	C
32	1a	1397	C
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
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	14	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	36	A

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Mol	Chain	Res	Type
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	56	C
54	1w	60	U
54	1w	62	C
54	1w	63	G
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
54	1w	75	C
55	1x	6	G
55	1x	9	G
55	1x	13	C
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	70	G
54	1y	2	C
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	23	A
54	1y	26	A
54	1y	34	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G

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Mol	Chain	Res	Type
54	1y	54	5MU
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C
54	1y	64	A
54	1y	65	G
54	1y	66	U
54	1y	70	G
54	1y	71	G
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A

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Mol	Chain	Res	Type
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	265	A
1	2A	271(J)	C
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	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	421	U
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	504	U
1	2A	505	A
1	2A	508	G

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Mol	Chain	Res	Type
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	589	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(D)	C
1	2A	652(U)	G
1	2A	654	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G

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Mol	Chain	Res	Type
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	832	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	878	A
1	2A	879	G
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	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
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	980	A
1	2A	983	A
1	2A	996	A
1	2A	999	U

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Mol	Chain	Res	Type
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1036	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1117	G
1	2A	1118	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1155	A
1	2A	1170	G
1	2A	1171	G
1	2A	1195	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A

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Mol	Chain	Res	Type
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1461	G
1	2A	1466	G
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	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A

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Mol	Chain	Res	Type
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1774	C
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	1861	G
1	2A	1877	A
1	2A	1878	G
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	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C

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Mol	Chain	Res	Type
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	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
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	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C

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Mol	Chain	Res	Type
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2150	U
1	2A	2151	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2303	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G

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Mol	Chain	Res	Type
1	2A	2334	G
1	2A	2336	A
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	2396	G
1	2A	2400	G
1	2A	2403	C
1	2A	2406	U
1	2A	2414	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	2448	A
1	2A	2459	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2534	A
1	2A	2536	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U

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Mol	Chain	Res	Type
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2638	G
1	2A	2646	C
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
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	2751	G
1	2A	2758	A
1	2A	2760	C
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2820	A
1	2A	2821	A
1	2A	2825	C
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U

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Mol	Chain	Res	Type
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	30	C
2	2B	32	C
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	94	C
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	40	C
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G

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Mol	Chain	Res	Type
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	287	U
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	345	C
32	2a	346	G
32	2a	350	G
32	2a	351	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

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Mol	Chain	Res	Type
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	457	C
32	2a	461	A
32	2a	470	C
32	2a	484	G
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	G7M
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	574	A
32	2a	575	G
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	601	C
32	2a	630	G
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A

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Mol	Chain	Res	Type
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	756	C
32	2a	759	A
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	870	U
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	962	C
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A

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Mol	Chain	Res	Type
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	990	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1050	G
32	2a	1053	G
32	2a	1064	G

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Mol	Chain	Res	Type
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A

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Mol	Chain	Res	Type
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1268	A
32	2a	1270	C
32	2a	1273	G
32	2a	1276	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1311	G
32	2a	1320	C
32	2a	1321	C
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1357	A
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1380	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	1503	A

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Mol	Chain	Res	Type
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
54	2w	4	C
54	2w	5	G
54	2w	12	U
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	59	U
54	2w	66	U
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	19	G
55	2x	47	U
55	2x	68	C
54	2y	15	G
54	2y	19	G
54	2y	24	G
54	2y	25	C
54	2y	27	G
54	2y	28	G
54	2y	30	G
54	2y	40	C
54	2y	45	U
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU

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Mol	Chain	Res	Type
54	2y	56	C
54	2y	58	A
54	2y	60	U
54	2y	62	C
54	2y	64	A
54	2y	65	G
54	2y	68	C
54	2y	69	G
54	2y	70	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	827	U
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2629	A
1	2A	196	A
1	2A	228	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U

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

86 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	$\#\|Z\| > 2$
54	G7M	2y	46	54	20,26,27	1.33	2 (10%)	17,39,42	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	0TD	1l	92	43	7,9,10	4.66	1 (14%)	6,11,13	6.05	3 (50%)
1	OMG	1A	2251	55,56,1	18,26,27	1.04	1 (5%)	19,38,41	0.93	2 (10%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	22,30,33	1.90	5 (22%)
54	PSU	2w	55	54,56	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
54	PSU	2y	55	54	18,21,22	1.34	3 (16%)	22,30,33	1.85	5 (22%)
54	PSU	2w	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
54	5MU	2y	54	54	19,22,23	1.49	4 (21%)	28,32,35	1.71	5 (17%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.74	3 (13%)
32	4OC	1a	1402	32	20,23,24	0.77	0	26,32,35	0.96	1 (3%)
32	4OC	2a	1402	32,56	20,23,24	0.76	0	26,32,35	1.04	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.43	2 (7%)
1	2MU	2A	2552	56,1	19,22,24	1.29	4 (21%)	26,31,36	1.65	5 (19%)
54	G7M	1y	46	54	20,26,27	1.31	1 (5%)	17,39,42	0.61	0
55	31H	1x	76	55,60,56	28,34,35	1.15	4 (14%)	23,47,50	1.41	3 (13%)
54	PSU	2y	39	54	18,21,22	1.41	2 (11%)	22,30,33	1.54	2 (9%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
1	5MC	1A	1962	56,1	18,22,23	0.92	2 (11%)	26,32,35	1.22	3 (11%)
55	5MC	2x	32	55	18,22,23	0.96	2 (11%)	26,32,35	1.25	3 (11%)
54	4SU	2y	8	54	18,21,22	1.69	4 (22%)	26,30,33	2.38	5 (19%)
32	G7M	1a	527	32,56	20,26,27	1.20	2 (10%)	17,39,42	0.60	0
32	G7M	2a	527	32,56	20,26,27	1.26	2 (10%)	17,39,42	0.50	0
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	28,32,35	2.18	5 (17%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	22,30,33	1.87	4 (18%)
32	5MC	2a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.26	3 (11%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
54	MIA	2y	37	54	18,24,32	1.14	2 (11%)	18,35,47	1.22	2 (11%)
1	OMG	2A	2251	55,1	18,26,27	0.97	1 (5%)	19,38,41	1.12	3 (15%)
32	5MC	1a	1404	32	18,22,23	1.05	2 (11%)	26,32,35	1.24	4 (15%)
1	8AH	1A	2503	56,1	20,26,27	0.84	1 (5%)	23,39,42	1.96	5 (21%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.47	2 (11%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.54	2 (11%)
1	5MC	2A	1962	56,1	18,22,23	0.94	2 (11%)	26,32,35	1.09	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.96	1 (3%)
55	31H	2x	76	55,56	28,34,35	1.11	3 (10%)	23,47,50	1.44	1 (4%)
55	PSU	1x	55	55,56	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MU	2A	1939	56,1	19,22,23	1.47	5 (26%)	28,32,35	2.24	5 (17%)
1	8AH	2A	2503	56,1	20,26,27	0.88	1 (5%)	23,39,42	1.94	4 (17%)
54	G7M	2w	46	54	20,26,27	1.26	2 (10%)	17,39,42	0.56	0
1	PSU	1A	1911	1	18,21,22	1.44	2 (11%)	22,30,33	1.84	4 (18%)
54	4SU	2w	8	54	18,21,22	1.69	4 (22%)	26,30,33	1.77	5 (19%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
1	OMC	2A	1920	1	19,22,23	0.84	0	26,31,34	0.92	0
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.85	3 (13%)
54	5MU	1w	54	54	19,22,23	1.41	5 (26%)	28,32,35	2.01	6 (21%)
55	5MU	1x	54	55,56	19,22,23	1.39	5 (26%)	28,32,35	2.21	8 (28%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	28,32,35	2.11	6 (21%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.80	3 (13%)
32	2MG	2a	1207	32,56	18,26,27	0.93	1 (5%)	16,38,41	1.02	2 (12%)
32	5MC	1a	967	32	18,22,23	0.96	1 (5%)	26,32,35	1.10	2 (7%)
32	5MC	2a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.11	3 (11%)
54	MIA	1y	37	54	18,24,32	1.15	2 (11%)	18,35,47	1.19	2 (11%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.49	3 (11%)
1	PSU	1A	2605	56,1	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
32	M2G	2a	966	32	20,27,28	1.40	3 (15%)	22,40,43	1.02	3 (13%)
54	5MU	1y	54	54	19,22,23	1.49	6 (31%)	28,32,35	1.78	5 (17%)
1	5MU	1A	1939	1	19,22,23	1.39	4 (21%)	28,32,35	2.23	6 (21%)
32	5MC	1a	1407	32	18,22,23	0.90	2 (11%)	26,32,35	1.10	3 (11%)
32	PSU	1a	516	32	18,21,22	1.39	2 (11%)	22,30,33	1.86	6 (27%)
54	MIA	2w	37	54	20,27,32	1.81	2 (10%)	22,39,47	1.93	7 (31%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	5MU	1A	1915	1	19,22,23	1.39	4 (21%)	28,32,35	2.12	6 (21%)
55	4SU	1x	8	55	18,21,22	2.16	5 (27%)	26,30,33	1.56	6 (23%)
1	5MC	1A	1942	56,1	18,22,23	0.95	2 (11%)	26,32,35	1.20	2 (7%)
32	MA6	1a	1519	32	19,26,27	0.82	0	18,38,41	1.67	3 (16%)
32	5MC	2a	1407	32,56	18,22,23	1.02	2 (11%)	26,32,35	1.16	3 (11%)
43	0TD	2l	92	43	7,9,10	4.87	1 (14%)	6,11,13	6.82	3 (50%)
32	5MC	1a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.25	2 (7%)
32	5MC	2a	1404	32	18,22,23	0.98	2 (11%)	26,32,35	1.15	2 (7%)
54	G7M	1w	46	54	20,26,27	1.25	2 (10%)	17,39,42	0.56	0
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	22,40,43	1.09	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	2A	1917	1	18,21,22	1.31	2 (11%)	22,30,33	1.80	3 (13%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.08	2 (12%)
55	5MC	1x	32	55	18,22,23	1.03	2 (11%)	26,32,35	1.31	4 (15%)
1	5MC	2A	1942	1	18,22,23	1.01	2 (11%)	26,32,35	1.19	3 (11%)
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	28,32,35	1.88	7 (25%)
54	PSU	1y	32	54	18,21,22	1.30	2 (11%)	22,30,33	1.83	3 (13%)
55	4SU	2x	8	55	18,21,22	1.92	7 (38%)	26,30,33	1.35	5 (19%)
54	MIA	1w	37	54	24,31,32	2.15	3 (12%)	26,44,47	2.60	9 (34%)
54	4SU	1y	8	54	18,21,22	1.74	5 (27%)	26,30,33	1.71	4 (15%)
1	2MU	1A	2552	56,1	19,22,24	1.29	4 (21%)	26,31,36	1.80	6 (23%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
32	MA6	2a	1518	32	19,26,27	0.83	0	18,38,41	1.40	2 (11%)
54	PSU	1w	32	54,56	18,21,22	1.30	2 (11%)	22,30,33	1.83	3 (13%)
54	4SU	1w	8	54	18,21,22	1.74	4 (22%)	26,30,33	2.07	5 (19%)

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
54	G7M	2y	46	54	-	0/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
1	OMG	1A	2251	55,56,1	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54,56	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	6/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
54	G7M	1y	46	54	-	1/3/25/26	0/3/3/3
55	31H	1x	76	55,60,56	-	4/18/40/41	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	3/3/25/26	0/3/3/3
32	G7M	2a	527	32,56	-	3/3/25/26	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	56,1	-	2/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	31H	2x	76	55,56	-	4/18/40/41	0/3/3/3
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	56,1	-	1/3/25/26	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	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	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/11/33/34	0/3/3/3
54	4SU	1y	8	54	-	2/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.62	1.69	1.82
43	1l	92	0TD	CB-SB	-11.89	1.70	1.82
54	1w	37	MIA	C13-C14	7.21	1.53	1.32
54	2w	37	MIA	C2-S10	-6.90	1.69	1.75
54	1w	37	MIA	C2-S10	-6.18	1.70	1.75
55	1x	8	4SU	C4-N3	-5.38	1.31	1.37
32	2a	966	M2G	C2-N3	4.53	1.36	1.30
54	2y	8	4SU	C4-S4	-4.48	1.59	1.68
54	1w	8	4SU	C4-S4	-4.43	1.60	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C4-N3	-4.41	1.32	1.37
32	1a	966	M2G	C2-N3	4.40	1.36	1.30
54	2w	8	4SU	C4-S4	-4.22	1.60	1.68
54	1y	46	G7M	C5-C4	4.15	1.47	1.39
54	1y	8	4SU	C4-S4	-4.14	1.60	1.68
55	1x	8	4SU	C4-S4	-4.12	1.60	1.68
54	2y	46	G7M	C5-C4	3.95	1.47	1.39
54	2w	46	G7M	C5-C4	3.86	1.46	1.39
54	1w	46	G7M	C5-C4	3.80	1.46	1.39
54	1y	39	PSU	C6-C5	3.78	1.39	1.35
55	1x	8	4SU	C2-N3	-3.78	1.31	1.38
32	2a	527	G7M	C5-C4	3.77	1.46	1.39
1	1A	1911	PSU	C6-C5	3.77	1.39	1.35
54	1w	55	PSU	C6-C5	3.76	1.39	1.35
54	2y	39	PSU	C6-C5	3.70	1.39	1.35
54	2w	39	PSU	C6-C5	3.70	1.39	1.35
54	2w	55	PSU	C6-C5	3.69	1.39	1.35
55	2x	8	4SU	C4-S4	-3.68	1.61	1.68
32	1a	527	G7M	C5-C4	3.66	1.46	1.39
54	1y	8	4SU	C4-N3	-3.60	1.33	1.37
54	1y	55	PSU	C6-C5	3.60	1.39	1.35
54	2y	32	PSU	C6-C5	3.59	1.39	1.35
54	2w	32	PSU	C6-C5	3.56	1.39	1.35
1	2A	2605	PSU	C6-C5	3.52	1.39	1.35
55	2x	55	PSU	C6-C5	3.39	1.39	1.35
32	2a	516	PSU	C6-C5	3.39	1.39	1.35
32	1a	516	PSU	C6-C5	3.38	1.39	1.35
54	1y	32	PSU	C6-C5	3.34	1.39	1.35
1	2A	1917	PSU	C6-C5	3.33	1.39	1.35
1	1A	1917	PSU	C6-C5	3.22	1.39	1.35
55	1x	8	4SU	C5-C4	-3.22	1.38	1.42
1	2A	1911	PSU	C6-C5	3.21	1.39	1.35
1	2A	1939	5MU	C4-N3	-3.18	1.32	1.38
54	1w	32	PSU	C6-C5	3.16	1.39	1.35
55	2x	8	4SU	C2-N3	-3.10	1.32	1.38
55	1x	55	PSU	C6-C5	3.07	1.38	1.35
1	1A	1939	5MU	C6-C5	3.07	1.39	1.34
1	1A	2251	OMG	C6-N1	-3.05	1.33	1.37
54	2y	54	5MU	C6-C5	3.04	1.39	1.34
32	2a	1404	5MC	C6-C5	2.99	1.39	1.34
55	2x	76	31H	C5-C4	-2.98	1.33	1.40
54	2w	8	4SU	C4-N3	-2.98	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	39	PSU	C6-C5	2.95	1.38	1.35
1	2A	1942	5MC	C6-C5	2.94	1.39	1.34
32	1a	1404	5MC	C6-C5	2.93	1.39	1.34
55	1x	76	31H	C5-C4	-2.92	1.33	1.40
54	2y	39	PSU	C4-N3	-2.91	1.33	1.38
54	1y	54	5MU	C4-N3	-2.90	1.33	1.38
1	1A	2552	2MU	C4-N3	-2.90	1.33	1.38
54	1w	8	4SU	C5-C4	-2.90	1.38	1.42
55	1x	32	5MC	C6-C5	2.90	1.39	1.34
54	1y	54	5MU	C6-C5	2.89	1.39	1.34
55	2x	8	4SU	C5-C4	-2.88	1.38	1.42
1	2A	1915	5MU	C6-C5	2.85	1.39	1.34
54	1w	8	4SU	C4-N3	-2.84	1.34	1.37
54	1y	37	MIA	C5-C4	2.83	1.48	1.40
32	1a	967	5MC	C6-C5	2.83	1.39	1.34
54	2y	54	5MU	C2-N1	2.82	1.43	1.38
54	2w	8	4SU	C5-C4	-2.82	1.38	1.42
54	2y	37	MIA	C5-C4	2.80	1.48	1.40
54	2y	55	PSU	C4-N3	-2.79	1.33	1.38
1	1A	1915	5MU	C6-C5	2.79	1.39	1.34
32	1a	966	M2G	C2-N2	2.79	1.40	1.35
32	2a	1407	5MC	C6-C5	2.77	1.39	1.34
32	2a	967	5MC	C6-C5	2.76	1.39	1.34
54	2w	37	MIA	C5-C4	2.76	1.48	1.40
32	2a	966	M2G	C2-N2	2.75	1.40	1.35
32	1a	1400	5MC	C6-C5	2.75	1.39	1.34
54	2y	8	4SU	C4-N3	-2.75	1.34	1.37
55	2x	54	5MU	C6-C5	2.74	1.39	1.34
32	1a	516	PSU	C4-N3	-2.72	1.33	1.38
32	1a	966	M2G	C6-N1	-2.70	1.33	1.37
55	2x	32	5MC	C6-C5	2.69	1.39	1.34
55	1x	54	5MU	C4-C5	2.68	1.49	1.44
54	2y	37	MIA	C2-N3	2.67	1.36	1.32
1	1A	1939	5MU	C4-N3	-2.67	1.33	1.38
1	1A	1942	5MC	C6-C5	2.67	1.39	1.34
1	2A	1939	5MU	C6-N1	-2.66	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.66	1.33	1.38
54	2w	54	5MU	C6-C5	2.66	1.39	1.34
55	2x	54	5MU	C4-N3	-2.65	1.33	1.38
1	1A	2605	PSU	C4-N3	-2.65	1.33	1.38
1	2A	1939	5MU	C6-C5	2.64	1.38	1.34
54	1y	37	MIA	C2-N3	2.64	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C6-C5	2.64	1.38	1.34
1	1A	2605	PSU	C6-C5	2.60	1.38	1.35
1	1A	1915	5MU	C4-N3	-2.59	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.59	1.34	1.37
1	2A	2251	OMG	C6-N1	-2.58	1.34	1.37
55	1x	55	PSU	C4-N3	-2.58	1.34	1.38
54	1w	39	PSU	C4-N3	-2.57	1.34	1.38
54	1y	55	PSU	C4-N3	-2.57	1.34	1.38
54	2y	54	5MU	C4-N3	-2.56	1.34	1.38
54	1w	32	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.56	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.55	1.34	1.38
55	1x	32	5MC	C6-N1	-2.54	1.33	1.38
55	2x	55	PSU	C4-N3	-2.54	1.34	1.38
54	1y	39	PSU	C4-N3	-2.54	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.54	1.34	1.38
1	2A	2503	8AH	C5-C4	2.53	1.47	1.40
1	2A	1915	5MU	C2-N1	2.53	1.42	1.38
1	1A	1962	5MC	C6-N1	-2.53	1.33	1.38
32	2a	1400	5MC	C6-C5	2.53	1.38	1.34
54	1w	46	G7M	C6-N1	-2.52	1.34	1.37
54	1w	54	5MU	C2-N1	2.52	1.42	1.38
54	1y	32	PSU	C4-N3	-2.52	1.34	1.38
54	1w	54	5MU	C6-C5	2.51	1.38	1.34
54	1y	54	5MU	C4-C5	2.50	1.48	1.44
54	2y	8	4SU	C2-N1	2.49	1.42	1.38
54	2w	55	PSU	C4-N3	-2.48	1.34	1.38
54	1w	37	MIA	C5-C4	2.48	1.47	1.40
55	2x	76	31H	C6-C5	-2.48	1.34	1.43
32	2a	527	G7M	C6-N1	-2.47	1.34	1.37
32	2a	1407	5MC	C6-N1	-2.46	1.33	1.38
54	1w	54	5MU	C4-C5	2.46	1.48	1.44
54	2y	46	G7M	C6-N1	-2.45	1.34	1.37
54	1y	8	4SU	C5-C4	-2.45	1.39	1.42
1	1A	1917	PSU	C4-N3	-2.45	1.34	1.38
55	1x	54	5MU	C4-N3	-2.45	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.44	1.34	1.38
54	2w	54	5MU	C4-N3	-2.44	1.34	1.38
1	2A	1915	5MU	C4-C5	2.43	1.48	1.44
54	2y	8	4SU	C5-C4	-2.43	1.39	1.42
54	1w	8	4SU	C2-N1	2.43	1.42	1.38
1	2A	1939	5MU	C2-N3	-2.43	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1962	5MC	C6-N1	-2.43	1.33	1.38
32	1a	1407	5MC	C6-C5	2.42	1.38	1.34
32	2a	1400	5MC	C6-N1	-2.42	1.33	1.38
1	2A	2552	2MU	C5-C4	2.41	1.49	1.43
1	1A	1915	5MU	C2-N1	2.41	1.42	1.38
32	2a	1498	UR3	C2-N1	2.40	1.42	1.38
54	2w	54	5MU	C4-C5	2.40	1.48	1.44
55	2x	54	5MU	C4-C5	2.39	1.48	1.44
1	2A	2552	2MU	C4-N3	-2.39	1.34	1.38
54	2w	32	PSU	C4-N3	-2.39	1.34	1.38
54	2y	55	PSU	C6-C5	2.38	1.38	1.35
32	1a	527	G7M	C6-N1	-2.37	1.34	1.37
32	2a	1207	2MG	C6-N1	-2.37	1.34	1.37
32	1a	1404	5MC	C6-N1	-2.36	1.34	1.38
55	1x	76	31H	C6-C5	-2.36	1.34	1.43
1	2A	1962	5MC	C6-C5	2.35	1.38	1.34
32	1a	1400	5MC	C6-N1	-2.33	1.34	1.38
32	2a	516	PSU	C4-N3	-2.33	1.34	1.38
54	2w	39	PSU	C4-N3	-2.31	1.34	1.38
55	1x	76	31H	C5-N7	-2.30	1.31	1.39
55	2x	32	5MC	C6-N1	-2.29	1.34	1.38
54	1y	54	5MU	C2-N1	2.29	1.42	1.38
1	1A	1915	5MU	C4-C5	2.28	1.48	1.44
1	2A	1942	5MC	C6-N1	-2.28	1.34	1.38
1	1A	1962	5MC	C6-C5	2.28	1.38	1.34
1	1A	1942	5MC	C6-N1	-2.27	1.34	1.38
54	1w	55	PSU	C4-N3	-2.27	1.34	1.38
1	1A	2552	2MU	C2-N3	-2.27	1.33	1.38
54	2y	32	PSU	C4-N3	-2.26	1.34	1.38
54	1w	54	5MU	C4-N3	-2.25	1.34	1.38
55	1x	8	4SU	O2-C2	2.25	1.27	1.23
54	1y	54	5MU	C2-N3	-2.25	1.34	1.38
54	1y	8	4SU	C2-N3	-2.23	1.34	1.38
54	2y	54	5MU	C4-C5	2.22	1.48	1.44
54	2w	46	G7M	C6-N1	-2.22	1.34	1.37
1	1A	1939	5MU	C6-N1	-2.19	1.34	1.38
55	2x	54	5MU	C2-N1	2.19	1.42	1.38
1	1A	2503	8AH	C5-C4	2.19	1.46	1.40
55	1x	54	5MU	C6-N1	-2.17	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.17	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.16	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C2-N1	2.15	1.41	1.38
55	1x	76	31H	O4'-C1'	2.13	1.44	1.41
1	2A	2605	PSU	C2-N3	-2.13	1.33	1.37
54	2w	8	4SU	C2-N3	-2.12	1.34	1.38
54	1w	54	5MU	C6-N1	-2.12	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.11	1.34	1.38
32	2a	967	5MC	C6-N1	-2.11	1.34	1.38
54	1y	54	5MU	C6-N1	-2.11	1.34	1.38
1	1A	2552	2MU	C2-N1	2.11	1.41	1.38
32	1a	1498	UR3	C6-C5	2.11	1.39	1.35
55	2x	8	4SU	O2-C2	2.11	1.26	1.23
32	2a	1498	UR3	C6-C5	2.10	1.39	1.35
55	2x	54	5MU	C6-N1	-2.08	1.34	1.38
1	2A	1939	5MU	C2-N1	2.08	1.41	1.38
32	2a	1404	5MC	C6-N1	-2.08	1.34	1.38
1	1A	2552	2MU	C5-C4	2.08	1.48	1.43
55	2x	8	4SU	C6-C5	2.07	1.39	1.35
54	2y	55	PSU	C2-N1	-2.05	1.34	1.36
1	2A	2552	2MU	C2-N1	2.03	1.41	1.38
55	2x	8	4SU	C2-N1	2.03	1.41	1.38
55	1x	54	5MU	C2-N1	2.03	1.41	1.38
32	2a	966	M2G	C6-N1	-2.03	1.34	1.37
54	1y	8	4SU	C6-C5	2.01	1.39	1.35
55	2x	76	31H	C5-N7	-2.00	1.32	1.39

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-16.16	73.21	102.44
43	1l	92	0TD	CSB-SB-CB	-14.16	76.83	102.44
54	1w	37	MIA	C12-C13-C14	-8.72	110.17	127.14
54	2y	8	4SU	C4-N3-C2	-7.19	120.36	127.34
1	2A	2503	8AH	C2-N3-C4	6.37	120.70	115.52
1	1A	2503	8AH	C2-N3-C4	6.12	120.50	115.52
54	2y	8	4SU	C5-C4-N3	6.11	120.36	114.69
54	1y	55	PSU	N1-C2-N3	6.08	122.02	115.13
32	2a	1498	UR3	C4-N3-C2	-5.97	118.94	124.56
1	2A	1911	PSU	N1-C2-N3	5.96	121.88	115.13
55	2x	55	PSU	N1-C2-N3	5.91	121.82	115.13
32	1a	516	PSU	N1-C2-N3	5.87	121.78	115.13
32	2a	516	PSU	N1-C2-N3	5.84	121.74	115.13
1	2A	2605	PSU	N1-C2-N3	5.83	121.74	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	55	PSU	N1-C2-N3	5.83	121.73	115.13
54	2w	39	PSU	N1-C2-N3	5.77	121.67	115.13
54	1w	39	PSU	N1-C2-N3	5.76	121.66	115.13
32	1a	1498	UR3	C4-N3-C2	-5.76	119.14	124.56
54	1w	55	PSU	N1-C2-N3	5.75	121.64	115.13
1	2A	1939	5MU	C4-N3-C2	-5.74	119.91	127.35
55	2x	76	31H	N3-C2-N1	-5.74	119.70	128.68
54	2w	55	PSU	N1-C2-N3	5.70	121.59	115.13
54	2w	32	PSU	N1-C2-N3	5.68	121.57	115.13
1	1A	1917	PSU	N1-C2-N3	5.67	121.55	115.13
1	2A	1917	PSU	N1-C2-N3	5.65	121.53	115.13
54	1w	32	PSU	N1-C2-N3	5.63	121.51	115.13
55	1x	54	5MU	C4-N3-C2	-5.60	120.11	127.35
1	1A	2605	PSU	N1-C2-N3	5.58	121.45	115.13
1	1A	1911	PSU	N1-C2-N3	5.57	121.44	115.13
54	1w	8	4SU	C4-N3-C2	-5.57	121.93	127.34
54	2y	32	PSU	N1-C2-N3	5.54	121.41	115.13
54	1y	39	PSU	N1-C2-N3	5.53	121.39	115.13
54	1w	8	4SU	C5-C4-N3	5.49	119.78	114.69
54	1y	32	PSU	N1-C2-N3	5.49	121.35	115.13
54	2y	55	PSU	N1-C2-N3	5.47	121.33	115.13
1	2A	1915	5MU	C4-N3-C2	-5.44	120.31	127.35
55	1x	76	31H	N3-C2-N1	-5.43	120.19	128.68
1	1A	1939	5MU	C4-N3-C2	-5.42	120.34	127.35
1	1A	2552	2MU	N3-C2-N1	5.35	121.99	114.89
1	1A	1915	5MU	C4-N3-C2	-5.34	120.44	127.35
1	1A	1915	5MU	N3-C2-N1	5.31	121.94	114.89
1	2A	1939	5MU	C5-C4-N3	5.30	119.83	115.31
55	2x	54	5MU	C4-N3-C2	-5.28	120.52	127.35
55	1x	54	5MU	N3-C2-N1	5.22	121.82	114.89
55	2x	54	5MU	N3-C2-N1	5.18	121.77	114.89
1	2A	1939	5MU	N3-C2-N1	5.18	121.76	114.89
1	1A	1939	5MU	C5-C4-N3	5.16	119.72	115.31
54	2w	8	4SU	C5-C4-N3	5.09	119.41	114.69
1	2A	1915	5MU	C5-C4-N3	5.04	119.61	115.31
32	1a	1519	MA6	N3-C2-N1	-5.03	120.82	128.68
1	1A	1939	5MU	O4-C4-C5	-5.01	119.09	124.90
1	2A	1915	5MU	N3-C2-N1	4.97	121.49	114.89
54	1w	54	5MU	C4-N3-C2	-4.96	120.93	127.35
32	2a	1519	MA6	N3-C2-N1	-4.92	120.99	128.68
54	2y	39	PSU	N1-C2-N3	4.89	120.67	115.13
54	1y	8	4SU	C4-N3-C2	-4.89	122.59	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	N3-C2-N1	-4.81	121.17	128.68
32	2a	1518	MA6	N3-C2-N1	-4.80	121.17	128.68
1	1A	2503	8AH	C5-C6-N1	-4.80	117.86	121.01
1	1A	1939	5MU	C5-C6-N1	-4.74	118.46	123.34
1	2A	2503	8AH	C5-C6-N1	-4.73	117.90	121.01
1	1A	1939	5MU	N3-C2-N1	4.68	121.10	114.89
1	2A	2552	2MU	N3-C2-N1	4.67	121.08	114.89
54	1y	8	4SU	C5-C4-N3	4.64	119.00	114.69
1	1A	2552	2MU	C4-N3-C2	-4.56	120.56	126.58
54	1w	54	5MU	N3-C2-N1	4.56	120.94	114.89
1	1A	1915	5MU	C5-C4-N3	4.52	119.17	115.31
54	2w	8	4SU	C4-N3-C2	-4.50	122.97	127.34
54	2w	54	5MU	C4-N3-C2	-4.45	121.59	127.35
54	1w	37	MIA	C2-N3-C4	4.44	121.44	115.32
55	1x	54	5MU	C5-C4-N3	4.44	119.10	115.31
1	2A	1915	5MU	O4-C4-C5	-4.43	119.76	124.90
1	2A	1939	5MU	C5-C6-N1	-4.40	118.81	123.34
54	1y	54	5MU	N3-C2-N1	4.38	120.71	114.89
55	2x	54	5MU	C5-C4-N3	4.35	119.02	115.31
54	2y	8	4SU	N3-C2-N1	4.31	120.61	114.89
54	2w	54	5MU	N3-C2-N1	4.30	120.60	114.89
54	1w	54	5MU	C5-C4-N3	4.28	118.97	115.31
54	1w	8	4SU	C5-C4-S4	-4.23	119.01	124.47
54	2y	8	4SU	C5-C4-S4	-4.21	119.04	124.47
55	2x	55	PSU	C4-N3-C2	-4.21	120.28	126.34
54	2w	37	MIA	C12-N6-C6	-4.20	119.25	122.87
54	1y	54	5MU	C4-N3-C2	-4.18	121.93	127.35
1	2A	2605	PSU	C4-N3-C2	-4.18	120.32	126.34
54	2w	54	5MU	C5-C4-N3	4.18	118.88	115.31
54	1w	37	MIA	C15-C14-C13	-4.13	110.72	122.65
1	2A	2552	2MU	C4-N3-C2	-4.11	121.15	126.58
1	1A	2605	PSU	C4-N3-C2	-4.09	120.45	126.34
54	2w	37	MIA	C2-N3-C4	4.06	120.92	115.32
1	2A	1911	PSU	C4-N3-C2	-4.06	120.50	126.34
1	1A	1915	5MU	O4-C4-C5	-4.05	120.20	124.90
1	2A	1942	5MC	C5-C6-N1	-4.03	119.19	123.34
55	1x	32	5MC	C5-C6-N1	-4.03	119.19	123.34
32	1a	1404	5MC	C5-C6-N1	-4.02	119.20	123.34
54	1w	54	5MU	O4-C4-C5	-4.01	120.25	124.90
55	1x	54	5MU	C5-C6-N1	-4.00	119.22	123.34
1	1A	1917	PSU	C4-N3-C2	-3.98	120.60	126.34
54	2w	39	PSU	C4-N3-C2	-3.96	120.64	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1939	5MU	O4-C4-C5	-3.94	120.33	124.90
32	1a	1400	5MC	C5-C6-N1	-3.94	119.28	123.34
32	2a	516	PSU	C4-N3-C2	-3.93	120.67	126.34
54	1y	55	PSU	C4-N3-C2	-3.93	120.68	126.34
32	2a	1404	5MC	C5-C6-N1	-3.93	119.30	123.34
55	2x	32	5MC	C5-C6-N1	-3.91	119.31	123.34
54	2y	55	PSU	C4-N3-C2	-3.91	120.70	126.34
32	1a	516	PSU	C4-N3-C2	-3.90	120.72	126.34
54	2y	54	5MU	N3-C2-N1	3.90	120.06	114.89
32	2a	1400	5MC	C5-C6-N1	-3.89	119.34	123.34
54	1w	32	PSU	C4-N3-C2	-3.86	120.77	126.34
32	1a	967	5MC	C5-C6-N1	-3.86	119.37	123.34
55	2x	54	5MU	O4-C4-C5	-3.85	120.43	124.90
54	1w	39	PSU	C4-N3-C2	-3.84	120.80	126.34
54	1y	54	5MU	C5-C4-N3	3.84	118.58	115.31
55	1x	55	PSU	C4-N3-C2	-3.83	120.81	126.34
54	1w	39	PSU	O2-C2-N1	-3.83	118.57	122.79
54	2y	54	5MU	C5-C4-N3	3.83	118.58	115.31
55	2x	54	5MU	C5-C6-N1	-3.83	119.40	123.34
54	1y	32	PSU	C4-N3-C2	-3.82	120.83	126.34
1	1A	1911	PSU	C4-N3-C2	-3.80	120.87	126.34
54	2w	37	MIA	C5-C6-N1	-3.80	117.66	120.81
54	2y	54	5MU	C4-N3-C2	-3.80	122.44	127.35
55	1x	8	4SU	C6-C5-C4	-3.77	116.69	119.95
55	1x	54	5MU	O4-C4-C5	-3.76	120.54	124.90
54	2w	32	PSU	C4-N3-C2	-3.75	120.93	126.34
32	2a	1407	5MC	C5-C6-N1	-3.71	119.52	123.34
55	1x	54	5MU	O2-C2-N1	-3.71	117.86	122.79
1	2A	1917	PSU	C4-N3-C2	-3.70	121.00	126.34
54	2w	54	5MU	O4-C4-C5	-3.68	120.64	124.90
54	1w	37	MIA	C16-C14-C13	-3.67	112.05	122.65
1	2A	1915	5MU	C5-C6-N1	-3.64	119.59	123.34
54	2y	54	5MU	O4-C4-C5	-3.61	120.72	124.90
54	1w	55	PSU	C4-N3-C2	-3.56	121.20	126.34
1	1A	1962	5MC	C5-C6-N1	-3.56	119.68	123.34
54	2y	32	PSU	C4-N3-C2	-3.56	121.21	126.34
54	2w	55	PSU	C4-N3-C2	-3.53	121.25	126.34
54	2y	32	PSU	O2-C2-N1	-3.53	118.91	122.79
1	1A	1942	5MC	C5-C6-N1	-3.52	119.72	123.34
54	2w	8	4SU	C5-C4-S4	-3.51	119.94	124.47
54	1y	39	PSU	C4-N3-C2	-3.51	121.28	126.34
54	2y	55	PSU	O2-C2-N1	-3.51	118.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	8	4SU	N3-C2-N1	3.48	119.51	114.89
54	1y	32	PSU	O2-C2-N1	-3.48	118.96	122.79
1	1A	2605	PSU	O2-C2-N1	-3.46	118.98	122.79
54	1y	54	5MU	C5-C6-N1	-3.44	119.80	123.34
1	2A	1911	PSU	O2-C2-N1	-3.44	119.00	122.79
55	1x	8	4SU	O2-C2-N1	3.40	127.31	122.79
54	2w	32	PSU	O2-C2-N1	-3.40	119.05	122.79
54	1w	54	5MU	C5-C6-N1	-3.39	119.85	123.34
1	2A	1962	5MC	C5-C6-N1	-3.39	119.85	123.34
54	1w	37	MIA	C5-C6-N1	-3.38	118.00	120.81
32	2a	1519	MA6	C4-C5-N7	-3.37	105.88	109.40
43	1l	92	0TD	OD2-CG-CB	3.34	120.37	113.15
32	1a	1519	MA6	C4-C5-N7	-3.33	105.93	109.40
32	2a	516	PSU	O2-C2-N1	-3.31	119.15	122.79
1	1A	1915	5MU	C5-C6-N1	-3.31	119.94	123.34
54	1w	37	MIA	C12-N6-C6	-3.30	117.66	122.55
32	1a	1407	5MC	C5-C6-N1	-3.30	119.95	123.34
54	2y	37	MIA	N3-C2-N1	-3.27	123.56	128.68
54	1y	55	PSU	O2-C2-N1	-3.27	119.19	122.79
55	1x	8	4SU	S4-C4-N3	-3.25	117.00	120.21
55	2x	8	4SU	C1'-N1-C2	3.25	123.46	117.57
54	1w	8	4SU	N3-C2-N1	3.25	119.20	114.89
43	2l	92	0TD	OD2-CG-CB	3.21	120.09	113.15
1	1A	1917	PSU	O2-C2-N1	-3.21	119.26	122.79
54	1y	37	MIA	N3-C2-N1	-3.20	123.67	128.68
55	1x	8	4SU	C5-C4-N3	3.20	117.66	114.69
55	1x	55	PSU	O2-C2-N1	-3.19	119.28	122.79
1	2A	1917	PSU	O2-C2-N1	-3.19	119.28	122.79
55	1x	32	5MC	C5-C4-N3	-3.19	118.23	121.67
54	1w	55	PSU	O2-C2-N1	-3.17	119.30	122.79
54	2w	55	PSU	O2-C2-N1	-3.15	119.32	122.79
54	1w	8	4SU	C1'-N1-C2	3.14	123.26	117.57
1	1A	1942	5MC	C5-C4-N3	-3.14	118.29	121.67
32	2a	967	5MC	C5-C6-N1	-3.10	120.15	123.34
54	1w	32	PSU	O2-C2-N1	-3.08	119.40	122.79
54	2w	54	5MU	C5-C6-N1	-3.01	120.25	123.34
54	2y	54	5MU	C5-C6-N1	-3.00	120.25	123.34
54	2w	39	PSU	O2-C2-N1	-2.95	119.54	122.79
1	2A	2503	8AH	C4-C5-N7	-2.90	106.53	109.47
32	1a	1400	5MC	C5-C4-N3	-2.88	118.57	121.67
1	1A	1939	5MU	O2-C2-N1	-2.86	118.98	122.79
1	2A	2552	2MU	C5-C4-N3	2.85	119.11	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C4-C5-N7	-2.83	106.45	109.40
32	1a	1518	MA6	C4-C5-N7	-2.83	106.45	109.40
54	1y	54	5MU	O4-C4-C5	-2.82	121.64	124.90
55	2x	8	4SU	O2-C2-N1	2.80	126.51	122.79
55	2x	54	5MU	O2-C2-N1	-2.79	119.08	122.79
54	2y	39	PSU	C4-N3-C2	-2.77	122.34	126.34
32	2a	1407	5MC	C5-C4-N3	-2.76	118.69	121.67
1	1A	1911	PSU	C6-C5-C4	-2.76	116.27	118.20
32	1a	1404	5MC	C5-C4-N3	-2.76	118.70	121.67
54	2w	8	4SU	N3-C2-N1	2.73	118.51	114.89
1	1A	1962	5MC	CM5-C5-C6	-2.72	119.22	122.85
54	2w	37	MIA	C11-S10-C2	-2.70	100.25	102.27
1	1A	2503	8AH	C2-N1-C6	2.70	122.28	118.08
32	2a	1518	MA6	C4-C5-N7	-2.69	106.59	109.40
54	1w	37	MIA	C2-N1-C6	2.68	121.98	117.19
55	2x	8	4SU	C5-C4-N3	2.67	117.17	114.69
1	1A	2552	2MU	C5-C4-N3	2.66	118.82	114.84
32	1a	1207	2MG	C8-N7-C5	2.64	108.02	102.99
1	2A	2251	OMG	C5-C6-N1	2.64	118.61	113.95
54	1y	37	MIA	C4-C5-N7	-2.62	106.67	109.40
32	2a	1404	5MC	C5-C4-N3	-2.59	118.88	121.67
32	1a	1402	4OC	C6-C5-C4	2.59	120.13	116.96
1	1A	1915	5MU	O2-C2-N1	-2.57	119.37	122.79
1	2A	1942	5MC	C5-C4-N3	-2.57	118.90	121.67
1	1A	2552	2MU	O4-C4-C5	-2.56	120.66	125.16
32	1a	966	M2G	C8-N7-C5	2.55	107.85	102.99
1	1A	1911	PSU	O2-C2-N1	-2.55	119.99	122.79
32	1a	966	M2G	C5-C6-N1	2.52	118.40	113.95
54	2w	37	MIA	C4-C5-N7	-2.51	106.78	109.40
55	2x	55	PSU	O2-C2-N1	-2.50	120.04	122.79
54	2w	37	MIA	C2-N1-C6	2.48	121.62	117.19
1	1A	1962	5MC	C5-C4-N3	-2.47	119.01	121.67
55	2x	32	5MC	C5-C4-N3	-2.45	119.03	121.67
1	1A	2503	8AH	C4-C5-N7	-2.44	107.00	109.47
32	1a	967	5MC	C5-C4-N3	-2.43	119.05	121.67
55	2x	8	4SU	C6-C5-C4	-2.42	117.86	119.95
1	2A	2503	8AH	C2-N1-C6	2.40	121.83	118.08
1	2A	2552	2MU	O4-C4-C5	-2.40	120.94	125.16
54	2w	8	4SU	C1'-N1-C2	2.39	121.90	117.57
43	2l	92	0TD	OD1-CG-CB	-2.39	117.43	122.44
32	2a	1400	5MC	O2-C2-N3	-2.39	118.44	122.33
32	2a	967	5MC	C5-C4-N3	-2.38	119.11	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	OD1-CG-CB	-2.37	117.47	122.44
32	1a	516	PSU	O4'-C1'-C2'	2.37	108.49	105.14
54	1w	37	MIA	N3-C2-N1	-2.36	122.64	126.98
1	1A	1920	OMC	O2-C2-N3	-2.36	118.50	122.33
1	2A	1962	5MC	C5-C4-N3	-2.34	119.14	121.67
32	1a	1519	MA6	C1'-N9-C4	-2.34	122.53	126.64
32	1a	1407	5MC	C5-C4-N3	-2.33	119.16	121.67
54	1y	39	PSU	O2-C2-N1	-2.33	120.23	122.79
32	2a	1207	2MG	C8-N7-C5	2.33	107.42	102.99
54	2y	8	4SU	C1'-N1-C2	2.33	121.78	117.57
54	2y	37	MIA	C4-C5-N7	-2.32	106.98	109.40
32	1a	1404	5MC	O2-C2-N3	-2.31	118.57	122.33
55	2x	32	5MC	O2-C2-N3	-2.31	118.58	122.33
54	2w	54	5MU	C5M-C5-C4	2.30	121.30	118.77
32	1a	516	PSU	O2-C2-N1	-2.30	120.26	122.79
1	1A	2605	PSU	C5-C6-N1	-2.30	118.66	122.11
55	2x	8	4SU	O2-C2-N3	-2.30	117.22	121.50
32	2a	1402	4OC	CM4-N4-C4	-2.28	117.99	122.45
32	2a	966	M2G	C8-N7-C5	2.28	107.33	102.99
32	2a	1402	4OC	O2-C2-N3	-2.27	118.64	122.33
55	1x	32	5MC	O2-C2-N3	-2.26	118.66	122.33
54	2w	37	MIA	C1'-N9-C4	2.25	130.59	126.64
32	1a	1498	UR3	C6-N1-C2	-2.25	119.78	121.79
55	1x	32	5MC	CM5-C5-C6	-2.25	119.85	122.85
1	2A	2605	PSU	O2-C2-N1	-2.24	120.33	122.79
55	1x	8	4SU	C1'-N1-C2	2.23	121.60	117.57
32	2a	1498	UR3	C3U-N3-C4	2.22	121.06	117.89
1	2A	2552	2MU	O2-C2-N1	-2.21	119.85	122.79
1	2A	2251	OMG	C8-N7-C5	2.20	107.18	102.99
1	2A	2605	PSU	C5-C6-N1	-2.19	118.83	122.11
32	2a	1402	4OC	C6-C5-C4	2.19	119.64	116.96
54	1y	8	4SU	C5-C4-S4	-2.18	121.65	124.47
55	1x	76	31H	CA-N-CN	-2.18	119.47	122.82
32	1a	1404	5MC	CM5-C5-C6	-2.16	119.96	122.85
55	1x	54	5MU	C5M-C5-C4	2.16	121.14	118.77
55	2x	55	PSU	C5-C6-N1	-2.16	118.87	122.11
55	1x	54	5MU	C5M-C5-C6	-2.16	119.97	122.85
1	1A	2251	OMG	C5-C6-N1	2.15	117.74	113.95
1	1A	2552	2MU	O2-C2-N1	-2.14	119.94	122.79
55	1x	76	31H	OCN-CN-N	-2.14	119.64	125.27
32	2a	966	M2G	C5-C6-N1	2.13	117.72	113.95
32	2a	1400	5MC	C5-C4-N3	-2.12	119.39	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2251	OMG	O6-C6-C5	-2.12	120.24	124.37
32	1a	1207	2MG	C5-C6-N1	2.11	117.67	113.95
32	1a	1498	UR3	C3U-N3-C4	2.10	120.89	117.89
54	2w	54	5MU	O2-C2-N1	-2.10	120.00	122.79
54	2y	55	PSU	O4'-C1'-C2'	2.08	108.08	105.14
32	1a	516	PSU	C5-C6-N1	-2.08	118.98	122.11
1	1A	2552	2MU	C2'-C1'-N1	-2.07	110.20	114.22
54	2y	55	PSU	C6-C5-C4	-2.07	116.75	118.20
1	2A	2605	PSU	O2-C2-N3	-2.06	117.93	121.82
32	2a	1207	2MG	C5-C6-N1	2.06	117.58	113.95
1	1A	2251	OMG	C8-N7-C5	2.05	106.90	102.99
1	2A	1911	PSU	C5-C6-N1	-2.05	119.03	122.11
32	1a	516	PSU	O2-C2-N3	-2.04	117.96	121.82
32	2a	966	M2G	O6-C6-C5	-2.04	120.39	124.37
54	1w	39	PSU	C5-C6-N1	-2.03	119.06	122.11
32	2a	516	PSU	O4'-C1'-C2'	2.03	108.01	105.14
54	1w	54	5MU	C5M-C5-C4	2.03	121.00	118.77
32	2a	1407	5MC	O2-C2-N3	-2.02	119.04	122.33
1	1A	2503	8AH	N6-C6-N1	2.02	122.55	117.07
32	2a	967	5MC	O2-C2-N3	-2.01	119.06	122.33
55	1x	8	4SU	O2-C2-N3	-2.01	117.75	121.50
32	1a	1407	5MC	O2-C2-N3	-2.00	119.07	122.33
1	2A	1942	5MC	O2-C2-N3	-2.00	119.08	122.33

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C3'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	1w	46	G7M	C4'-C5'-O5'-P
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	CB-CA-N-CN
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
55	2x	76	31H	C3'-C4'-C5'-O5'
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
55	1x	76	31H	C4'-C5'-O5'-P
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	2503	8AH	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C1'-C5-C4
1	1A	2503	8AH	C4'-C5'-O5'-P
54	2y	55	PSU	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
43	2l	92	0TD	CG-CB-SB-CSB
1	2A	1917	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
1	1A	2503	8AH	O4'-C4'-C5'-O5'
54	2y	8	4SU	C2'-C1'-N1-C2

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 2714 ligands modelled in this entry, 2710 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
57	6IF	2A	3831	-	30,34,34	1.04	2 (6%)	32,49,49	1.89	4 (12%)
57	6IF	1A	4084	-	30,34,34	1.00	1 (3%)	32,49,49	1.67	4 (12%)
59	SF4	2d	303	35	0,12,12	-	-	-		
59	SF4	1d	302	35	0,12,12	-	-	-		

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
57	6IF	2A	3831	-	-	0/22/65/65	0/3/3/3
57	6IF	1A	4084	-	-	1/22/65/65	0/3/3/3
59	SF4	2d	303	35	-	-	0/6/5/5
59	SF4	1d	302	35	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4084	6IF	OAF-CAE	3.35	1.49	1.44
57	2A	3831	6IF	OAV-CB	3.03	1.45	1.42
57	2A	3831	6IF	CD2-CAY	-2.32	1.51	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2A	3831	6IF	CBB-CBA-CAY	-7.56	109.57	116.03
57	1A	4084	6IF	CBB-CBA-CAY	-5.46	111.36	116.03
57	2A	3831	6IF	CD1-CG-CB	-4.93	97.70	103.80
57	1A	4084	6IF	CD1-CG-CB	-4.58	98.13	103.80
57	1A	4084	6IF	CD2-CAY-CAX	-3.00	109.39	113.89
57	2A	3831	6IF	CAA-OAF-CAE	-2.73	110.42	114.12
57	1A	4084	6IF	CAK-CAI-CAG	-2.44	111.11	114.26
57	2A	3831	6IF	CD2-CAY-CAX	-2.25	110.52	113.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

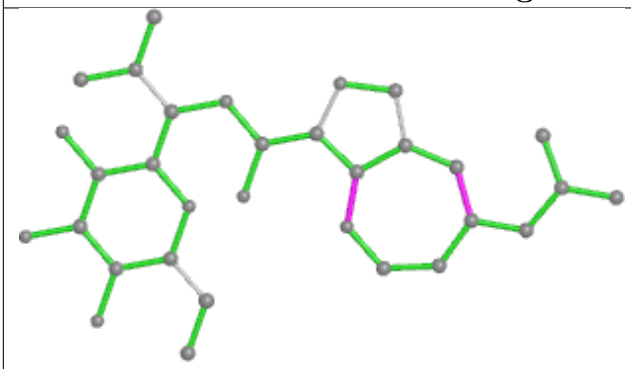
Mol	Chain	Res	Type	Atoms
57	1A	4084	6IF	CAE-CAG-NAH-C

There are no ring outliers.

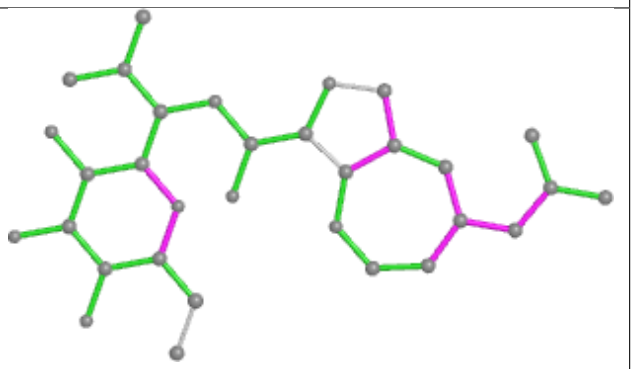
No monomer is involved in short contacts.

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.

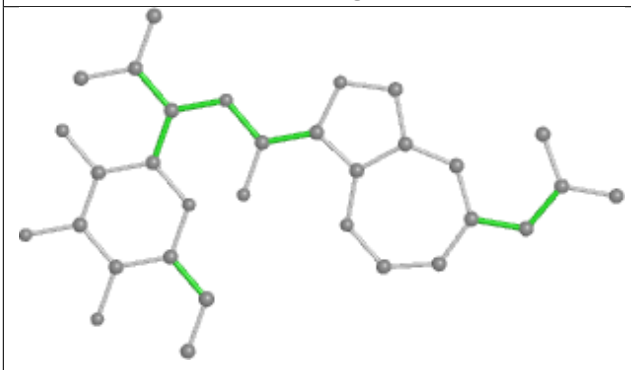
Ligand 6IF 2A 3831



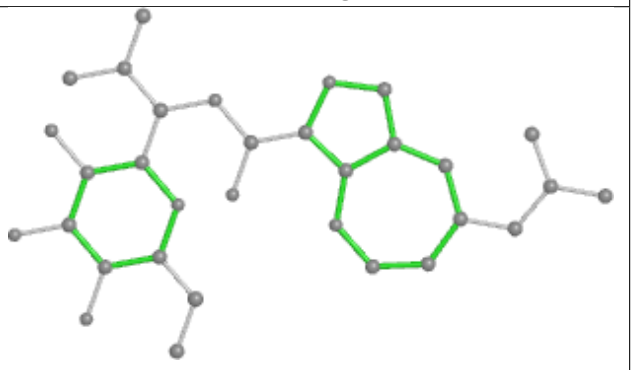
Bond lengths



Bond angles

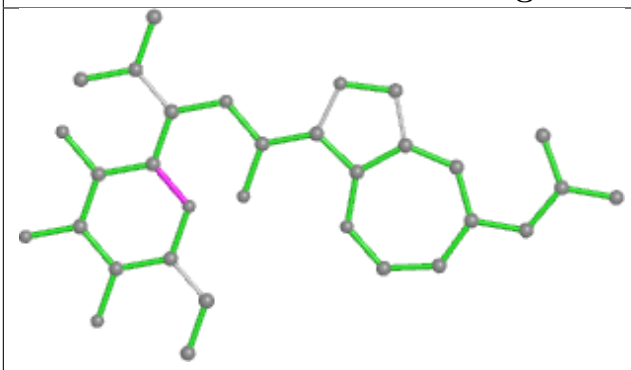


Torsions

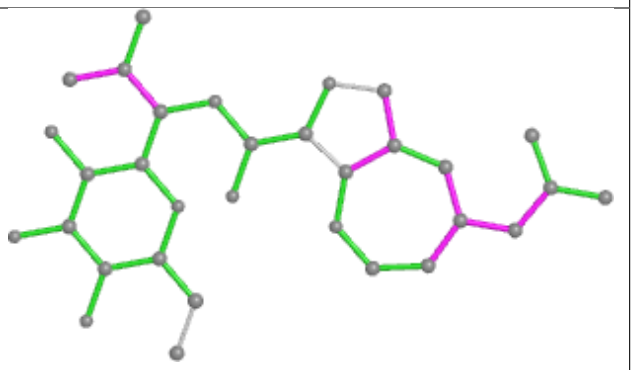


Rings

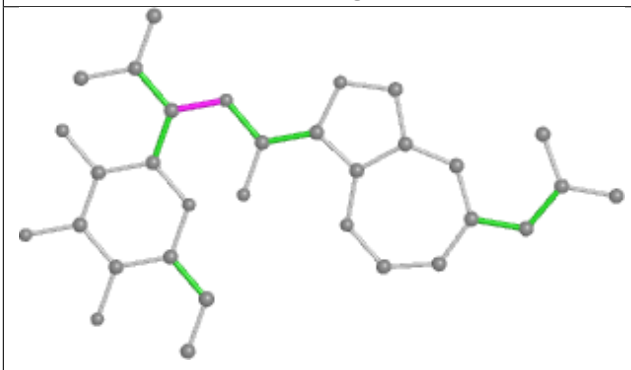
Ligand 6IF 1A 4084



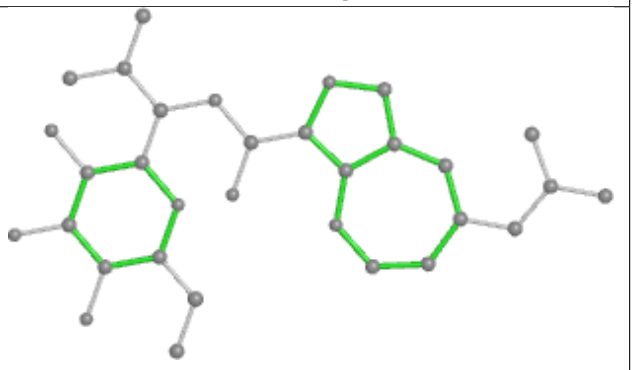
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

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%)	0.39	117 (4%) 37 44	23, 40, 97, 111	0
1	2A	2789/2915 (95%)	0.35	112 (4%) 38 45	39, 60, 95, 110	0
2	1B	120/121 (99%)	-0.03	0 100 100	35, 54, 67, 88	0
2	2B	120/121 (99%)	-0.13	0 100 100	67, 77, 85, 93	0
3	1D	275/276 (99%)	0.65	2 (0%) 87 90	25, 39, 53, 76	0
3	2D	275/276 (99%)	0.83	4 (1%) 73 79	32, 52, 65, 80	0
4	1E	204/206 (99%)	0.48	1 (0%) 91 94	24, 42, 61, 78	0
4	2E	204/206 (99%)	0.66	15 (7%) 14 18	40, 61, 74, 82	0
5	1F	202/210 (96%)	0.35	1 (0%) 91 94	23, 46, 70, 85	0
5	2F	202/210 (96%)	0.61	8 (3%) 38 45	38, 69, 78, 84	0
6	1G	181/182 (99%)	0.38	3 (1%) 70 76	42, 59, 72, 85	0
6	2G	181/182 (99%)	0.52	11 (6%) 21 25	63, 77, 84, 89	0
7	1H	174/180 (96%)	0.32	2 (1%) 80 85	42, 57, 67, 75	0
7	2H	174/180 (96%)	2.90	127 (72%) 0 0	67, 84, 92, 97	0
8	1I	146/148 (98%)	0.28	2 (1%) 75 81	53, 74, 83, 87	0
8	2I	146/148 (98%)	0.57	15 (10%) 6 8	53, 73, 84, 87	0
9	1N	140/140 (100%)	0.48	1 (0%) 87 90	29, 41, 64, 74	0
9	2N	140/140 (100%)	1.00	19 (13%) 3 3	51, 68, 80, 88	0
10	1O	122/122 (100%)	0.45	2 (1%) 72 78	31, 44, 61, 66	0
10	2O	122/122 (100%)	0.71	7 (5%) 23 28	49, 61, 73, 76	0
11	1P	149/150 (99%)	0.47	1 (0%) 87 90	24, 51, 72, 79	0
11	2P	149/150 (99%)	1.35	38 (25%) 0 0	41, 68, 84, 92	0
12	1Q	141/141 (100%)	0.52	3 (2%) 63 70	32, 44, 61, 75	0
12	2Q	141/141 (100%)	1.23	30 (21%) 0 0	50, 69, 79, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.46	0 100 100	28, 38, 50, 63	0
13	2R	118/118 (100%)	0.59	6 (5%) 28 33	46, 55, 64, 71	0
14	1S	110/112 (98%)	0.33	2 (1%) 68 74	43, 54, 65, 69	0
14	2S	110/112 (98%)	1.03	20 (18%) 1 1	64, 72, 81, 87	0
15	1T	131/146 (89%)	0.39	1 (0%) 86 89	37, 49, 74, 80	0
15	2T	131/146 (89%)	0.80	13 (9%) 7 9	53, 64, 77, 82	0
16	1U	116/118 (98%)	0.61	1 (0%) 84 88	24, 32, 47, 63	0
16	2U	116/118 (98%)	0.69	4 (3%) 45 52	48, 66, 75, 80	0
17	1V	101/101 (100%)	0.29	0 100 100	24, 41, 56, 63	0
17	2V	101/101 (100%)	0.49	5 (4%) 28 34	46, 73, 81, 91	0
18	1W	112/113 (99%)	0.53	2 (1%) 68 74	26, 34, 52, 85	0
18	2W	112/113 (99%)	0.60	2 (1%) 68 74	43, 52, 70, 82	0
19	1X	95/96 (98%)	0.62	1 (1%) 80 85	28, 42, 65, 81	0
19	2X	95/96 (98%)	0.60	3 (3%) 47 55	48, 60, 79, 88	0
20	1Y	107/110 (97%)	0.50	2 (1%) 66 73	40, 53, 69, 79	0
20	2Y	107/110 (97%)	0.80	11 (10%) 6 8	62, 72, 83, 90	0
21	1Z	154/206 (74%)	0.47	7 (4%) 33 40	43, 67, 86, 94	0
21	2Z	160/206 (77%)	1.51	51 (31%) 0 0	66, 83, 92, 96	0
22	10	83/85 (97%)	1.15	8 (9%) 8 10	33, 41, 65, 86	0
22	20	83/85 (97%)	1.46	19 (22%) 0 0	48, 65, 77, 89	0
23	11	97/98 (98%)	0.76	3 (3%) 49 56	31, 47, 72, 76	0
23	21	97/98 (98%)	0.73	5 (5%) 27 32	43, 56, 75, 81	0
24	12	70/72 (97%)	0.57	0 100 100	39, 52, 63, 73	0
24	22	70/72 (97%)	0.37	3 (4%) 35 42	61, 71, 78, 82	0
25	13	59/60 (98%)	0.42	0 100 100	28, 39, 65, 78	0
25	23	59/60 (98%)	1.04	8 (13%) 3 3	59, 69, 80, 87	0
26	14	69/71 (97%)	0.33	3 (4%) 35 42	56, 77, 88, 91	0
26	24	69/71 (97%)	0.58	10 (14%) 2 3	74, 85, 92, 95	0
27	15	59/60 (98%)	0.41	1 (1%) 70 76	23, 33, 57, 63	0
27	25	59/60 (98%)	0.47	0 100 100	43, 56, 66, 77	0
28	16	53/54 (98%)	0.51	2 (3%) 40 47	37, 45, 60, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.30	11 (20%) 1 0	53, 61, 69, 76	0
29	17	48/49 (97%)	0.76	3 (6%) 20 23	25, 32, 54, 66	0
29	27	48/49 (97%)	1.01	4 (8%) 11 13	37, 44, 68, 73	0
30	18	64/65 (98%)	0.55	0 100 100	31, 38, 45, 60	0
30	28	64/65 (98%)	1.50	15 (23%) 0 0	47, 56, 63, 68	0
31	19	37/37 (100%)	0.81	3 (8%) 12 15	32, 44, 59, 62	0
31	29	37/37 (100%)	1.85	16 (43%) 0 0	61, 70, 78, 83	0
32	1a	1488/1521 (97%)	0.30	61 (4%) 37 44	35, 68, 94, 109	0
32	2a	1491/1521 (98%)	0.33	79 (5%) 26 31	51, 77, 96, 108	0
33	1b	231/256 (90%)	1.20	49 (21%) 0 0	66, 78, 87, 93	0
33	2b	231/256 (90%)	1.79	81 (35%) 0 0	75, 86, 92, 98	0
34	1c	206/239 (86%)	1.03	40 (19%) 1 1	61, 72, 83, 85	0
34	2c	206/239 (86%)	1.46	70 (33%) 0 0	74, 83, 88, 93	0
35	1d	208/209 (99%)	0.58	10 (4%) 30 37	54, 71, 79, 84	0
35	2d	208/209 (99%)	0.67	13 (6%) 20 23	63, 71, 78, 84	0
36	1e	148/162 (91%)	0.48	2 (1%) 75 81	51, 65, 75, 82	0
36	2e	148/162 (91%)	0.98	21 (14%) 2 3	66, 76, 84, 90	0
37	1f	100/101 (99%)	0.34	1 (1%) 82 86	58, 70, 76, 79	0
37	2f	100/101 (99%)	0.33	0 100 100	56, 69, 77, 87	0
38	1g	155/156 (99%)	1.03	28 (18%) 1 1	61, 70, 83, 88	0
38	2g	155/156 (99%)	1.08	25 (16%) 1 2	70, 78, 86, 91	0
39	1h	137/138 (99%)	0.51	7 (5%) 28 33	56, 67, 74, 79	0
39	2h	137/138 (99%)	1.06	23 (16%) 1 1	67, 78, 82, 85	0
40	1i	127/128 (99%)	2.22	58 (45%) 0 0	52, 77, 84, 88	0
40	2i	127/128 (99%)	2.89	79 (62%) 0 0	71, 84, 90, 94	0
41	1j	97/105 (92%)	1.26	25 (25%) 0 0	58, 75, 84, 87	0
41	2j	96/105 (91%)	2.66	56 (58%) 0 0	73, 84, 92, 94	0
42	1k	114/129 (88%)	0.64	7 (6%) 21 25	45, 67, 76, 83	0
42	2k	114/129 (88%)	0.39	4 (3%) 44 51	56, 74, 83, 86	0
43	1l	121/132 (91%)	0.49	2 (1%) 70 76	46, 54, 68, 74	0
43	2l	121/132 (91%)	0.83	15 (12%) 4 5	58, 68, 79, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.72	8 (6%) 18 22	56, 70, 78, 91	0
44	2m	122/126 (96%)	1.18	24 (19%) 1 1	71, 81, 87, 94	0
45	1n	60/61 (98%)	1.59	19 (31%) 0 0	60, 67, 75, 77	0
45	2n	60/61 (98%)	4.45	54 (90%) 0 0	77, 83, 87, 93	0
46	1o	88/89 (98%)	0.53	2 (2%) 60 67	51, 66, 75, 80	0
46	2o	88/89 (98%)	0.62	3 (3%) 45 52	61, 73, 82, 86	0
47	1p	82/88 (93%)	1.40	23 (28%) 0 0	58, 72, 79, 87	0
47	2p	82/88 (93%)	1.22	14 (17%) 1 1	60, 71, 78, 81	0
48	1q	99/105 (94%)	0.72	4 (4%) 38 45	53, 67, 78, 78	0
48	2q	99/105 (94%)	0.84	10 (10%) 7 8	63, 74, 82, 85	0
49	1r	68/88 (77%)	0.45	2 (2%) 51 59	58, 67, 80, 81	0
49	2r	68/88 (77%)	0.44	2 (2%) 51 59	65, 72, 79, 86	0
50	1s	83/93 (89%)	0.68	6 (7%) 15 18	66, 73, 80, 82	0
50	2s	83/93 (89%)	1.60	29 (34%) 0 0	77, 85, 89, 91	0
51	1t	96/106 (90%)	1.60	36 (37%) 0 0	61, 72, 80, 84	0
51	2t	96/106 (90%)	1.81	39 (40%) 0 0	61, 73, 83, 86	0
52	1u	23/27 (85%)	1.82	10 (43%) 0 0	61, 66, 72, 74	0
52	2u	23/27 (85%)	2.83	15 (65%) 0 0	74, 79, 81, 83	0
53	1v	13/24 (54%)	1.42	3 (23%) 0 0	51, 55, 88, 94	0
53	2v	13/24 (54%)	1.65	6 (46%) 0 0	67, 77, 90, 101	0
54	1w	66/76 (86%)	0.59	10 (15%) 2 2	54, 85, 99, 106	0
54	1y	67/76 (88%)	0.72	9 (13%) 3 4	40, 93, 101, 103	0
54	2w	63/76 (82%)	0.48	8 (12%) 3 4	75, 94, 104, 106	0
54	2y	66/76 (86%)	1.31	20 (30%) 0 0	54, 98, 103, 105	0
55	1x	71/77 (92%)	0.06	0 100 100	34, 62, 81, 91	0
55	2x	71/77 (92%)	-0.09	1 (1%) 75 81	49, 77, 88, 100	0
All	All	20868/21748 (95%)	0.65	1879 (9%) 9 11	23, 65, 90, 111	0

All (1879) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	24.9
44	2m	124	PRO	17.8

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	16.4
1	2A	652(V)	C	13.8
1	2A	652(U)	G	13.6
1	1A	652(C)	G	13.0
1	2A	652(C)	G	12.8
1	2A	653	A	12.4
1	1A	653	A	12.3
45	2n	34	TYR	11.5
44	1m	123	ALA	11.4
1	2A	652(T)	C	11.0
1	2A	654	A	10.7
22	20	2	ALA	10.6
1	2A	2802	G	10.6
1	1A	652(V)	C	10.5
45	2n	38	GLY	10.3
45	2n	25	VAL	10.3
45	2n	39	LEU	10.2
1	1A	652(U)	G	10.2
41	2j	65	LEU	9.4
22	10	3	HIS	9.4
38	2g	82	GLY	9.1
38	1g	80	VAL	9.0
1	1A	652(S)	C	8.9
45	2n	12	ARG	8.9
45	2n	2	ALA	8.6
41	2j	47	PHE	8.6
40	1i	106	ALA	8.4
1	1A	652(T)	C	8.4
21	2Z	170	THR	8.4
1	1A	654	A	8.3
44	2m	122	LYS	8.3
33	2b	122	PHE	8.0
38	2g	156	TRP	7.9
1	2A	2146	C	7.8
22	10	2	ALA	7.8
1	2A	652(D)	C	7.7
7	2H	52	VAL	7.7
40	2i	14	VAL	7.6
41	2j	63	PHE	7.5
40	1i	19	LEU	7.4
7	2H	35	VAL	7.4
22	10	4	LYS	7.3

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Mol	Chain	Res	Type	RSRZ
50	2s	80	TYR	7.1
32	2a	1033	G	7.0
33	2b	165	VAL	7.0
7	2H	72	ILE	7.0
40	2i	115	GLY	7.0
33	2b	121	LEU	7.0
40	2i	114	TYR	6.8
22	10	6	GLY	6.7
38	1g	79	ARG	6.7
21	2Z	149	SER	6.6
1	2A	2145	C	6.6
1	2A	1509	C	6.6
32	2a	1001(A)	G	6.5
45	2n	61	TRP	6.5
1	1A	1094	U	6.5
40	2i	90	PRO	6.5
20	2Y	1	MET	6.4
40	2i	128	ARG	6.4
45	2n	11	LYS	6.4
33	2b	187	LEU	6.4
1	2A	2127	G	6.3
32	1a	1001(A)	G	6.3
54	1w	71	G	6.3
40	2i	7	THR	6.3
41	2j	59	SER	6.3
52	2u	16	GLY	6.3
33	2b	29	ALA	6.3
32	1a	1030(B)	C	6.2
54	2y	36	A	6.2
40	1i	8	GLY	6.2
1	2A	2801(A)	A	6.2
40	1i	14	VAL	6.0
21	2Z	106	GLY	6.0
45	2n	57	ARG	6.0
32	1a	1036	G	6.0
7	2H	121	ILE	6.0
40	2i	86	VAL	6.0
7	2H	105	LEU	6.0
23	11	2	SER	6.0
38	2g	80	VAL	5.9
51	2t	63	ILE	5.9
33	1b	133	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
34	2c	8	ILE	5.9
34	2c	182	ILE	5.9
1	2A	2112	G	5.8
40	2i	127	LYS	5.8
44	2m	121	LYS	5.8
32	1a	1030	C	5.8
32	1a	1030(A)	G	5.8
45	2n	29	ARG	5.8
40	2i	49	PRO	5.8
41	2j	44	VAL	5.7
45	2n	37	PHE	5.7
7	2H	48	GLY	5.7
7	2H	24	VAL	5.7
7	2H	125	VAL	5.7
45	2n	31	ARG	5.7
32	2a	1030(A)	G	5.7
33	2b	92	TYR	5.6
1	1A	1096	A	5.6
40	1i	15	ALA	5.6
1	1A	888	C	5.6
38	2g	154	TYR	5.6
32	1a	1003	G	5.6
7	2H	123	PHE	5.6
1	2A	885	C	5.6
45	2n	6	LEU	5.5
32	1a	204	U	5.5
1	2A	2793	G	5.5
32	2a	1002	G	5.5
1	2A	2138	C	5.5
32	2a	1034	G	5.5
40	1i	81	ILE	5.5
1	2A	2154	G	5.5
32	2a	1035	A	5.5
38	1g	85	TYR	5.5
14	2S	58	LEU	5.5
23	11	98	LEU	5.5
32	2a	1030(B)	C	5.4
45	2n	35	ARG	5.4
22	20	3	HIS	5.4
1	1A	652(E)	G	5.4
7	2H	102	ALA	5.4
40	2i	36	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
7	2H	2	SER	5.4
22	20	4	LYS	5.4
7	2H	128	PRO	5.4
33	2b	34	ALA	5.4
38	1g	156	TRP	5.4
45	2n	42	ILE	5.4
32	2a	1532	U	5.3
41	2j	98	ILE	5.3
45	1n	2	ALA	5.3
1	2A	2111	C	5.3
21	2Z	139	VAL	5.3
38	1g	154	TYR	5.3
45	2n	13	THR	5.3
41	2j	55	LYS	5.3
45	2n	22	THR	5.3
11	2P	109	GLY	5.3
50	2s	36	ARG	5.3
32	1a	1030(C)	G	5.3
33	2b	70	PHE	5.3
1	1A	1095	A	5.3
32	2a	1003	G	5.3
40	2i	102	LEU	5.3
51	2t	25	ARG	5.2
45	2n	55	GLY	5.2
40	2i	125	TYR	5.2
54	1w	20	U	5.2
1	1A	2145	C	5.2
52	2u	14	TRP	5.2
40	1i	66	ARG	5.2
7	2H	98	LEU	5.2
1	1A	1057	A	5.2
21	2Z	152	ALA	5.2
1	1A	652(F)	G	5.2
1	1A	896	A	5.2
32	2a	1257	U	5.2
33	2b	161	ALA	5.1
33	2b	127	ILE	5.1
7	2H	115	VAL	5.1
1	2A	2128	C	5.1
32	1a	1034	G	5.1
32	2a	1036	G	5.1
41	2j	10	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2147	G	5.0
40	2i	9	ARG	5.0
7	2H	133	VAL	5.0
1	2A	2125	G	5.0
38	2g	7	ALA	5.0
7	2H	37	VAL	5.0
1	1A	884	C	5.0
41	2j	66	ARG	5.0
34	2c	6	HIS	5.0
45	2n	4	LYS	5.0
51	1t	68	LYS	5.0
21	2Z	144	LEU	5.0
1	2A	884	C	5.0
1	2A	2126	A	5.0
11	2P	91	PHE	5.0
1	2A	2115	G	4.9
1	2A	2133	G	4.9
40	2i	108	VAL	4.9
54	2y	21	A	4.9
40	2i	109	VAL	4.9
45	2n	49	HIS	4.9
40	1i	65	VAL	4.9
7	2H	100	GLY	4.9
7	2H	54	ARG	4.9
4	2E	196	VAL	4.9
51	2t	24	LEU	4.9
33	2b	215	LEU	4.9
41	2j	34	VAL	4.9
32	1a	1029	C	4.8
7	2H	157	TYR	4.8
40	2i	62	TYR	4.8
42	1k	25	TYR	4.8
40	2i	82	ALA	4.8
41	2j	38	ILE	4.8
1	1A	652(D)	C	4.8
21	2Z	96	VAL	4.8
40	2i	10	ARG	4.8
45	2n	36	PHE	4.8
45	2n	10	ALA	4.8
40	1i	47	LEU	4.8
33	2b	214	ILE	4.8
7	2H	6	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
45	1n	61	TRP	4.8
1	2A	229	A	4.8
1	2A	2804	C	4.8
12	2Q	32	TYR	4.7
7	2H	101	ARG	4.7
7	2H	99	VAL	4.7
51	2t	59	ALA	4.7
7	2H	82	GLY	4.7
1	1A	1509	C	4.7
45	2n	53	LEU	4.7
23	21	2	SER	4.7
31	29	16	VAL	4.7
1	1A	1058	G	4.7
1	1A	1087	G	4.7
54	2w	72	C	4.7
44	2m	42	ALA	4.7
21	1Z	149	SER	4.7
33	2b	201	ILE	4.7
40	2i	66	ARG	4.6
52	2u	15	ARG	4.6
32	1a	1532	U	4.6
34	1c	13	GLY	4.6
41	2j	72	VAL	4.6
32	1a	1002	G	4.6
54	2w	73	A	4.6
40	1i	109	VAL	4.6
1	1A	1068	G	4.6
33	2b	48	MET	4.6
34	2c	145	GLY	4.6
1	2A	2113	U	4.6
43	2l	64	TYR	4.6
32	2a	1001	A	4.6
50	1s	71	LEU	4.6
34	2c	193	TYR	4.6
38	2g	81	GLY	4.6
40	2i	19	LEU	4.6
41	2j	85	LEU	4.6
45	2n	44	LEU	4.6
1	1A	885	C	4.6
1	2A	883	G	4.6
7	2H	145	ALA	4.6
21	2Z	51	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
32	1a	1447	A	4.6
41	2j	71	LEU	4.6
47	2p	19	ILE	4.6
40	2i	28	VAL	4.5
26	24	49	PHE	4.5
33	2b	211	ILE	4.5
34	2c	5	ILE	4.5
40	1i	28	VAL	4.5
34	1c	87	LEU	4.5
1	1A	1098	A	4.5
40	1i	113	LYS	4.5
54	1y	36	A	4.5
47	1p	1	MET	4.5
53	1v	12	A	4.5
54	2w	4	C	4.5
34	2c	23	TYR	4.5
38	2g	79	ARG	4.5
7	2H	71	LEU	4.5
21	2Z	155	LEU	4.5
7	2H	29	PRO	4.5
32	2a	1039	C	4.5
1	2A	2119	A	4.4
36	2e	12	LEU	4.4
51	2t	41	ILE	4.4
32	1a	1031	G	4.4
43	2l	39	VAL	4.4
1	2A	2155	G	4.4
6	1G	139	LEU	4.4
45	2n	51	GLY	4.4
51	1t	69	GLY	4.4
25	23	29	ARG	4.4
34	2c	14	ILE	4.4
33	2b	123	ALA	4.4
40	2i	5	TYR	4.4
50	2s	35	SER	4.4
34	1c	14	ILE	4.3
40	2i	8	GLY	4.3
45	2n	23	ARG	4.3
1	2A	2803	C	4.3
32	2a	1149	C	4.3
50	2s	12	ASP	4.3
33	2b	66	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
50	2s	79	THR	4.3
32	2a	1031	G	4.3
14	2S	3	ARG	4.3
52	2u	6	ARG	4.3
34	1c	193	TYR	4.3
22	10	7	LEU	4.3
40	2i	17	VAL	4.3
38	1g	82	GLY	4.3
1	1A	2159	G	4.3
7	2H	171	LEU	4.3
33	1b	165	VAL	4.3
7	2H	47	GLU	4.3
12	2Q	66	ILE	4.3
39	2h	134	ILE	4.3
31	29	13	LYS	4.3
11	2P	79	ARG	4.3
32	2a	1030(C)	G	4.3
26	24	50	VAL	4.3
1	1A	2174	C	4.3
1	2A	645	C	4.3
1	2A	888	C	4.3
45	2n	7	ILE	4.3
28	26	5	VAL	4.3
7	2H	175	LYS	4.3
44	2m	104	ARG	4.3
39	2h	2	LEU	4.3
51	2t	26	ASN	4.3
14	2S	29	PHE	4.3
32	1a	1032	G	4.3
38	1g	83	ALA	4.3
38	2g	4	ARG	4.3
7	2H	89	ILE	4.2
34	2c	157	ILE	4.2
33	2b	164	VAL	4.2
41	2j	49	VAL	4.2
1	1A	1093	G	4.2
32	1a	1035	A	4.2
53	1v	24	A	4.2
7	2H	67	LEU	4.2
28	26	10	LEU	4.2
7	2H	51	ARG	4.2
33	1b	232	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
45	2n	59	ALA	4.2
21	2Z	153	SER	4.2
1	1A	2128	C	4.2
1	1A	2151	G	4.2
1	2A	896	A	4.2
1	2A	2897	U	4.2
51	2t	62	LEU	4.2
34	2c	178	LEU	4.2
40	1i	117	HIS	4.2
32	2a	1030	C	4.2
7	2H	49	VAL	4.2
21	2Z	126	VAL	4.2
34	2c	7	PRO	4.2
1	1A	1064	C	4.2
1	2A	2170	A	4.2
7	1H	174	GLY	4.2
14	2S	14	VAL	4.2
33	2b	81	VAL	4.2
38	2g	85	TYR	4.2
44	2m	120	LYS	4.2
7	2H	169	VAL	4.2
53	2v	24	A	4.2
33	2b	118	LEU	4.1
41	2j	39	PRO	4.1
40	2i	93	ARG	4.1
12	2Q	109	VAL	4.1
40	2i	53	VAL	4.1
51	1t	80	ARG	4.1
54	1w	75	C	4.1
45	2n	24	CYS	4.1
1	2A	652(E)	G	4.1
32	1a	1026	G	4.1
7	2H	17	VAL	4.1
33	2b	152	PHE	4.1
34	1c	184	TYR	4.1
1	2A	1026	U	4.1
40	2i	124	GLN	4.1
40	1i	20	ARG	4.1
40	2i	27	THR	4.1
33	1b	188	ALA	4.1
40	1i	119	ALA	4.1
38	1g	84	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
39	2h	94	TYR	4.1
40	1i	4	TYR	4.1
40	2i	65	VAL	4.1
34	2c	155	GLY	4.1
41	2j	51	ARG	4.1
32	1a	1257	U	4.1
45	1n	60	SER	4.1
32	1a	1030(D)	A	4.1
34	2c	13	GLY	4.1
45	2n	56	VAL	4.1
1	2A	2173	A	4.0
38	2g	83	ALA	4.0
40	2i	63	ILE	4.0
50	2s	63	THR	4.0
54	2w	71	G	4.0
1	1A	2138	C	4.0
1	1A	2173	A	4.0
39	2h	58	TYR	4.0
1	1A	1059	G	4.0
32	2a	1021	G	4.0
21	2Z	145	GLU	4.0
11	2P	77	ARG	4.0
40	2i	70	LYS	4.0
32	2a	1531	A	4.0
33	2b	68	ILE	4.0
54	2y	60	U	4.0
40	2i	105	ASP	4.0
33	2b	203	GLY	4.0
32	2a	1030(D)	A	4.0
7	2H	131	VAL	4.0
40	1i	37	PHE	3.9
40	1i	59	PHE	3.9
35	1d	73	ARG	3.9
40	2i	16	ARG	3.9
41	2j	67	THR	3.9
40	1i	82	ALA	3.9
40	2i	4	TYR	3.9
33	1b	61	LEU	3.9
41	2j	50	ILE	3.9
54	1y	20	U	3.9
54	2y	57	G	3.9
47	1p	21	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
45	2n	30	ALA	3.9
32	1a	1531	A	3.9
47	1p	59	TRP	3.9
7	2H	43	VAL	3.9
7	2H	113	VAL	3.9
47	2p	20	VAL	3.9
45	2n	58	LYS	3.9
51	1t	55	ILE	3.9
34	2c	201	TYR	3.9
40	1i	5	TYR	3.9
38	2g	16	LEU	3.9
51	1t	74	LYS	3.9
33	1b	214	ILE	3.9
40	2i	103	THR	3.9
51	2t	83	ARG	3.9
41	2j	64	GLU	3.9
1	1A	1060	U	3.9
34	2c	160	ALA	3.9
7	2H	30	LYS	3.9
38	2g	78	ARG	3.9
50	2s	13	ASP	3.9
7	2H	96	ALA	3.9
50	2s	14	HIS	3.9
41	2j	62	HIS	3.8
7	2H	165	ALA	3.8
32	2a	1032	G	3.8
45	2n	46	GLU	3.8
7	2H	7	LEU	3.8
21	2Z	148	ASP	3.8
22	20	5	LYS	3.8
40	2i	79	LEU	3.8
40	2i	80	GLY	3.8
33	2b	17	PHE	3.8
33	1b	222	ILE	3.8
51	1t	41	ILE	3.8
40	1i	110	GLU	3.8
32	1a	1033	G	3.8
26	24	32	TYR	3.8
41	2j	26	ALA	3.8
1	2A	2169	A	3.8
32	1a	1001	A	3.8
4	2E	115	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
14	2S	20	ARG	3.8
33	1b	136	VAL	3.8
34	2c	207	VAL	3.8
39	2h	133	LEU	3.8
40	2i	78	LYS	3.8
1	1A	2131	G	3.8
1	2A	2129	C	3.8
1	2A	2139	C	3.8
21	2Z	95	PRO	3.8
40	1i	33	PHE	3.8
40	2i	81	ILE	3.8
40	2i	126	SER	3.8
50	2s	50	ALA	3.8
54	1w	1	G	3.8
34	1c	124	ILE	3.8
39	2h	9	MET	3.8
1	2A	614(A)	U	3.8
1	2A	2131	G	3.8
33	2b	94	ASN	3.8
7	2H	64	LEU	3.8
40	2i	104	ARG	3.7
45	2n	50	LYS	3.7
1	2A	2110	G	3.7
54	2y	34	G	3.7
29	27	46	VAL	3.7
51	1t	62	LEU	3.7
41	2j	46	ARG	3.7
45	2n	14	PRO	3.7
45	2n	16	PHE	3.7
34	2c	194	GLY	3.7
41	2j	61	GLU	3.7
29	17	48	LYS	3.7
51	1t	14	LYS	3.7
6	2G	3	LEU	3.7
7	2H	103	LEU	3.7
51	1t	20	LEU	3.7
1	2A	1112	G	3.7
50	2s	31	ILE	3.7
1	1A	2132	U	3.7
45	1n	57	ARG	3.7
52	2u	22	ARG	3.7
21	2Z	141	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
36	2e	90	VAL	3.7
40	2i	64	THR	3.7
1	1A	1099	G	3.7
1	2A	2805	G	3.7
32	2a	1024	G	3.7
34	1c	65	ALA	3.7
32	2a	1004	A	3.7
41	2j	56	HIS	3.7
41	2j	74	ILE	3.7
52	2u	13	ILE	3.7
52	2u	18	TYR	3.7
30	28	29	LYS	3.7
34	2c	198	VAL	3.7
41	2j	36	GLY	3.7
39	2h	83	ILE	3.7
1	2A	2151	G	3.7
45	2n	40	CYS	3.7
40	2i	73	GLN	3.7
12	2Q	104	PHE	3.7
33	1b	211	ILE	3.7
1	2A	2132	U	3.7
1	2A	2144	U	3.7
1	1A	2170	A	3.7
1	2A	614(B)	G	3.7
22	20	6	GLY	3.7
38	1g	99	LEU	3.7
1	2A	2794	C	3.7
7	2H	146	ALA	3.7
32	2a	1116	C	3.7
33	1b	28	PHE	3.6
21	2Z	133	ILE	3.6
34	1c	39	ILE	3.6
1	1A	1097	U	3.6
52	1u	14	TRP	3.6
38	1g	4	ARG	3.6
51	1t	22	ARG	3.6
7	2H	36	PRO	3.6
41	1j	41	PRO	3.6
7	2H	107	VAL	3.6
40	1i	26	VAL	3.6
7	2H	41	MET	3.6
40	2i	77	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
9	2N	83	LYS	3.6
8	2I	38	LEU	3.6
12	2Q	17	LEU	3.6
21	2Z	140	ASP	3.6
1	1A	1086	A	3.6
32	2a	1286	A	3.6
1	2A	2123	G	3.6
1	2A	2896	C	3.6
38	1g	81	GLY	3.6
40	2i	123	PRO	3.6
7	2H	94	TYR	3.6
22	20	7	LEU	3.6
34	2c	12	LEU	3.6
40	1i	79	LEU	3.6
7	2H	141	VAL	3.6
1	1A	2110	G	3.6
1	2A	2153	G	3.6
12	2Q	113	GLN	3.6
26	24	63	TYR	3.6
34	1c	179	ARG	3.6
34	2c	18	TRP	3.6
40	2i	37	PHE	3.6
41	2j	6	ILE	3.6
42	2k	25	TYR	3.6
7	2H	32	GLU	3.6
30	28	23	VAL	3.6
47	2p	59	TRP	3.6
1	2A	6	A	3.6
1	2A	2174	C	3.6
11	2P	45	LEU	3.6
51	2t	13	LEU	3.6
7	2H	122	THR	3.6
40	2i	43	ALA	3.6
47	2p	2	VAL	3.6
50	2s	70	LYS	3.6
32	2a	1447	A	3.5
33	2b	51	LEU	3.5
11	2P	76	LYS	3.5
1	1A	2162	G	3.5
52	1u	18	TYR	3.5
16	2U	2	PRO	3.5
8	2I	12	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
21	2Z	125	LEU	3.5
33	2b	98	LEU	3.5
40	1i	11	LYS	3.5
41	1j	40	LEU	3.5
49	2r	66	LEU	3.5
50	2s	71	LEU	3.5
19	2X	68	ARG	3.5
51	2t	28	ALA	3.5
7	2H	124	GLU	3.5
7	2H	164	TYR	3.5
33	2b	31	TYR	3.5
40	2i	88	TYR	3.5
1	1A	1082	U	3.5
40	2i	6	GLY	3.5
1	1A	2140	C	3.5
7	2H	76	VAL	3.5
39	1h	93	VAL	3.5
45	1n	56	VAL	3.5
33	2b	33	TYR	3.5
9	2N	71	ILE	3.5
41	1j	47	PHE	3.5
48	1q	27	PHE	3.5
54	2y	19	G	3.5
40	1i	108	VAL	3.5
40	1i	10	ARG	3.5
32	2a	1150	U	3.5
39	2h	112	LEU	3.5
1	2A	2156	G	3.5
40	1i	76	ALA	3.5
50	2s	38	SER	3.5
21	2Z	122	ARG	3.5
41	1j	46	ARG	3.5
52	1u	10	ARG	3.5
31	29	37	GLY	3.5
52	2u	21	TYR	3.5
1	1A	2803	C	3.5
44	1m	121	LYS	3.5
33	1b	137	ARG	3.5
40	2i	121	ARG	3.5
44	1m	2	ALA	3.5
33	2b	71	VAL	3.5
33	1b	132	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
34	2c	4	LYS	3.5
1	1A	2801(A)	A	3.4
30	28	41	ILE	3.4
41	2j	96	ILE	3.4
7	2H	70	THR	3.4
52	2u	5	ASP	3.4
7	2H	38	SER	3.4
29	27	1	MET	3.4
41	1j	57	LYS	3.4
36	2e	22	GLY	3.4
17	2V	72	VAL	3.4
45	2n	8	GLU	3.4
9	2N	61	ARG	3.4
14	2S	13	ARG	3.4
28	26	28	ARG	3.4
41	2j	11	PHE	3.4
1	1A	1067	A	3.4
51	1t	53	LEU	3.4
1	1A	2161	C	3.4
32	1a	1028	C	3.4
41	2j	60	ARG	3.4
7	2H	13	LYS	3.4
15	2T	48	ILE	3.4
40	1i	77	ILE	3.4
21	2Z	169	GLU	3.4
33	2b	37	ASN	3.4
34	2c	60	ALA	3.4
54	1y	19	G	3.4
7	2H	77	LYS	3.4
32	1a	1027	C	3.4
41	2j	13	HIS	3.4
1	2A	272(A)	U	3.4
33	2b	145	LEU	3.4
35	2d	161	ASN	3.4
53	2v	12	A	3.4
1	1A	1092	C	3.4
31	29	25	VAL	3.4
3	2D	38	LYS	3.4
7	2H	88	LEU	3.4
11	2P	123	LEU	3.4
28	26	11	LEU	3.4
30	28	16	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
33	2b	32	ILE	3.4
45	2n	41	ARG	3.4
34	2c	188	LEU	3.4
51	1t	63	ILE	3.4
21	2Z	173	ALA	3.4
40	2i	15	ALA	3.4
41	2j	48	THR	3.4
1	2A	2792	G	3.4
1	2A	2894	G	3.4
9	2N	140	VAL	3.4
50	2s	67	VAL	3.4
8	2I	13	GLY	3.3
48	2q	80	GLY	3.3
33	2b	216	SER	3.3
41	1j	50	ILE	3.3
40	2i	75	ASP	3.3
33	2b	75	LYS	3.3
54	2y	58	A	3.3
1	1A	2897	U	3.3
50	2s	52	TYR	3.3
41	1j	98	ILE	3.3
7	2H	106	THR	3.3
54	1y	47	U	3.3
45	2n	26	ARG	3.3
34	1c	206	GLU	3.3
21	2Z	151	HIS	3.3
40	1i	88	TYR	3.3
1	1A	2896	C	3.3
32	2a	1249	C	3.3
33	1b	187	LEU	3.3
7	2H	20	ALA	3.3
7	2H	46	GLU	3.3
7	2H	92	ILE	3.3
54	2y	56	C	3.3
54	1w	44	G	3.3
7	2H	114	VAL	3.3
50	2s	45	VAL	3.3
7	2H	55	PRO	3.3
12	2Q	2	LEU	3.3
30	28	2	PRO	3.3
33	2b	183	PRO	3.3
45	2n	54	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
41	2j	87	THR	3.3
44	2m	78	ILE	3.3
1	1A	887	A	3.3
7	2H	132	ARG	3.3
12	2Q	6	ARG	3.3
7	2H	56	SER	3.3
7	2H	87	LEU	3.3
34	1c	8	ILE	3.3
35	2d	70	ILE	3.3
40	2i	59	PHE	3.3
41	1j	11	PHE	3.3
1	1A	2143	C	3.3
54	1y	35	A	3.3
47	1p	27	LYS	3.3
5	1F	89	VAL	3.3
1	2A	2160	G	3.2
7	2H	112	PRO	3.2
11	2P	122	PRO	3.2
33	2b	69	LEU	3.2
22	20	69	PHE	3.2
40	1i	52	ALA	3.2
40	2i	18	PHE	3.2
51	2t	76	ALA	3.2
1	1A	1081	U	3.2
51	2t	9	ASN	3.2
1	1A	2146	C	3.2
32	2a	1038	C	3.2
53	2v	15	A	3.2
20	2Y	55	TYR	3.2
21	2Z	165	VAL	3.2
6	2G	39	ILE	3.2
40	2i	33	PHE	3.2
7	2H	34	GLU	3.2
32	2a	1115	C	3.2
33	2b	93	VAL	3.2
7	2H	33	LEU	3.2
36	2e	21	ALA	3.2
34	2c	10	PHE	3.2
34	2c	57	ILE	3.2
9	2N	1	MET	3.2
1	2A	2117	A	3.2
12	2Q	114	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
33	2b	55	PHE	3.2
12	2Q	60	ARG	3.2
40	1i	116	LYS	3.2
1	2A	2157	G	3.2
32	1a	1023	G	3.2
45	1n	51	GLY	3.2
38	1g	151	TYR	3.2
22	20	75	LEU	3.2
7	2H	4	ILE	3.2
38	2g	6	ARG	3.2
40	2i	30	GLY	3.2
31	29	15	LYS	3.2
32	2a	470	C	3.2
34	2c	91	LEU	3.2
1	2A	2114	A	3.2
45	2n	3	ARG	3.2
54	2y	35	A	3.2
22	20	45	PHE	3.2
35	2d	5	ILE	3.2
40	1i	75	ASP	3.2
33	2b	232	PRO	3.2
22	10	5	LYS	3.2
33	2b	139	LYS	3.2
51	2t	68	LYS	3.2
40	1i	86	VAL	3.2
41	1j	44	VAL	3.2
44	1m	87	TYR	3.1
50	2s	30	LEU	3.2
1	1A	1100	C	3.1
7	2H	159	GLU	3.1
32	2a	1117	G	3.1
32	1a	1286	A	3.1
32	2a	969	A	3.1
40	2i	72	GLY	3.1
41	1j	36	GLY	3.1
33	1b	19	HIS	3.1
6	2G	29	TRP	3.1
38	2g	76	ARG	3.1
41	1j	43	ARG	3.1
44	2m	88	ARG	3.1
7	2H	50	VAL	3.1
33	2b	136	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
11	2P	110	TYR	3.1
26	24	67	TYR	3.1
1	1A	1056	G	3.1
1	2A	2149	G	3.1
1	2A	2165	G	3.1
34	1c	12	LEU	3.1
44	2m	87	TYR	3.1
33	2b	227	GLY	3.1
10	2O	69	ILE	3.1
54	2w	74	C	3.1
1	1A	2112	G	3.1
1	1A	2117	A	3.1
32	2a	1224	G	3.1
34	2c	170	GLN	3.1
28	26	52	VAL	3.1
36	2e	16	THR	3.1
46	2o	60	VAL	3.1
51	1t	72	LEU	3.1
51	2t	72	LEU	3.1
45	2n	60	SER	3.1
1	1A	1026	U	3.1
1	1A	2113	U	3.1
4	2E	134	ILE	3.1
33	2b	58	ILE	3.1
11	2P	108	LYS	3.1
54	1w	72	C	3.1
1	2A	2171	A	3.1
1	1A	2793	G	3.1
40	2i	106	ALA	3.1
45	2n	43	CYS	3.1
50	2s	41	VAL	3.1
28	26	42	TRP	3.1
40	1i	126	SER	3.1
7	2H	65	HIS	3.1
17	2V	70	ILE	3.1
46	1o	69	TYR	3.1
47	2p	9	PHE	3.1
32	1a	201	C	3.1
26	24	68	ARG	3.1
1	2A	652(B)	A	3.1
8	1I	35	LEU	3.1
33	2b	138	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
34	2c	101	LEU	3.1
34	2c	200	ALA	3.1
40	1i	50	LEU	3.1
21	1Z	1	MET	3.1
33	2b	41	ILE	3.1
33	2b	131	PRO	3.1
12	2Q	10	ARG	3.1
34	1c	190	ARG	3.1
1	1A	2129	C	3.1
4	1E	195	LEU	3.1
11	2P	149	GLU	3.0
1	1A	2109	U	3.0
1	2A	2166	G	3.0
11	2P	65	ARG	3.0
14	2S	12	PHE	3.0
15	2T	22	PHE	3.0
20	1Y	1	MET	3.0
28	26	54	ILE	3.0
32	1a	79	G	3.0
38	2g	27	ILE	3.0
50	2s	62	ILE	3.0
51	2t	57	ARG	3.0
54	2y	18	G	3.0
7	2H	78	GLY	3.0
34	1c	60	ALA	3.0
41	2j	40	LEU	3.0
1	1A	1065	U	3.0
34	2c	184	TYR	3.0
1	1A	2115	G	3.0
40	2i	68	GLY	3.0
46	2o	61	GLY	3.0
47	1p	6	LEU	3.0
14	2S	46	VAL	3.0
7	2H	148	ILE	3.0
34	1c	128	PHE	3.0
47	1p	33	ILE	3.0
39	2h	65	TYR	3.0
34	2c	22	TRP	3.0
40	2i	87	GLN	3.0
1	2A	2162	G	3.0
7	1H	2	SER	3.0
33	1b	98	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
33	1b	213	LEU	3.0
41	2j	27	ALA	3.0
41	2j	32	ALA	3.0
1	1A	2108	C	3.0
36	2e	8	GLU	3.0
1	2A	2118	U	3.0
11	2P	118	GLY	3.0
12	2Q	15	GLY	3.0
45	1n	42	ILE	3.0
7	2H	23	ARG	3.0
31	29	22	ARG	3.0
31	29	12	ASP	3.0
21	1Z	170	THR	3.0
1	1A	2152	G	3.0
1	1A	2154	G	3.0
45	2n	18	VAL	3.0
45	2n	27	CYS	3.0
32	2a	1027	C	3.0
45	2n	52	GLN	3.0
31	19	26	ILE	3.0
34	2c	176	HIS	3.0
1	1A	1077	A	3.0
7	2H	58	GLU	3.0
32	2a	1005	A	3.0
34	2c	20	SER	3.0
33	1b	215	LEU	3.0
40	2i	76	ALA	3.0
7	2H	10	PRO	3.0
36	2e	128	PRO	3.0
7	2H	45	VAL	3.0
33	1b	229	VAL	3.0
1	1A	2125	G	3.0
1	2A	2159	G	3.0
32	1a	102	G	3.0
47	1p	80	PHE	3.0
9	2N	10	GLU	3.0
34	2c	206	GLU	3.0
32	2a	1180	A	3.0
33	1b	118	LEU	3.0
44	2m	90	LEU	3.0
51	1t	13	LEU	3.0
52	2u	8	THR	3.0

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Mol	Chain	Res	Type	RSRZ
20	2Y	50	ARG	3.0
33	2b	97	TRP	3.0
8	2I	1	MET	2.9
1	1A	2124	G	2.9
1	1A	2139	C	2.9
1	1A	2141	G	2.9
1	2A	2120	G	2.9
33	1b	233	SER	2.9
54	2w	3	C	2.9
4	2E	52	LEU	2.9
6	1G	146	TYR	2.9
21	2Z	69	THR	2.9
29	17	47	ARG	2.9
51	1t	12	ALA	2.9
13	2R	69	ASP	2.9
38	1g	141	VAL	2.9
11	2P	75	ILE	2.9
21	2Z	124	ILE	2.9
50	2s	40	ILE	2.9
1	1A	2111	C	2.9
32	2a	1114	C	2.9
1	2A	882	G	2.9
7	2H	129	THR	2.9
21	2Z	172	ALA	2.9
34	1c	71	ALA	2.9
36	2e	119	LEU	2.9
45	2n	21	TYR	2.9
7	2H	44	VAL	2.9
51	2t	73	HIS	2.9
21	2Z	92	SER	2.9
38	2g	84	ASN	2.9
32	1a	92	C	2.9
40	2i	85	LEU	2.9
32	2a	1220	G	2.9
31	29	20	HIS	2.9
7	2H	3	ARG	2.9
7	2H	69	ARG	2.9
40	2i	20	ARG	2.9
40	2i	41	VAL	2.9
48	2q	35	VAL	2.9
44	2m	101	GLN	2.9
21	2Z	104	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
30	28	24	ALA	2.9
48	1q	98	LEU	2.9
14	2S	36	TYR	2.9
33	1b	135	GLN	2.9
12	2Q	103	MET	2.9
33	1b	93	VAL	2.9
44	1m	122	LYS	2.9
54	2y	53	G	2.9
1	2A	271(K)	U	2.9
33	1b	200	ILE	2.9
35	2d	158	ILE	2.9
42	2k	86	GLY	2.9
9	2N	82	LEU	2.9
40	1i	46	ALA	2.9
50	2s	37	ARG	2.9
52	2u	10	ARG	2.9
33	2b	135	GLN	2.9
1	2A	2164	C	2.9
54	1y	56	C	2.9
15	2T	28	VAL	2.9
21	2Z	98	MET	2.9
26	24	51	ASP	2.9
1	1A	1063	G	2.9
1	2A	2124	G	2.9
1	2A	2319	G	2.9
14	2S	35	ILE	2.9
34	2c	39	ILE	2.9
36	2e	45	PHE	2.9
54	1w	73	A	2.9
34	1c	47	LEU	2.9
44	1m	103	THR	2.9
52	2u	17	THR	2.9
33	1b	31	TYR	2.9
1	1A	2794	C	2.8
21	1Z	165	VAL	2.8
25	23	6	VAL	2.8
39	2h	131	GLY	2.8
41	2j	58	ASP	2.8
8	2I	35	LEU	2.8
11	2P	101	VAL	2.8
29	27	47	ARG	2.8
31	29	19	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	179	ARG	2.8
45	1n	34	TYR	2.8
48	2q	85	VAL	2.8
51	1t	38	LYS	2.8
36	2e	120	THR	2.8
39	1h	133	LEU	2.8
47	2p	74	LEU	2.8
1	1A	2119	A	2.8
7	2H	174	GLY	2.8
22	20	44	ARG	2.8
34	1c	148	GLY	2.8
34	2c	2	GLY	2.8
41	2j	35	SER	2.8
4	2E	167	VAL	2.8
35	1d	170	VAL	2.8
16	2U	17	ILE	2.8
21	2Z	171	ILE	2.8
32	2a	1006	C	2.8
33	2b	39	ILE	2.8
33	2b	40	HIS	2.8
51	1t	59	ALA	2.8
4	2E	195	LEU	2.8
33	2b	133	LYS	2.8
45	2n	15	LYS	2.8
50	1s	15	LEU	2.8
7	2H	95	ARG	2.8
40	2i	83	ARG	2.8
51	2t	23	ARG	2.8
47	1p	2	VAL	2.8
40	1i	125	TYR	2.8
33	1b	131	PRO	2.8
21	2Z	137	ILE	2.8
1	1A	897	C	2.8
12	2Q	59	ARG	2.8
33	2b	67	THR	2.8
14	2S	32	LEU	2.8
34	2c	204	LEU	2.8
51	1t	24	LEU	2.8
33	1b	48	MET	2.8
12	2Q	63	LYS	2.8
40	2i	116	LYS	2.8
1	2A	1113	U	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2116	G	2.8
1	2A	2895	U	2.8
32	1a	202	U	2.8
32	1a	1025	U	2.8
32	2a	1202	G	2.8
38	2g	32	ARG	2.8
39	2h	45	ILE	2.8
54	2w	45	U	2.8
33	1b	70	PHE	2.8
42	2k	89	ALA	2.8
51	2t	77	ALA	2.8
1	2A	2179	C	2.8
34	2c	33	LEU	2.8
40	1i	115	GLY	2.8
45	1n	39	LEU	2.8
40	2i	71	SER	2.8
34	1c	72	LYS	2.8
7	2H	26	VAL	2.8
34	1c	195	VAL	2.8
36	2e	105	VAL	2.8
1	2A	1847	A	2.8
40	2i	61	ALA	2.8
41	1j	20	ALA	2.8
1	1A	2802	G	2.8
1	2A	2161	C	2.8
7	2H	85	LYS	2.7
32	2a	1219	U	2.7
47	1p	38	TYR	2.7
52	2u	2	GLY	2.7
54	2y	59	U	2.7
40	2i	13	ALA	2.7
40	2i	122	ALA	2.7
34	2c	142	MET	2.7
12	2Q	102	VAL	2.7
33	2b	132	LYS	2.7
43	2l	55	VAL	2.7
10	2O	79	PHE	2.7
26	14	59	PHE	2.7
33	1b	148	TYR	2.7
33	2b	88	ALA	2.7
40	2i	101	PHE	2.7
24	22	60	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
51	2t	22	ARG	2.7
51	2t	79	ARG	2.7
41	1j	59	SER	2.7
29	27	48	LYS	2.7
9	2N	98	VAL	2.7
43	2l	58	VAL	2.7
7	2H	59	ARG	2.7
51	1t	83	ARG	2.7
22	20	60	PHE	2.7
33	2b	185	ILE	2.7
48	1q	36	ILE	2.7
8	2I	54	GLN	2.7
40	1i	58	HIS	2.7
23	21	28	GLY	2.7
1	2A	889	C	2.7
32	1a	345	C	2.7
33	2b	36	ARG	2.7
51	2t	86	ARG	2.7
1	1A	2166	G	2.7
1	1A	2792	G	2.7
32	1a	1456	G	2.7
47	1p	7	ALA	2.7
33	1b	11	LEU	2.7
34	2c	154	SER	2.7
36	2e	20	GLN	2.7
39	1h	6	ILE	2.7
47	2p	33	ILE	2.7
7	2H	61	HIS	2.7
41	2j	68	HIS	2.7
7	2H	8	PRO	2.7
11	2P	111	ARG	2.7
32	1a	1503	A	2.7
36	2e	10	MET	2.7
40	1i	9	ARG	2.7
34	1c	198	VAL	2.7
1	1A	1078	U	2.7
32	2a	204	U	2.7
34	2c	189	ALA	2.7
52	1u	8	THR	2.7
52	1u	17	THR	2.7
21	2Z	76	LEU	2.7
44	2m	4	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
46	1o	57	LEU	2.7
47	1p	19	ILE	2.7
7	2H	12	PRO	2.7
48	2q	33	GLY	2.7
7	2H	25	LYS	2.7
30	28	25	MET	2.7
40	1i	112	LYS	2.7
47	1p	48	TRP	2.7
1	2A	652(A)	A	2.7
34	2c	37	GLN	2.7
8	2I	19	VAL	2.7
21	2Z	100	VAL	2.7
1	2A	2167	U	2.7
32	2a	1037	C	2.7
45	1n	48	ALA	2.7
50	2s	48	THR	2.7
34	2c	186	PHE	2.7
40	1i	85	LEU	2.7
7	2H	62	LYS	2.7
18	1W	112	GLY	2.7
28	26	21	TYR	2.7
54	1y	34	G	2.7
34	1c	18	TRP	2.7
42	1k	42	TRP	2.7
6	2G	160	VAL	2.6
7	2H	16	SER	2.6
7	2H	68	THR	2.6
11	2P	89	ALA	2.6
35	2d	73	ARG	2.6
40	1i	120	ARG	2.6
51	2t	8	ARG	2.6
38	2g	24	THR	2.6
32	1a	1446	U	2.6
41	1j	55	LYS	2.6
33	1b	149	LEU	2.6
1	1A	2123	G	2.6
54	2y	44	G	2.6
26	14	58	ARG	2.6
9	2N	46	VAL	2.6
33	1b	15	VAL	2.6
9	2N	73	THR	2.6
14	2S	5	THR	2.6

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Mol	Chain	Res	Type	RSRZ
5	2F	134	GLY	2.6
33	1b	154	LEU	2.6
34	1c	196	LEU	2.6
21	2Z	48	PHE	2.6
50	2s	49	ILE	2.6
32	2a	1223	C	2.6
39	1h	5	PRO	2.6
51	2t	98	PRO	2.6
33	2b	220	ASP	2.6
33	1b	226	ARG	2.6
40	1i	121	ARG	2.6
42	1k	126	ARG	2.6
51	2t	74	LYS	2.6
5	2F	113	ALA	2.6
22	20	63	VAL	2.6
25	23	47	VAL	2.6
1	1A	271(K)	U	2.6
11	2P	148	LEU	2.6
33	1b	126	GLU	2.6
44	2m	66	LEU	2.6
4	2E	77	ILE	2.6
38	1g	32	ARG	2.6
40	1i	107	ARG	2.6
30	28	64	TYR	2.6
25	23	51	ALA	2.6
34	1c	68	VAL	2.6
34	1c	100	ALA	2.6
47	1p	62	VAL	2.6
1	2A	2109	U	2.6
1	2A	2148	G	2.6
34	1c	52	LEU	2.6
9	2N	85	ILE	2.6
34	2c	134	ILE	2.6
41	2j	29	ARG	2.6
51	1t	15	ARG	2.6
7	2H	83	TYR	2.6
47	1p	58	TYR	2.6
51	2t	30	LYS	2.6
25	23	25	ALA	2.6
38	2g	119	ARG	2.6
51	1t	67	ALA	2.6
7	2H	39	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
11	2P	62	LEU	2.6
28	26	36	LEU	2.6
48	1q	28	PRO	2.6
22	10	57	PHE	2.6
34	2c	124	ILE	2.6
34	2c	167	TRP	2.6
42	1k	125	PHE	2.6
50	1s	31	ILE	2.6
7	2H	86	GLU	2.6
32	1a	70	G	2.6
53	2v	23	A	2.6
33	2b	8	LYS	2.6
47	1p	39	TYR	2.6
50	2s	68	GLY	2.6
21	2Z	79	ARG	2.6
34	2c	172	ARG	2.6
52	2u	9	ARG	2.6
7	2H	79	VAL	2.6
7	2H	21	PRO	2.6
35	2d	64	LEU	2.6
39	2h	132	GLU	2.6
51	2t	84	LEU	2.6
3	2D	276	LYS	2.6
1	1A	2147	G	2.6
1	2A	2152	G	2.6
22	20	77	ARG	2.6
32	1a	93	G	2.6
32	1a	162	A	2.6
32	1a	1024	G	2.6
20	2Y	65	ALA	2.5
7	2H	19	VAL	2.5
44	2m	103	THR	2.5
11	2P	59	LEU	2.5
13	2R	4	LEU	2.5
31	29	17	ILE	2.5
39	2h	35	ILE	2.5
41	2j	33	GLN	2.5
44	1m	4	ILE	2.5
50	1s	40	ILE	2.5
51	2t	17	ARG	2.5
21	2Z	147	GLY	2.5
30	28	34	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2158	A	2.5
1	1A	2168	G	2.5
9	2N	5	VAL	2.5
51	1t	84	LEU	2.5
12	2Q	19	GLY	2.5
15	2T	76	PHE	2.5
33	2b	163	PHE	2.5
33	2b	140	HIS	2.5
20	2Y	5	MET	2.5
51	2t	14	LYS	2.5
32	1a	1037	C	2.5
33	1b	201	ILE	2.5
41	2j	54	PHE	2.5
43	2l	32	PHE	2.5
45	1n	50	LYS	2.5
51	1t	33	ILE	2.5
12	2Q	41	TRP	2.5
38	2g	40	ALA	2.5
43	2l	41	ARG	2.5
45	1n	12	ARG	2.5
4	2E	181	LEU	2.5
25	23	23	LEU	2.5
33	2b	197	VAL	2.5
1	2A	2172	U	2.5
50	2s	69	HIS	2.5
1	1A	2106	G	2.5
7	2H	151	ILE	2.5
34	1c	57	ILE	2.5
38	1g	42	ILE	2.5
34	2c	138	VAL	2.5
41	1j	72	VAL	2.5
41	2j	88	LEU	2.5
47	2p	79	VAL	2.5
32	2a	1040	U	2.5
31	29	26	ILE	2.5
32	2a	91	C	2.5
24	22	1	MET	2.5
38	1g	78	ARG	2.5
45	2n	17	LYS	2.5
7	2H	126	PRO	2.5
39	2h	135	CYS	2.5
8	2I	75	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
20	1Y	67	LEU	2.5
34	1c	188	LEU	2.5
34	2c	64	VAL	2.5
39	1h	112	LEU	2.5
45	2n	33	VAL	2.5
22	20	57	PHE	2.5
52	1u	13	ILE	2.5
1	1A	889	C	2.5
1	2A	2141	G	2.5
33	1b	134	GLU	2.5
33	2b	19	HIS	2.4
34	2c	196	LEU	2.4
51	2t	21	LYS	2.4
51	1t	70	SER	2.4
33	1b	55	PHE	2.4
33	2b	172	ILE	2.4
39	2h	111	ILE	2.4
1	1A	2158	A	2.4
32	1a	1157	A	2.4
32	2a	983	A	2.4
41	2j	73	ASP	2.4
32	2a	1452	C	2.4
55	2x	34	C	2.4
33	1b	227	GLY	2.4
34	2c	185	GLY	2.4
42	1k	88	GLY	2.4
34	1c	15	THR	2.4
34	2c	21	ARG	2.4
51	1t	32	ALA	2.4
51	1t	66	ALA	2.4
23	21	98	LEU	2.4
32	2a	1023	G	2.4
51	2t	20	LEU	2.4
28	16	5	VAL	2.4
1	1A	2130	U	2.4
5	2F	90	PHE	2.4
38	2g	120	ILE	2.4
1	1A	1103	A	2.4
1	1A	2169	A	2.4
6	2G	136	ARG	2.4
11	2P	39	LYS	2.4
11	2P	81	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
40	2i	42	ARG	2.4
1	1A	2107	C	2.4
1	1A	2136	C	2.4
1	2A	2107	C	2.4
32	2a	1192	C	2.4
21	2Z	70	LEU	2.4
11	2P	83	VAL	2.4
7	2H	57	ASP	2.4
32	1a	90	U	2.4
34	1c	48	TYR	2.4
48	2q	95	TYR	2.4
12	2Q	18	LYS	2.4
12	2Q	22	LYS	2.4
54	2y	15	G	2.4
11	2P	15	ARG	2.4
35	2d	75	PHE	2.4
47	1p	25	ARG	2.4
50	1s	74	PHE	2.4
23	21	63	ALA	2.4
33	2b	47	THR	2.4
34	2c	53	ALA	2.4
51	2t	12	ALA	2.4
1	2A	2175	C	2.4
21	2Z	150	LEU	2.4
36	2e	31	LEU	2.4
4	2E	104	VAL	2.4
34	1c	207	VAL	2.4
39	2h	19	VAL	2.4
40	1i	17	VAL	2.4
43	2l	101	VAL	2.4
48	2q	23	VAL	2.4
7	2H	60	ARG	2.4
35	1d	122	ARG	2.4
41	2j	9	ARG	2.4
21	2Z	99	TYR	2.4
11	1P	44	GLY	2.4
28	26	20	ASN	2.4
35	2d	90	GLY	2.4
44	2m	119	GLY	2.4
1	2A	2168	G	2.4
15	2T	60	THR	2.4
38	2g	25	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
10	2O	81	ASP	2.4
43	2l	28	LYS	2.4
32	2a	1007	C	2.4
32	2a	1248	A	2.4
48	2q	22	LEU	2.4
50	2s	81	ARG	2.4
9	2N	69	GLN	2.4
39	2h	93	VAL	2.4
4	2E	6	GLY	2.4
34	1c	2	GLY	2.4
35	1d	138	TYR	2.4
35	1d	207	TYR	2.4
21	2Z	164	ALA	2.4
1	2A	11	G	2.4
31	29	11	CYS	2.4
32	2a	1068	G	2.4
7	2H	80	SER	2.4
35	1d	3	ARG	2.4
8	2I	9	LEU	2.4
14	1S	4	LEU	2.4
1	1A	2804	C	2.4
1	2A	2143	C	2.4
4	2E	7	VAL	2.4
7	2H	74	ASN	2.4
11	2P	125	VAL	2.4
32	2a	1119	C	2.4
41	2j	94	VAL	2.4
51	2t	29	LYS	2.4
7	2H	162	ILE	2.4
36	1e	128	PRO	2.4
33	1b	120	ALA	2.4
35	2d	168	ARG	2.4
33	1b	78	GLN	2.4
38	1g	24	THR	2.4
47	1p	65	GLN	2.4
7	2H	63	SER	2.4
9	2N	67	LEU	2.4
47	1p	49	LEU	2.4
51	1t	43	LEU	2.4
32	1a	66	G	2.3
32	2a	1061	G	2.3
43	1l	23	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	55	VAL	2.3
34	2c	153	VAL	2.3
45	1n	25	VAL	2.3
21	2Z	130	PRO	2.3
38	1g	153	HIS	2.3
41	2j	41	PRO	2.3
12	2Q	65	PHE	2.3
28	26	50	ARG	2.3
34	2c	190	ARG	2.3
43	2l	7	ILE	2.3
40	1i	36	TYR	2.3
40	1i	45	ALA	2.3
47	2p	77	ALA	2.3
30	28	26	LYS	2.3
4	2E	49	LEU	2.3
36	1e	22	GLY	2.3
40	1i	96	LEU	2.3
32	1a	220	G	2.3
32	1a	1186	G	2.3
9	2N	44	PRO	2.3
32	2a	961	U	2.3
40	2i	107	ARG	2.3
15	2T	1	MET	2.3
1	1A	1054	A	2.3
1	1A	2175	C	2.3
32	1a	344	A	2.3
33	2b	95	GLN	2.3
34	2c	202	ILE	2.3
35	2d	146	ILE	2.3
41	1j	64	GLU	2.3
40	1i	18	PHE	2.3
45	1n	36	PHE	2.3
45	1n	15	LYS	2.3
40	2i	69	GLY	2.3
13	2R	65	LEU	2.3
34	2c	32	LEU	2.3
34	2c	34	LEU	2.3
38	1g	16	LEU	2.3
38	1g	124	LEU	2.3
31	29	9	ARG	2.3
12	2Q	27	VAL	2.3
33	1b	71	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	174	PRO	2.3
39	2h	86	ILE	2.3
47	1p	36	ILE	2.3
40	1i	101	PHE	2.3
1	2A	2135	A	2.3
13	2R	21	TYR	2.3
32	1a	160	A	2.3
46	2o	69	TYR	2.3
7	2H	31	GLY	2.3
12	2Q	33	GLY	2.3
47	2p	69	THR	2.3
52	1u	11	GLY	2.3
34	2c	40	ARG	2.3
38	1g	3	ARG	2.3
40	1i	102	LEU	2.3
51	1t	79	ARG	2.3
3	1D	38	LYS	2.3
17	2V	74	LYS	2.3
40	1i	70	LYS	2.3
40	2i	117	HIS	2.3
45	1n	49	HIS	2.3
15	2T	70	VAL	2.3
27	15	60	VAL	2.3
3	2D	270	ILE	2.3
15	2T	50	ILE	2.3
20	2Y	75	ILE	2.3
21	1Z	120	ILE	2.3
33	2b	223	ILE	2.3
45	1n	7	ILE	2.3
1	1A	1076	C	2.3
11	2P	102	ARG	2.3
36	2e	99	GLY	2.3
1	1A	1084	A	2.3
1	2A	887	A	2.3
32	2a	998	G	2.3
32	2a	1092	A	2.3
32	2a	1287	A	2.3
54	2y	65	G	2.3
21	2Z	50	GLN	2.3
34	2c	28	GLN	2.3
49	1r	79	LEU	2.3
7	2H	168	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
6	2G	159	VAL	2.3
7	2H	144	VAL	2.3
21	2Z	47	VAL	2.3
33	1b	97	TRP	2.3
12	2Q	64	ILE	2.3
30	28	58	ILE	2.3
30	28	18	ALA	2.3
40	1i	64	THR	2.3
51	1t	64	ASP	2.3
14	2S	92	TYR	2.3
32	1a	163	C	2.3
32	1a	217	C	2.3
32	2a	1112	C	2.3
5	2F	32	LEU	2.3
11	2P	105	LEU	2.3
22	20	62	LEU	2.3
1	2A	881	G	2.3
1	2A	1114	G	2.3
32	1a	216	G	2.3
32	2a	965	A	2.3
21	1Z	169	GLU	2.3
35	2d	49	ARG	2.3
39	2h	26	VAL	2.3
40	2i	26	VAL	2.3
1	1A	2172	U	2.3
41	1j	60	ARG	2.3
12	2Q	72	LYS	2.3
30	28	15	LYS	2.3
36	2e	109	ILE	2.3
12	2Q	121	ALA	2.3
30	28	55	ALA	2.3
33	1b	163	PHE	2.3
33	2b	188	ALA	2.3
34	2c	65	ALA	2.3
4	2E	105	THR	2.3
34	2c	177	THR	2.3
51	1t	71	THR	2.3
51	2t	16	HIS	2.3
12	2Q	37	LEU	2.3
21	2Z	163	LEU	2.3
25	23	28	LEU	2.3
32	1a	470	C	2.3

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Mol	Chain	Res	Type	RSRZ
34	1c	43	LEU	2.3
1	1A	229	A	2.2
1	1A	2062	A	2.2
11	2P	107	LYS	2.2
12	1Q	6	ARG	2.2
12	2Q	5	ARG	2.2
32	1a	171	A	2.2
32	1a	197	A	2.2
38	1g	155	ARG	2.2
38	2g	155	ARG	2.2
40	1i	78	LYS	2.2
1	1A	1089	G	2.2
1	1A	2116	G	2.2
7	2H	15	VAL	2.2
7	2H	135	GLY	2.2
31	19	25	VAL	2.2
39	2h	129	VAL	2.2
38	1g	86	GLN	2.2
41	2j	21	GLN	2.2
52	1u	2	GLY	2.2
52	2u	11	GLY	2.2
26	24	66	SER	2.2
33	2b	233	SER	2.2
8	2I	79	ILE	2.2
12	1Q	44	ALA	2.2
20	2Y	38	ILE	2.2
36	2e	84	PHE	2.2
38	2g	147	ALA	2.2
40	1i	61	ALA	2.2
7	2H	167	GLU	2.2
7	2H	138	LYS	2.2
19	1X	95	LEU	2.2
22	20	46	LYS	2.2
33	1b	138	LEU	2.2
32	2a	218	C	2.2
32	1a	161	A	2.2
38	2g	13	GLN	2.2
53	1v	13	A	2.2
1	2A	9	U	2.2
11	2P	94	GLU	2.2
33	1b	50	GLU	2.2
54	2y	52	G	2.2

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Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	2.2
34	1c	113	ALA	2.2
40	2i	55	ALA	2.2
8	1I	40	THR	2.2
41	1j	66	ARG	2.2
47	2p	18	ARG	2.2
51	2t	80	ARG	2.2
44	2m	64	TRP	2.2
11	2P	78	PRO	2.2
44	2m	97	PRO	2.2
34	2c	181	ASN	2.2
7	2H	14	GLY	2.2
1	1A	2142	C	2.2
1	2A	2137	C	2.2
9	2N	84	LYS	2.2
54	1y	58	A	2.2
48	2q	65	ILE	2.2
20	2Y	60	PHE	2.2
32	1a	1368	G	2.2
54	1w	70	G	2.2
13	2R	10	LEU	2.2
20	2Y	90	LEU	2.2
31	29	30	PRO	2.2
36	2e	133	TYR	2.2
22	20	67	VAL	2.2
45	1n	41	ARG	2.2
54	1w	2	C	2.2
21	2Z	57	ILE	2.2
32	2a	1093	A	2.2
36	2e	131	ILE	2.2
39	1h	86	ILE	2.2
33	1b	17	PHE	2.2
9	2N	45	ASN	2.2
14	2S	33	LYS	2.2
41	2j	37	PRO	2.2
41	2j	52	GLY	2.2
47	2p	73	LEU	2.2
21	2Z	72	ARG	2.2
31	29	24	TYR	2.2
33	2b	24	TRP	2.2
12	2Q	97	VAL	2.2
16	2U	8	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2142	C	2.2
31	29	28	GLU	2.2
32	2a	1122	U	2.2
38	1g	11	GLN	2.2
40	2i	46	ALA	2.2
45	2n	20	ALA	2.2
33	2b	162	ILE	2.2
7	2H	142	GLY	2.2
40	1i	56	LEU	2.2
47	1p	66	PRO	2.2
34	2c	59	ARG	2.2
41	2j	45	ARG	2.2
42	1k	91	ARG	2.2
48	2q	32	TYR	2.2
43	2l	68	ALA	2.2
32	2a	1043	C	2.2
41	2j	12	ASP	2.2
54	1w	74	C	2.2
45	2n	19	ARG	2.2
11	2P	6	LEU	2.2
19	2X	92	LEU	2.2
34	2c	87	LEU	2.2
10	1O	112	MET	2.1
34	1c	201	TYR	2.1
42	2k	59	TYR	2.1
48	2q	42	TYR	2.1
52	1u	21	TYR	2.1
4	2E	150	VAL	2.1
10	2O	102	VAL	2.1
15	2T	72	VAL	2.1
17	2V	5	VAL	2.1
32	2a	79	G	2.1
34	1c	168	ALA	2.1
7	2H	22	GLY	2.1
33	1b	228	GLY	2.1
34	1c	171	GLY	2.1
36	2e	76	ILE	2.1
41	1j	10	GLY	2.1
44	2m	102	ARG	2.1
8	2I	4	ILE	2.1
43	2l	85	ILE	2.1
51	2t	71	THR	2.1

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Mol	Chain	Res	Type	RSRZ
12	2Q	39	PRO	2.1
21	2Z	136	PHE	2.1
39	2h	36	LEU	2.1
1	1A	1070	A	2.1
1	1A	2176	A	2.1
53	2v	14	A	2.1
12	1Q	59	ARG	2.1
5	2F	166	ALA	2.1
6	2G	169	ALA	2.1
16	1U	9	VAL	2.1
16	2U	67	ALA	2.1
32	2a	202	U	2.1
34	2c	63	ASN	2.1
41	2j	93	GLY	2.1
43	2l	56	ALA	2.1
51	1t	76	ALA	2.1
1	1A	2148	G	2.1
1	1A	2160	G	2.1
15	2T	102	ILE	2.1
20	2Y	54	LYS	2.1
32	2a	1154	G	2.1
8	2I	30	LEU	2.1
21	2Z	102	LEU	2.1
43	2l	60	LEU	2.1
44	2m	70	LEU	2.1
49	1r	78	LEU	2.1
51	1t	18	GLN	2.1
1	1A	886	C	2.1
14	2S	43	GLU	2.1
32	2a	977	A	2.1
36	2e	24	ARG	2.1
52	1u	15	ARG	2.1
22	20	65	GLY	2.1
5	2F	193	VAL	2.1
7	2H	90	LYS	2.1
11	2P	93	GLY	2.1
20	2Y	42	VAL	2.1
22	10	38	VAL	2.1
22	20	79	VAL	2.1
33	2b	74	LYS	2.1
41	2j	20	ALA	2.1
43	1l	64	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
43	2l	69	TYR	2.1
44	2m	7	VAL	2.1
54	2y	33	U	2.1
10	2O	19	ILE	2.1
38	1g	13	GLN	2.1
41	1j	38	ILE	2.1
6	1G	152	LEU	2.1
15	1T	114	LEU	2.1
50	2s	15	LEU	2.1
1	1A	2127	G	2.1
1	2A	100	G	2.1
13	2R	14	SER	2.1
32	2a	485	G	2.1
32	2a	1356	G	2.1
1	2A	2140	C	2.1
32	1a	67	C	2.1
32	2a	1045	C	2.1
47	1p	68	ASP	2.1
6	2G	75	LYS	2.1
50	2s	82	GLY	2.1
3	2D	18	VAL	2.1
5	2F	37	VAL	2.1
10	1O	115	VAL	2.1
33	2b	77	ALA	2.1
7	2H	154	PRO	2.1
7	2H	18	GLU	2.1
26	24	59	PHE	2.1
33	2b	23	ARG	2.1
34	1c	101	LEU	2.1
39	2h	39	LEU	2.1
41	1j	65	LEU	2.1
45	2n	47	LEU	2.1
47	2p	6	LEU	2.1
23	21	38	SER	2.1
50	2s	53	ASN	2.1
1	1A	2133	G	2.1
9	2N	105	GLY	2.1
32	1a	1118	C	2.1
32	2a	980	C	2.1
32	2a	1018	C	2.1
4	2E	28	ALA	2.1
1	1A	2135	A	2.1

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Mol	Chain	Res	Type	RSRZ
6	2G	92	VAL	2.1
26	24	57	GLU	2.1
32	1a	1005	A	2.1
7	2H	97	ARG	2.1
39	1h	3	THR	2.1
39	2h	17	THR	2.1
7	2H	172	LYS	2.1
33	2b	200	ILE	2.1
5	2F	24	LEU	2.1
6	2G	133	LEU	2.1
35	1d	110	PHE	2.1
49	2r	26	LEU	2.1
18	2W	60	ASN	2.1
26	14	17	GLY	2.1
41	1j	93	GLY	2.1
14	2S	84	GLN	2.1
41	1j	97	GLU	2.1
15	2T	111	ARG	2.1
21	2Z	156	LYS	2.1
35	1d	76	ARG	2.1
51	1t	25	ARG	2.1
51	2t	58	LYS	2.1
9	2N	9	VAL	2.1
32	1a	1196	U	2.1
33	1b	190	THR	2.1
38	1g	91	VAL	2.1
44	2m	15	VAL	2.1
44	2m	105	THR	2.1
51	2t	88	VAL	2.1
53	2v	13	A	2.1
11	2P	88	LEU	2.1
14	2S	4	LEU	2.1
21	2Z	157	LEU	2.1
30	28	32	LEU	2.1
35	1d	101	LEU	2.1
41	1j	54	PHE	2.1
11	2P	38	GLN	2.1
51	2t	90	GLN	2.1
11	2P	92	GLU	2.1
25	23	35	ARG	2.1
28	16	28	ARG	2.1
33	1b	147	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	11	ARG	2.1
38	1g	115	ARG	2.1
41	2j	57	LYS	2.1
19	2X	1	MET	2.0
8	2I	100	ALA	2.0
32	2a	962	C	2.0
33	2b	186	ALA	2.0
35	1d	136	PRO	2.0
51	1t	40	ALA	2.0
21	2Z	161	VAL	2.0
34	1c	66	VAL	2.0
35	2d	148	VAL	2.0
43	2l	90	VAL	2.0
50	1s	33	THR	2.0
1	2A	1042	G	2.0
32	2a	1026	G	2.0
42	1k	75	TYR	2.0
54	1y	57	G	2.0
1	2A	2758	A	2.0
17	2V	35	LEU	2.0
11	2P	82	GLY	2.0
32	2a	1225	A	2.0
33	2b	141	GLU	2.0
34	1c	32	LEU	2.0
47	2p	65	GLN	2.0
6	2G	182	LYS	2.0
41	1j	39	PRO	2.0
47	1p	24	ALA	2.0
1	1A	614(A)	U	2.0
1	1A	2137	C	2.0
32	1a	1137	C	2.0
44	2m	60	VAL	2.0
51	1t	16	HIS	2.0
24	22	8	LYS	2.0
9	1N	116	LEU	2.0
14	1S	48	LEU	2.0
14	2S	48	LEU	2.0
15	2T	6	LEU	2.0
18	1W	92	ARG	2.0
23	11	76	ARG	2.0
33	2b	115	LEU	2.0
35	2d	206	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
54	2y	63	G	2.0
38	1g	20	ASP	2.0
10	2O	1	MET	2.0
11	2P	97	PRO	2.0
33	2b	101	MET	2.0
8	2I	104	GLN	2.0
10	2O	76	ALA	2.0
14	2S	51	ALA	2.0
40	2i	52	ALA	2.0
45	1n	59	ALA	2.0
47	1p	22	THR	2.0
51	1t	29	LYS	2.0
51	2t	81	LYS	2.0
8	2I	92	VAL	2.0
21	1Z	139	VAL	2.0
31	19	16	VAL	2.0
37	1f	6	VAL	2.0
14	2S	17	ARG	2.0
11	2P	100	LEU	2.0
18	2W	6	ILE	2.0
33	2b	42	ILE	2.0
54	2y	48	C	2.0
15	2T	45	PHE	2.0
33	2b	205	ASP	2.0
1	1A	883	G	2.0
32	2a	1191	A	2.0
54	2w	44	G	2.0
54	2y	64	A	2.0
29	17	1	MET	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	G7M	1y	46	24/25	0.76	0.22	84,96,103,119	0
54	G7M	2y	46	24/25	0.76	0.20	96,100,104,123	0
54	G7M	1w	46	24/25	0.77	0.20	78,90,109,132	0
54	PSU	1y	55	20/21	0.78	0.30	92,99,105,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	2y	55	20/21	0.78	0.34	92,102,113,117	0
54	4SU	2w	8	20/21	0.79	0.17	86,94,103,115	0
54	G7M	2w	46	24/25	0.80	0.20	85,96,111,121	0
54	5MU	2y	54	21/22	0.82	0.27	88,94,104,118	0
54	5MU	1y	54	21/22	0.82	0.29	88,93,102,111	0
54	MIA	2y	37	22/30	0.83	0.26	85,91,97,107	0
54	PSU	2y	32	20/21	0.83	0.22	84,89,98,101	0
54	4SU	1y	8	20/21	0.84	0.16	91,94,105,106	0
54	4SU	2y	8	20/21	0.85	0.15	93,99,109,120	0
54	PSU	2y	39	20/21	0.87	0.22	86,90,99,105	0
54	PSU	1w	55	20/21	0.88	0.20	61,77,81,85	0
54	PSU	1y	39	20/21	0.88	0.20	83,86,92,99	0
54	PSU	2w	55	20/21	0.89	0.16	79,88,95,101	0
54	PSU	1y	32	20/21	0.89	0.24	80,86,93,94	0
54	MIA	2w	37	25/30	0.90	0.23	67,77,83,100	0
55	PSU	2x	55	20/21	0.90	0.17	68,74,83,92	0
54	MIA	1y	37	22/30	0.90	0.21	80,88,92,96	0
43	0TD	2l	92	10/11	0.91	0.16	62,65,71,79	0
32	2MG	2a	1207	24/25	0.92	0.18	77,86,89,89	0
54	5MU	2w	54	21/22	0.92	0.15	73,80,83,90	0
54	4SU	1w	8	20/21	0.92	0.16	77,84,90,93	0
55	4SU	2x	8	20/21	0.92	0.14	77,81,85,87	0
54	PSU	2w	39	20/21	0.93	0.23	70,79,84,85	0
55	5MU	2x	54	21/22	0.93	0.20	73,78,84,92	0
32	PSU	2a	516	20/21	0.93	0.14	67,73,77,77	0
54	PSU	2w	32	20/21	0.93	0.22	76,83,92,96	0
32	5MC	2a	967	21/22	0.93	0.21	66,71,78,82	0
1	PSU	2A	1917	20/21	0.93	0.15	57,66,72,73	0
54	MIA	1w	37	29/30	0.94	0.31	44,56,68,91	0
43	0TD	1l	92	10/11	0.94	0.15	48,54,56,67	0
32	G7M	2a	527	24/25	0.94	0.15	60,64,70,83	0
32	M2G	2a	966	25/26	0.94	0.27	65,69,79,83	0
1	5MU	2A	1915	21/22	0.94	0.16	60,67,70,77	0
54	PSU	1w	32	20/21	0.94	0.21	59,65,72,74	0
32	MA6	2a	1519	24/25	0.95	0.21	58,66,69,74	0
54	5MU	1w	54	21/22	0.95	0.15	53,68,73,74	0
32	2MG	1a	1207	24/25	0.95	0.13	63,69,74,75	0
55	5MC	1x	32	21/22	0.95	0.20	50,57,60,74	0
55	PSU	1x	55	20/21	0.95	0.15	56,62,68,71	0
1	PSU	2A	1911	20/21	0.95	0.17	57,60,65,66	0
32	5MC	2a	1400	21/22	0.95	0.29	68,73,78,85	0
32	4OC	2a	1402	22/23	0.95	0.19	56,66,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMC	2A	1920	21/22	0.95	0.18	52,61,64,68	0
1	5MC	2A	1962	21/22	0.95	0.21	40,49,58,64	0
54	PSU	1w	39	20/21	0.96	0.19	58,63,70,77	0
55	5MC	2x	32	21/22	0.96	0.20	66,74,78,86	0
55	4SU	1x	8	20/21	0.96	0.16	48,64,70,76	0
32	5MC	2a	1404	21/22	0.96	0.17	52,60,63,65	0
1	5MU	1A	1915	21/22	0.96	0.17	52,59,62,64	0
32	UR3	2a	1498	21/22	0.96	0.22	57,64,66,67	0
1	PSU	1A	1917	20/21	0.96	0.16	46,55,59,59	0
32	MA6	2a	1518	24/25	0.96	0.19	58,67,71,73	0
32	5MC	1a	967	21/22	0.96	0.24	49,54,60,62	0
32	PSU	1a	516	20/21	0.96	0.16	54,60,66,66	0
1	PSU	1A	1911	20/21	0.97	0.20	43,48,57,58	0
32	4OC	1a	1402	22/23	0.97	0.19	43,47,51,57	0
55	31H	1x	76	32/33	0.97	0.20	25,34,43,47	10
32	5MC	2a	1407	21/22	0.97	0.19	53,58,61,64	0
32	MA6	1a	1519	24/25	0.97	0.18	39,44,49,53	0
32	G7M	1a	527	24/25	0.97	0.19	43,49,56,60	0
55	5MU	1x	54	21/22	0.97	0.14	60,66,72,74	0
1	5MC	1A	1942	21/22	0.97	0.20	38,46,51,53	0
1	5MC	2A	1942	21/22	0.97	0.19	54,57,63,64	0
55	31H	2x	76	32/33	0.97	0.24	44,50,56,60	0
1	OMG	2A	2251	24/25	0.97	0.21	43,47,50,54	0
1	2MU	2A	2552	21/23	0.97	0.20	41,48,52,60	0
1	PSU	2A	2605	20/21	0.97	0.19	39,46,49,51	0
32	MA6	1a	1518	24/25	0.98	0.21	36,43,46,47	0
1	5MU	1A	1939	21/22	0.98	0.19	30,35,39,39	0
1	5MU	2A	1939	21/22	0.98	0.20	35,39,47,49	0
32	5MC	1a	1400	21/22	0.98	0.19	46,52,58,62	0
32	M2G	1a	966	25/26	0.98	0.21	47,54,57,67	0
1	5MC	1A	1962	21/22	0.98	0.19	30,40,43,46	0
32	5MC	1a	1404	21/22	0.98	0.18	35,42,47,48	0
1	OMG	1A	2251	24/25	0.98	0.21	26,29,31,34	0
32	5MC	1a	1407	21/22	0.98	0.20	36,42,48,49	0
1	8AH	2A	2503	24/25	0.98	0.22	36,43,48,52	0
32	UR3	1a	1498	21/22	0.98	0.19	39,44,47,49	0
1	PSU	1A	2605	20/21	0.98	0.20	27,31,35,36	0
1	OMC	1A	1920	21/22	0.98	0.18	38,48,55,59	0
1	2MU	1A	2552	21/23	0.99	0.22	27,31,34,38	0
1	8AH	1A	2503	24/25	0.99	0.23	19,29,34,38	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, 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
56	MG	2A	3006	1/1	0.41	0.26	68,68,68,68	0
56	MG	1A	3984	1/1	0.43	0.13	78,78,78,78	0
56	MG	1A	3990	1/1	0.45	0.41	66,66,66,66	0
56	MG	2a	1681	1/1	0.47	0.14	73,73,73,73	0
56	MG	2A	3732	1/1	0.49	0.12	83,83,83,83	0
56	MG	2A	3522	1/1	0.49	0.22	70,70,70,70	0
56	MG	2A	3266	1/1	0.52	0.31	75,75,75,75	0
56	MG	2F	307	1/1	0.53	0.27	68,68,68,68	0
56	MG	1A	3627	1/1	0.53	0.11	58,58,58,58	0
56	MG	2A	3829	1/1	0.54	0.48	69,69,69,69	0
56	MG	1A	3377	1/1	0.54	0.26	71,71,71,71	0
56	MG	1A	3669	1/1	0.54	0.25	38,38,38,38	0
56	MG	1A	3544	1/1	0.55	0.23	60,60,60,60	0
56	MG	1A	3331	1/1	0.55	0.76	64,64,64,64	0
56	MG	1A	3425	1/1	0.55	0.41	61,61,61,61	0
56	MG	1a	1745	1/1	0.57	0.25	83,83,83,83	0
56	MG	1A	3539	1/1	0.57	0.30	54,54,54,54	0
56	MG	2A	3360	1/1	0.58	0.19	73,73,73,73	0
56	MG	1A	3241	1/1	0.58	0.16	67,67,67,67	0
56	MG	2A	3282	1/1	0.58	0.31	65,65,65,65	0
56	MG	2A	3401	1/1	0.59	0.17	81,81,81,81	0
56	MG	2A	3224	1/1	0.59	0.42	61,61,61,61	0
56	MG	1A	3979	1/1	0.59	0.19	74,74,74,74	0
56	MG	2A	3556	1/1	0.60	0.21	37,37,37,37	0
56	MG	18	105	1/1	0.60	0.25	68,68,68,68	0
56	MG	2A	3380	1/1	0.60	0.32	66,66,66,66	0
56	MG	1A	3915	1/1	0.60	0.16	49,49,49,49	0
56	MG	1A	4022	1/1	0.60	0.17	61,61,61,61	0
56	MG	1A	3891	1/1	0.61	0.11	57,57,57,57	0
56	MG	1A	3996	1/1	0.61	0.12	58,58,58,58	0
56	MG	2A	3453	1/1	0.61	0.12	73,73,73,73	0
56	MG	1A	3461	1/1	0.62	0.34	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3382	1/1	0.62	0.20	86,86,86,86	0
56	MG	1A	3905	1/1	0.62	0.18	66,66,66,66	0
56	MG	2G	201	1/1	0.62	0.14	72,72,72,72	0
56	MG	20	101	1/1	0.62	0.22	76,76,76,76	0
56	MG	2A	3663	1/1	0.62	0.09	73,73,73,73	0
56	MG	2A	3597	1/1	0.63	0.12	88,88,88,88	0
56	MG	1A	3914	1/1	0.63	0.15	61,61,61,61	0
56	MG	2v	102	1/1	0.63	0.23	78,78,78,78	0
56	MG	2A	3027	1/1	0.64	0.40	76,76,76,76	0
56	MG	2A	3210	1/1	0.64	0.27	68,68,68,68	0
56	MG	1G	3603	1/1	0.64	0.16	64,64,64,64	0
56	MG	1a	1762	1/1	0.64	0.11	66,66,66,66	0
56	MG	1A	3821	1/1	0.64	0.15	60,60,60,60	0
56	MG	28	102	1/1	0.65	0.19	72,72,72,72	0
56	MG	2a	1604	1/1	0.65	0.23	74,74,74,74	0
56	MG	1A	3833	1/1	0.65	0.25	57,57,57,57	0
56	MG	2a	1739	1/1	0.65	0.21	78,78,78,78	0
56	MG	1P	206	1/1	0.65	0.32	55,55,55,55	0
56	MG	2A	3375	1/1	0.66	0.26	57,57,57,57	0
56	MG	2A	3082	1/1	0.66	0.26	60,60,60,60	0
56	MG	1F	313	1/1	0.66	0.37	59,59,59,59	0
56	MG	1A	3313	1/1	0.66	0.20	64,64,64,64	0
56	MG	1A	3910	1/1	0.66	0.11	71,71,71,71	0
56	MG	2A	3281	1/1	0.66	0.27	72,72,72,72	0
56	MG	1A	3444	1/1	0.66	0.26	66,66,66,66	0
56	MG	2a	1732	1/1	0.66	0.16	84,84,84,84	0
56	MG	2A	3320	1/1	0.66	0.30	70,70,70,70	0
56	MG	2t	201	1/1	0.66	0.10	57,57,57,57	0
56	MG	2v	101	1/1	0.66	0.19	69,69,69,69	0
56	MG	2A	3064	1/1	0.66	0.13	71,71,71,71	0
56	MG	1a	1764	1/1	0.67	0.15	83,83,83,83	0
56	MG	2A	3534	1/1	0.67	0.36	87,87,87,87	0
56	MG	1A	3173	1/1	0.67	0.23	52,52,52,52	0
56	MG	1A	3569	1/1	0.67	0.21	72,72,72,72	0
56	MG	1A	3800	1/1	0.67	0.19	62,62,62,62	0
56	MG	2A	3506	1/1	0.67	0.23	41,41,41,41	0
56	MG	1A	3466	1/1	0.68	0.23	57,57,57,57	0
56	MG	2A	3043	1/1	0.68	0.19	74,74,74,74	0
56	MG	2A	3747	1/1	0.68	0.19	59,59,59,59	0
56	MG	1a	1678	1/1	0.68	0.12	75,75,75,75	0
56	MG	1A	3237	1/1	0.68	0.18	71,71,71,71	0
56	MG	2A	3773	1/1	0.69	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	3821	1/1	0.69	0.14	65,65,65,65	0
56	MG	1A	3937	1/1	0.69	0.49	83,83,83,83	0
56	MG	2A	3261	1/1	0.69	0.22	66,66,66,66	0
56	MG	1A	3958	1/1	0.69	0.11	54,54,54,54	0
56	MG	1a	1629	1/1	0.69	0.27	70,70,70,70	0
56	MG	1a	1668	1/1	0.69	0.53	56,56,56,56	0
56	MG	1A	3976	1/1	0.69	0.19	50,50,50,50	0
56	MG	2A	3324	1/1	0.69	0.31	81,81,81,81	0
56	MG	2A	3642	1/1	0.69	0.16	78,78,78,78	0
56	MG	1A	3546	1/1	0.69	0.57	51,51,51,51	0
56	MG	2a	1792	1/1	0.69	0.13	61,61,61,61	0
56	MG	2a	1802	1/1	0.69	0.13	80,80,80,80	0
56	MG	2A	3671	1/1	0.69	0.20	60,60,60,60	0
56	MG	2A	3167	1/1	0.69	0.13	82,82,82,82	0
56	MG	1A	3395	1/1	0.69	0.31	58,58,58,58	0
56	MG	1x	116	1/1	0.70	0.16	82,82,82,82	0
56	MG	2a	1691	1/1	0.70	0.12	73,73,73,73	0
56	MG	2B	216	1/1	0.70	0.14	69,69,69,69	0
56	MG	2A	3070	1/1	0.70	0.28	67,67,67,67	0
56	MG	1A	3772	1/1	0.70	0.47	59,59,59,59	0
56	MG	2A	3062	1/1	0.70	0.22	66,66,66,66	0
56	MG	2A	3409	1/1	0.70	0.40	74,74,74,74	0
56	MG	2A	3335	1/1	0.70	0.25	78,78,78,78	0
56	MG	2a	1617	1/1	0.70	0.30	68,68,68,68	0
56	MG	2y	105	1/1	0.70	0.07	86,86,86,86	0
56	MG	1A	3386	1/1	0.71	0.21	69,69,69,69	0
56	MG	1A	3797	1/1	0.71	0.20	45,45,45,45	0
56	MG	2A	3219	1/1	0.71	0.42	62,62,62,62	0
56	MG	1a	1743	1/1	0.71	0.13	71,71,71,71	0
56	MG	1A	3020	1/1	0.71	0.24	59,59,59,59	0
56	MG	1A	3252	1/1	0.71	0.17	62,62,62,62	0
56	MG	1A	3710	1/1	0.71	0.16	78,78,78,78	0
56	MG	2A	3696	1/1	0.71	0.14	45,45,45,45	0
56	MG	1A	3864	1/1	0.71	0.13	52,52,52,52	0
56	MG	2A	3134	1/1	0.71	0.14	68,68,68,68	0
56	MG	1A	4027	1/1	0.72	0.20	52,52,52,52	0
56	MG	2a	1680	1/1	0.72	0.13	72,72,72,72	0
56	MG	2A	3588	1/1	0.72	0.32	59,59,59,59	0
56	MG	2A	3292	1/1	0.72	0.17	74,74,74,74	0
56	MG	2B	214	1/1	0.72	0.17	68,68,68,68	0
56	MG	1F	309	1/1	0.72	0.19	54,54,54,54	0
56	MG	1A	3390	1/1	0.72	0.33	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	2A	3469	1/1	0.72	0.14	43,43,43,43	0
56	MG	2A	3098	1/1	0.72	0.10	79,79,79,79	0
56	MG	1a	1658	1/1	0.72	0.20	70,70,70,70	0
56	MG	1A	3994	1/1	0.72	0.17	63,63,63,63	0
56	MG	2w	103	1/1	0.72	0.09	74,74,74,74	0
56	MG	2a	1613	1/1	0.72	0.14	70,70,70,70	0
56	MG	2A	3608	1/1	0.73	0.41	72,72,72,72	0
56	MG	1A	3454	1/1	0.73	0.40	59,59,59,59	0
56	MG	1A	3479	1/1	0.73	0.38	57,57,57,57	0
56	MG	1A	3198	1/1	0.73	0.10	62,62,62,62	0
56	MG	1A	3751	1/1	0.73	0.13	42,42,42,42	0
56	MG	2a	1771	1/1	0.73	0.15	71,71,71,71	0
56	MG	1a	1706	1/1	0.73	0.12	74,74,74,74	0
56	MG	1A	3619	1/1	0.73	0.24	51,51,51,51	0
56	MG	2A	3759	1/1	0.73	0.17	62,62,62,62	0
56	MG	2A	3326	1/1	0.73	0.20	55,55,55,55	0
56	MG	2A	3779	1/1	0.73	0.12	61,61,61,61	0
56	MG	2A	3787	1/1	0.73	0.16	47,47,47,47	0
56	MG	2a	1646	1/1	0.73	0.11	67,67,67,67	0
56	MG	1a	1605	1/1	0.74	0.12	68,68,68,68	0
56	MG	1A	3696	1/1	0.74	0.15	67,67,67,67	0
56	MG	1A	3904	1/1	0.74	0.17	37,37,37,37	0
56	MG	2A	3465	1/1	0.74	0.17	54,54,54,54	0
56	MG	2A	3755	1/1	0.74	0.14	60,60,60,60	0
56	MG	1A	4012	1/1	0.74	0.12	56,56,56,56	0
56	MG	2A	3768	1/1	0.74	0.17	59,59,59,59	0
56	MG	2a	1688	1/1	0.74	0.12	76,76,76,76	0
56	MG	1a	1787	1/1	0.74	0.08	85,85,85,85	0
56	MG	1x	112	1/1	0.74	0.11	78,78,78,78	0
56	MG	1A	3281	1/1	0.74	0.18	50,50,50,50	0
56	MG	2A	3329	1/1	0.74	0.38	69,69,69,69	0
56	MG	1y	101	1/1	0.74	0.10	76,76,76,76	0
56	MG	2a	1801	1/1	0.74	0.24	69,69,69,69	0
56	MG	2B	202	1/1	0.74	0.85	70,70,70,70	0
56	MG	1a	1681	1/1	0.74	0.21	66,66,66,66	0
56	MG	1a	1691	1/1	0.74	0.14	74,74,74,74	0
56	MG	1A	3817	1/1	0.74	0.09	70,70,70,70	0
56	MG	2A	3645	1/1	0.74	0.15	73,73,73,73	0
56	MG	2A	3396	1/1	0.74	0.23	59,59,59,59	0
56	MG	2a	1638	1/1	0.75	0.27	75,75,75,75	0
56	MG	1A	3207	1/1	0.75	0.23	52,52,52,52	0
56	MG	1A	3242	1/1	0.75	0.23	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	1670	1/1	0.75	0.10	79,79,79,79	0
56	MG	2A	3249	1/1	0.75	0.33	72,72,72,72	0
56	MG	1A	3647	1/1	0.75	0.22	49,49,49,49	0
56	MG	2A	3643	1/1	0.75	0.16	75,75,75,75	0
56	MG	2B	211	1/1	0.75	0.13	72,72,72,72	0
56	MG	1a	1797	1/1	0.75	0.15	62,62,62,62	0
56	MG	2A	3273	1/1	0.75	0.27	67,67,67,67	0
56	MG	1U	203	1/1	0.75	0.48	59,59,59,59	0
56	MG	1A	3060	1/1	0.75	0.14	57,57,57,57	0
56	MG	2A	3285	1/1	0.75	0.24	71,71,71,71	0
56	MG	1A	3603	1/1	0.75	0.20	54,54,54,54	0
56	MG	1A	3934	1/1	0.75	0.12	72,72,72,72	0
56	MG	2A	3188	1/1	0.75	0.21	62,62,62,62	0
56	MG	2A	3192	1/1	0.75	0.19	58,58,58,58	0
56	MG	1A	3403	1/1	0.76	0.20	61,61,61,61	0
56	MG	2A	3332	1/1	0.76	0.29	73,73,73,73	0
56	MG	1A	3715	1/1	0.76	0.19	47,47,47,47	0
56	MG	1A	3409	1/1	0.76	0.24	63,63,63,63	0
56	MG	1A	4044	1/1	0.76	0.21	81,81,81,81	0
56	MG	2A	3379	1/1	0.76	0.29	69,69,69,69	0
56	MG	1A	4083	1/1	0.76	0.25	64,64,64,64	0
56	MG	2a	1737	1/1	0.76	0.09	77,77,77,77	0
56	MG	1A	3562	1/1	0.76	0.35	58,58,58,58	0
56	MG	2a	1752	1/1	0.76	0.21	76,76,76,76	0
56	MG	2A	3165	1/1	0.76	0.11	68,68,68,68	0
56	MG	2a	1779	1/1	0.76	0.17	72,72,72,72	0
56	MG	2a	1791	1/1	0.76	0.19	66,66,66,66	0
56	MG	1A	3917	1/1	0.76	0.16	57,57,57,57	0
56	MG	2a	1800	1/1	0.76	0.17	46,46,46,46	0
56	MG	2A	3436	1/1	0.76	0.14	73,73,73,73	0
56	MG	1A	3518	1/1	0.76	0.20	62,62,62,62	0
56	MG	2q	203	1/1	0.76	0.23	78,78,78,78	0
56	MG	2A	3312	1/1	0.76	0.10	82,82,82,82	0
56	MG	1A	3134	1/1	0.76	0.20	45,45,45,45	0
56	MG	1A	4009	1/1	0.76	0.17	53,53,53,53	0
56	MG	2a	1616	1/1	0.76	0.14	78,78,78,78	0
56	MG	2x	104	1/1	0.76	0.20	71,71,71,71	0
56	MG	1Y	201	1/1	0.76	0.14	52,52,52,52	0
56	MG	2A	3670	1/1	0.77	0.20	62,62,62,62	0
56	MG	1A	3519	1/1	0.77	0.18	61,61,61,61	0
56	MG	1a	1646	1/1	0.77	0.14	71,71,71,71	0
56	MG	2A	3721	1/1	0.77	0.28	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	3071	1/1	0.77	0.22	76,76,76,76	0
56	MG	2A	3741	1/1	0.77	0.17	63,63,63,63	0
56	MG	1a	1783	1/1	0.77	0.09	65,65,65,65	0
56	MG	1B	210	1/1	0.77	0.16	57,57,57,57	0
56	MG	2a	1705	1/1	0.77	0.25	77,77,77,77	0
56	MG	1A	4002	1/1	0.77	0.09	54,54,54,54	0
56	MG	2A	3765	1/1	0.77	0.11	75,75,75,75	0
56	MG	1A	3343	1/1	0.77	0.41	57,57,57,57	0
56	MG	1A	3317	1/1	0.77	0.17	47,47,47,47	0
56	MG	2A	3184	1/1	0.77	0.36	67,67,67,67	0
56	MG	1A	4019	1/1	0.77	0.23	44,44,44,44	0
56	MG	2A	3533	1/1	0.77	0.15	66,66,66,66	0
56	MG	2A	3325	1/1	0.77	0.34	70,70,70,70	0
56	MG	2A	3538	1/1	0.77	0.14	71,71,71,71	0
56	MG	1A	3505	1/1	0.77	0.23	47,47,47,47	0
56	MG	2A	3207	1/1	0.77	0.21	66,66,66,66	0
56	MG	1A	3249	1/1	0.77	0.11	66,66,66,66	0
56	MG	1A	4043	1/1	0.77	0.32	62,62,62,62	0
56	MG	2A	3346	1/1	0.77	0.18	66,66,66,66	0
56	MG	2A	3060	1/1	0.77	0.32	60,60,60,60	0
56	MG	1A	3907	1/1	0.77	0.13	52,52,52,52	0
56	MG	2A	3647	1/1	0.77	0.12	67,67,67,67	0
56	MG	2y	104	1/1	0.77	0.12	93,93,93,93	0
56	MG	2A	3255	1/1	0.77	0.17	69,69,69,69	0
56	MG	1a	1663	1/1	0.78	0.24	61,61,61,61	0
56	MG	1A	3753	1/1	0.78	0.14	85,85,85,85	0
56	MG	1A	3429	1/1	0.78	0.24	53,53,53,53	0
56	MG	1A	3986	1/1	0.78	0.12	75,75,75,75	0
56	MG	1A	3776	1/1	0.78	0.16	63,63,63,63	0
56	MG	2a	1759	1/1	0.78	0.22	73,73,73,73	0
56	MG	2A	3330	1/1	0.78	0.40	67,67,67,67	0
56	MG	1A	3882	1/1	0.78	0.13	64,64,64,64	0
56	MG	1A	3564	1/1	0.78	0.33	53,53,53,53	0
56	MG	2A	3163	1/1	0.78	0.20	63,63,63,63	0
56	MG	2a	1798	1/1	0.78	0.10	79,79,79,79	0
56	MG	1a	1736	1/1	0.78	0.12	62,62,62,62	0
56	MG	2A	3584	1/1	0.78	0.24	55,55,55,55	0
56	MG	1A	3253	1/1	0.78	0.19	41,41,41,41	0
56	MG	2a	1811	1/1	0.78	0.10	88,88,88,88	0
56	MG	2q	201	1/1	0.78	0.39	69,69,69,69	0
56	MG	1A	3816	1/1	0.78	0.18	75,75,75,75	0
56	MG	2a	1635	1/1	0.78	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3284	1/1	0.78	0.20	71,71,71,71	0
56	MG	2A	3056	1/1	0.78	0.23	68,68,68,68	0
56	MG	1A	3483	1/1	0.78	0.22	57,57,57,57	0
56	MG	2w	104	1/1	0.78	0.22	74,74,74,74	0
56	MG	2A	3803	1/1	0.78	0.21	60,60,60,60	0
56	MG	2A	3811	1/1	0.78	0.07	64,64,64,64	0
56	MG	2A	3202	1/1	0.78	0.15	73,73,73,73	0
56	MG	2A	3247	1/1	0.79	0.20	67,67,67,67	0
56	MG	2a	1692	1/1	0.79	0.14	69,69,69,69	0
56	MG	2A	3818	1/1	0.79	0.30	75,75,75,75	0
56	MG	1A	3548	1/1	0.79	0.21	42,42,42,42	0
56	MG	2A	3156	1/1	0.79	0.41	68,68,68,68	0
56	MG	2A	3490	1/1	0.79	0.23	55,55,55,55	0
56	MG	2B	204	1/1	0.79	0.29	68,68,68,68	0
56	MG	2B	208	1/1	0.79	0.11	69,69,69,69	0
56	MG	1A	3630	1/1	0.79	0.16	31,31,31,31	0
56	MG	2A	3683	1/1	0.79	0.23	88,88,88,88	0
56	MG	2A	3694	1/1	0.79	0.16	48,48,48,48	0
56	MG	1A	3421	1/1	0.79	0.32	68,68,68,68	0
56	MG	2A	3269	1/1	0.79	0.28	67,67,67,67	0
56	MG	1A	3900	1/1	0.79	0.17	49,49,49,49	0
56	MG	1A	3200	1/1	0.79	0.17	38,38,38,38	0
56	MG	1A	3681	1/1	0.79	0.11	55,55,55,55	0
56	MG	2a	1610	1/1	0.79	0.13	71,71,71,71	0
56	MG	1A	3568	1/1	0.79	0.19	37,37,37,37	0
56	MG	1l	201	1/1	0.79	0.14	69,69,69,69	0
56	MG	1A	3175	1/1	0.79	0.14	54,54,54,54	0
56	MG	1A	3122	1/1	0.79	0.21	73,73,73,73	0
56	MG	2A	3620	1/1	0.79	0.20	54,54,54,54	0
56	MG	2A	3641	1/1	0.79	0.14	74,74,74,74	0
56	MG	2a	1657	1/1	0.79	0.16	63,63,63,63	0
56	MG	2x	103	1/1	0.79	0.18	71,71,71,71	0
56	MG	1A	3337	1/1	0.79	0.33	72,72,72,72	0
56	MG	2y	103	1/1	0.79	0.10	81,81,81,81	0
56	MG	2A	3800	1/1	0.79	0.22	74,74,74,74	0
56	MG	2A	3120	1/1	0.79	0.25	58,58,58,58	0
56	MG	2A	3724	1/1	0.80	0.11	45,45,45,45	0
56	MG	2A	3153	1/1	0.80	0.08	69,69,69,69	0
56	MG	1A	4054	1/1	0.80	0.12	37,37,37,37	0
56	MG	1A	3824	1/1	0.80	0.23	49,49,49,49	0
56	MG	1x	102	1/1	0.80	0.23	62,62,62,62	0
56	MG	1B	204	1/1	0.80	0.34	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1684	1/1	0.80	0.18	62,62,62,62	0
56	MG	2a	1685	1/1	0.80	0.36	70,70,70,70	0
56	MG	2A	3303	1/1	0.80	0.27	63,63,63,63	0
56	MG	2A	3182	1/1	0.80	0.24	59,59,59,59	0
56	MG	1B	207	1/1	0.80	0.20	71,71,71,71	0
56	MG	1A	3481	1/1	0.80	0.21	54,54,54,54	0
56	MG	2a	1718	1/1	0.80	0.14	77,77,77,77	0
56	MG	1A	3310	1/1	0.80	0.17	49,49,49,49	0
56	MG	2A	3579	1/1	0.80	0.14	52,52,52,52	0
56	MG	2A	3194	1/1	0.80	0.17	66,66,66,66	0
56	MG	1A	3335	1/1	0.80	0.16	53,53,53,53	0
56	MG	1A	3796	1/1	0.80	0.22	87,87,87,87	0
56	MG	1A	3131	1/1	0.80	0.20	41,41,41,41	0
56	MG	1U	202	1/1	0.80	0.30	53,53,53,53	0
56	MG	1A	3968	1/1	0.80	0.14	58,58,58,58	0
56	MG	2A	3347	1/1	0.80	0.23	66,66,66,66	0
56	MG	2A	3358	1/1	0.80	0.11	76,76,76,76	0
56	MG	1A	3293	1/1	0.80	0.20	60,60,60,60	0
56	MG	1a	1759	1/1	0.80	0.14	76,76,76,76	0
56	MG	2A	3655	1/1	0.80	0.21	64,64,64,64	0
56	MG	2F	304	1/1	0.80	0.16	67,67,67,67	0
56	MG	1A	3470	1/1	0.80	0.15	52,52,52,52	0
56	MG	1A	3473	1/1	0.80	0.24	65,65,65,65	0
56	MG	2P	201	1/1	0.80	0.19	63,63,63,63	0
56	MG	2W	201	1/1	0.80	0.23	68,68,68,68	0
56	MG	2A	3384	1/1	0.80	0.24	59,59,59,59	0
56	MG	2A	3682	1/1	0.80	0.09	78,78,78,78	0
56	MG	2A	3264	1/1	0.80	0.22	63,63,63,63	0
56	MG	2a	1609	1/1	0.80	0.21	69,69,69,69	0
56	MG	1a	1777	1/1	0.80	0.06	58,58,58,58	0
56	MG	1A	3347	1/1	0.80	0.22	49,49,49,49	0
56	MG	2A	3716	1/1	0.80	0.07	62,62,62,62	0
56	MG	1a	1642	1/1	0.80	0.17	65,65,65,65	0
56	MG	2A	3731	1/1	0.81	0.10	61,61,61,61	0
56	MG	1A	3980	1/1	0.81	0.13	78,78,78,78	0
56	MG	2A	3274	1/1	0.81	0.20	58,58,58,58	0
56	MG	1A	3139	1/1	0.81	0.19	34,34,34,34	0
56	MG	1a	1613	1/1	0.81	0.09	67,67,67,67	0
56	MG	1A	4075	1/1	0.81	0.15	65,65,65,65	0
56	MG	2a	1682	1/1	0.81	0.39	68,68,68,68	0
56	MG	1A	4081	1/1	0.81	0.13	46,46,46,46	0
56	MG	2A	3286	1/1	0.81	0.35	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3288	1/1	0.81	0.24	56,56,56,56	0
56	MG	1A	3306	1/1	0.81	0.10	55,55,55,55	0
56	MG	1w	105	1/1	0.81	0.16	79,79,79,79	0
56	MG	1A	3339	1/1	0.81	0.19	55,55,55,55	0
56	MG	1A	3224	1/1	0.81	0.24	55,55,55,55	0
56	MG	1A	3262	1/1	0.81	0.21	63,63,63,63	0
56	MG	1B	230	1/1	0.81	0.29	79,79,79,79	0
56	MG	1A	3667	1/1	0.81	0.23	56,56,56,56	0
56	MG	2A	3604	1/1	0.81	0.12	82,82,82,82	0
56	MG	2a	1755	1/1	0.81	0.13	74,74,74,74	0
56	MG	2A	3021	1/1	0.81	0.12	79,79,79,79	0
56	MG	1A	3952	1/1	0.81	0.15	35,35,35,35	0
56	MG	2a	1777	1/1	0.81	0.16	70,70,70,70	0
56	MG	2A	3042	1/1	0.81	0.16	58,58,58,58	0
56	MG	1A	3953	1/1	0.81	0.16	58,58,58,58	0
56	MG	2A	3049	1/1	0.81	0.11	54,54,54,54	0
56	MG	2A	3223	1/1	0.81	0.66	58,58,58,58	0
56	MG	2F	303	1/1	0.81	0.23	49,49,49,49	0
56	MG	2A	3354	1/1	0.81	0.10	69,69,69,69	0
56	MG	2A	3357	1/1	0.81	0.14	74,74,74,74	0
56	MG	1O	204	1/1	0.81	0.22	63,63,63,63	0
56	MG	1a	1733	1/1	0.81	0.27	71,71,71,71	0
56	MG	1A	3172	1/1	0.81	0.25	44,44,44,44	0
56	MG	2A	3063	1/1	0.81	0.14	65,65,65,65	0
56	MG	27	102	1/1	0.81	0.28	77,77,77,77	0
56	MG	1A	3381	1/1	0.81	0.21	57,57,57,57	0
56	MG	1A	3284	1/1	0.81	0.20	47,47,47,47	0
56	MG	1A	3333	1/1	0.81	0.22	72,72,72,72	0
56	MG	2A	3268	1/1	0.81	0.18	72,72,72,72	0
56	MG	2a	1611	1/1	0.81	0.19	76,76,76,76	0
56	MG	2A	3719	1/1	0.81	0.11	55,55,55,55	0
56	MG	11	106	1/1	0.81	0.12	50,50,50,50	0
56	MG	2A	3413	1/1	0.81	0.20	68,68,68,68	0
56	MG	2A	3088	1/1	0.82	0.26	80,80,80,80	0
56	MG	2A	3725	1/1	0.82	0.14	72,72,72,72	0
56	MG	2A	3271	1/1	0.82	0.16	76,76,76,76	0
56	MG	1A	3094	1/1	0.82	0.08	67,67,67,67	0
56	MG	1A	4006	1/1	0.82	0.20	37,37,37,37	0
56	MG	2a	1673	1/1	0.82	0.26	64,64,64,64	0
56	MG	2a	1675	1/1	0.82	0.17	68,68,68,68	0
56	MG	2A	3746	1/1	0.82	0.22	70,70,70,70	0
56	MG	1A	3300	1/1	0.82	0.24	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	1A	3006	1/1	0.82	0.19	69,69,69,69	0
56	MG	2A	3154	1/1	0.82	0.12	59,59,59,59	0
56	MG	1A	3637	1/1	0.82	0.15	23,23,23,23	0
56	MG	1A	3644	1/1	0.82	0.13	30,30,30,30	0
56	MG	1A	3375	1/1	0.82	0.18	46,46,46,46	0
56	MG	1A	3936	1/1	0.82	0.11	63,63,63,63	0
56	MG	2A	3299	1/1	0.82	0.29	64,64,64,64	0
56	MG	1A	3664	1/1	0.82	0.21	34,34,34,34	0
56	MG	1A	4047	1/1	0.82	0.19	80,80,80,80	0
56	MG	2A	3314	1/1	0.82	0.23	62,62,62,62	0
56	MG	1A	3453	1/1	0.82	0.14	44,44,44,44	0
56	MG	2A	3323	1/1	0.82	0.15	67,67,67,67	0
56	MG	2a	1754	1/1	0.82	0.27	83,83,83,83	0
56	MG	2A	3592	1/1	0.82	0.18	38,38,38,38	0
56	MG	1a	1655	1/1	0.82	0.11	72,72,72,72	0
56	MG	1A	4071	1/1	0.82	0.21	69,69,69,69	0
56	MG	1A	3491	1/1	0.82	0.23	65,65,65,65	0
56	MG	1A	3675	1/1	0.82	0.21	51,51,51,51	0
56	MG	2B	212	1/1	0.82	0.18	74,74,74,74	0
56	MG	1A	3235	1/1	0.82	0.35	60,60,60,60	0
56	MG	2A	3217	1/1	0.82	0.23	67,67,67,67	0
56	MG	2E	303	1/1	0.82	0.15	70,70,70,70	0
56	MG	1A	3291	1/1	0.82	0.25	55,55,55,55	0
56	MG	1A	3850	1/1	0.82	0.22	42,42,42,42	0
56	MG	2a	1803	1/1	0.82	0.12	81,81,81,81	0
56	MG	1a	1690	1/1	0.82	0.23	52,52,52,52	0
56	MG	2A	3225	1/1	0.82	0.20	63,63,63,63	0
56	MG	2A	3230	1/1	0.82	0.26	62,62,62,62	0
56	MG	1A	3587	1/1	0.82	0.15	39,39,39,39	0
56	MG	2A	3359	1/1	0.82	0.15	64,64,64,64	0
56	MG	1A	3410	1/1	0.82	0.15	58,58,58,58	0
56	MG	2A	3373	1/1	0.82	0.15	64,64,64,64	0
56	MG	1F	303	1/1	0.82	0.24	67,67,67,67	0
56	MG	2A	3695	1/1	0.82	0.24	49,49,49,49	0
56	MG	1A	3721	1/1	0.82	0.18	25,25,25,25	0
56	MG	1A	3722	1/1	0.82	0.12	52,52,52,52	0
56	MG	1A	3729	1/1	0.82	0.23	34,34,34,34	0
56	MG	1A	3733	1/1	0.82	0.18	24,24,24,24	0
56	MG	2A	3101	1/1	0.83	0.16	63,63,63,63	0
56	MG	2A	3103	1/1	0.83	0.15	59,59,59,59	0
56	MG	2A	3113	1/1	0.83	0.25	57,57,57,57	0
56	MG	1A	3633	1/1	0.83	0.13	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	3633	1/1	0.83	0.10	72,72,72,72	0
56	MG	1E	302	1/1	0.83	0.52	51,51,51,51	0
56	MG	2A	3318	1/1	0.83	0.26	66,66,66,66	0
56	MG	1A	3903	1/1	0.83	0.18	37,37,37,37	0
56	MG	1A	3360	1/1	0.83	0.28	59,59,59,59	0
56	MG	1a	1744	1/1	0.83	0.09	74,74,74,74	0
56	MG	1A	3991	1/1	0.83	0.15	50,50,50,50	0
56	MG	1a	1751	1/1	0.83	0.20	63,63,63,63	0
56	MG	2a	1627	1/1	0.83	0.14	73,73,73,73	0
56	MG	2A	3166	1/1	0.83	0.15	70,70,70,70	0
56	MG	1A	3369	1/1	0.83	0.12	56,56,56,56	0
56	MG	1A	3373	1/1	0.83	0.63	46,46,46,46	0
56	MG	1A	3649	1/1	0.83	0.24	61,61,61,61	0
56	MG	2A	3187	1/1	0.83	0.18	64,64,64,64	0
56	MG	1A	3301	1/1	0.83	0.52	44,44,44,44	0
56	MG	1A	3248	1/1	0.83	0.18	40,40,40,40	0
56	MG	1A	3799	1/1	0.83	0.13	55,55,55,55	0
56	MG	1Z	301	1/1	0.83	0.18	68,68,68,68	0
56	MG	1A	3212	1/1	0.83	0.26	54,54,54,54	0
56	MG	1A	3670	1/1	0.83	0.25	61,61,61,61	0
56	MG	2A	3216	1/1	0.83	0.23	57,57,57,57	0
56	MG	1A	3350	1/1	0.83	0.35	53,53,53,53	0
56	MG	1A	3938	1/1	0.83	0.13	48,48,48,48	0
56	MG	2a	1698	1/1	0.83	0.16	51,51,51,51	0
56	MG	2a	1702	1/1	0.83	0.21	70,70,70,70	0
56	MG	2A	3733	1/1	0.83	0.19	72,72,72,72	0
56	MG	1a	1618	1/1	0.83	0.11	59,59,59,59	0
56	MG	1A	3939	1/1	0.83	0.08	60,60,60,60	0
56	MG	2A	3395	1/1	0.83	0.22	61,61,61,61	0
56	MG	2A	3003	1/1	0.83	0.34	60,60,60,60	0
56	MG	1A	3948	1/1	0.83	0.15	36,36,36,36	0
56	MG	1A	4049	1/1	0.83	0.29	37,37,37,37	0
56	MG	1a	1653	1/1	0.83	0.11	57,57,57,57	0
56	MG	2A	3772	1/1	0.83	0.20	58,58,58,58	0
56	MG	2A	3415	1/1	0.83	0.32	66,66,66,66	0
56	MG	2A	3033	1/1	0.83	0.25	45,45,45,45	0
56	MG	1A	3484	1/1	0.83	0.22	65,65,65,65	0
56	MG	2a	1780	1/1	0.83	0.19	70,70,70,70	0
56	MG	1A	3433	1/1	0.83	0.32	67,67,67,67	0
56	MG	1A	3355	1/1	0.83	0.23	38,38,38,38	0
56	MG	2A	3470	1/1	0.83	0.12	49,49,49,49	0
56	MG	2A	3813	1/1	0.83	0.38	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3387	1/1	0.83	0.28	48,48,48,48	0
56	MG	2A	3498	1/1	0.83	0.11	50,50,50,50	0
56	MG	1A	3624	1/1	0.83	0.21	26,26,26,26	0
56	MG	2A	3508	1/1	0.83	0.18	44,44,44,44	0
56	MG	1A	3358	1/1	0.83	0.27	63,63,63,63	0
56	MG	1A	3528	1/1	0.83	0.29	46,46,46,46	0
56	MG	1a	1682	1/1	0.83	0.15	63,63,63,63	0
56	MG	1a	1686	1/1	0.83	0.10	67,67,67,67	0
56	MG	2A	3543	1/1	0.83	0.14	47,47,47,47	0
56	MG	1A	3981	1/1	0.83	0.12	59,59,59,59	0
56	MG	2D	305	1/1	0.83	0.60	57,57,57,57	0
56	MG	1B	221	1/1	0.83	0.18	75,75,75,75	0
56	MG	2A	3085	1/1	0.83	0.35	78,78,78,78	0
56	MG	2x	108	1/1	0.83	0.14	56,56,56,56	0
56	MG	2A	3587	1/1	0.83	0.19	63,63,63,63	0
56	MG	1a	1700	1/1	0.83	0.15	63,63,63,63	0
56	MG	1a	1704	1/1	0.83	0.20	64,64,64,64	0
56	MG	1A	3257	1/1	0.84	0.27	65,65,65,65	0
56	MG	2A	3648	1/1	0.84	0.17	67,67,67,67	0
56	MG	2A	3654	1/1	0.84	0.15	44,44,44,44	0
56	MG	1a	1647	1/1	0.84	0.16	67,67,67,67	0
56	MG	2A	3661	1/1	0.84	0.20	54,54,54,54	0
56	MG	1B	229	1/1	0.84	0.26	69,69,69,69	0
56	MG	1A	3836	1/1	0.84	0.20	44,44,44,44	0
56	MG	1B	231	1/1	0.84	0.10	81,81,81,81	0
56	MG	1a	1792	1/1	0.84	0.09	57,57,57,57	0
56	MG	1B	238	1/1	0.84	0.20	65,65,65,65	0
56	MG	1A	3424	1/1	0.84	0.14	68,68,68,68	0
56	MG	1v	101	1/1	0.84	0.22	74,74,74,74	0
56	MG	1w	102	1/1	0.84	0.22	69,69,69,69	0
56	MG	2A	3710	1/1	0.84	0.09	69,69,69,69	0
56	MG	2a	1667	1/1	0.84	0.08	72,72,72,72	0
56	MG	2A	3399	1/1	0.84	0.45	64,64,64,64	0
56	MG	1A	3940	1/1	0.84	0.14	62,62,62,62	0
56	MG	1A	3401	1/1	0.84	0.19	71,71,71,71	0
56	MG	2A	3410	1/1	0.84	0.32	57,57,57,57	0
56	MG	1x	109	1/1	0.84	0.15	68,68,68,68	0
56	MG	2A	3283	1/1	0.84	0.26	64,64,64,64	0
56	MG	2A	3157	1/1	0.84	0.08	68,68,68,68	0
56	MG	2A	3447	1/1	0.84	0.15	52,52,52,52	0
56	MG	2A	3452	1/1	0.84	0.35	61,61,61,61	0
56	MG	1a	1680	1/1	0.84	0.34	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3164	1/1	0.84	0.23	68,68,68,68	0
56	MG	1A	3744	1/1	0.84	0.35	60,60,60,60	0
56	MG	1A	3499	1/1	0.84	0.13	62,62,62,62	0
56	MG	2a	1712	1/1	0.84	0.22	69,69,69,69	0
56	MG	2A	3298	1/1	0.84	0.49	65,65,65,65	0
56	MG	2a	1730	1/1	0.84	0.09	63,63,63,63	0
56	MG	2A	3002	1/1	0.84	0.36	68,68,68,68	0
56	MG	2A	3301	1/1	0.84	0.48	63,63,63,63	0
56	MG	1A	3895	1/1	0.84	0.12	35,35,35,35	0
56	MG	2A	3517	1/1	0.84	0.18	59,59,59,59	0
56	MG	2A	3784	1/1	0.84	0.07	63,63,63,63	0
56	MG	2A	3786	1/1	0.84	0.21	65,65,65,65	0
56	MG	1A	3504	1/1	0.84	0.26	46,46,46,46	0
56	MG	2A	3529	1/1	0.84	0.17	67,67,67,67	0
56	MG	1A	3465	1/1	0.84	0.24	54,54,54,54	0
56	MG	2A	3317	1/1	0.84	0.54	67,67,67,67	0
56	MG	2A	3022	1/1	0.84	0.27	59,59,59,59	0
56	MG	2A	3541	1/1	0.84	0.32	71,71,71,71	0
56	MG	1A	3596	1/1	0.84	0.15	30,30,30,30	0
56	MG	1A	3226	1/1	0.84	0.27	58,58,58,58	0
56	MG	1A	3431	1/1	0.84	0.57	52,52,52,52	0
56	MG	1A	3623	1/1	0.84	0.15	29,29,29,29	0
56	MG	1A	3002	1/1	0.84	0.38	60,60,60,60	0
56	MG	2A	3328	1/1	0.84	0.18	65,65,65,65	0
56	MG	2A	3052	1/1	0.84	0.23	61,61,61,61	0
56	MG	1A	3706	1/1	0.84	0.10	55,55,55,55	0
56	MG	2A	3331	1/1	0.84	0.09	64,64,64,64	0
56	MG	1B	203	1/1	0.84	0.20	45,45,45,45	0
56	MG	2A	3613	1/1	0.84	0.12	60,60,60,60	0
56	MG	2A	3617	1/1	0.84	0.15	56,56,56,56	0
56	MG	1A	3149	1/1	0.84	0.25	40,40,40,40	0
56	MG	2A	3343	1/1	0.84	0.20	66,66,66,66	0
56	MG	1A	3447	1/1	0.84	0.23	49,49,49,49	0
56	MG	1a	1752	1/1	0.84	0.13	68,68,68,68	0
56	MG	1A	3482	1/1	0.84	0.20	50,50,50,50	0
56	MG	2W	203	1/1	0.84	0.27	54,54,54,54	0
56	MG	2A	3238	1/1	0.84	0.20	72,72,72,72	0
56	MG	25	103	1/1	0.84	0.28	70,70,70,70	0
56	MG	2A	3610	1/1	0.85	0.17	79,79,79,79	0
56	MG	2A	3327	1/1	0.85	0.11	65,65,65,65	0
56	MG	2Q	203	1/1	0.85	0.21	61,61,61,61	0
56	MG	1x	106	1/1	0.85	0.17	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	1A	3704	1/1	0.85	0.22	30,30,30,30	0
56	MG	1A	3861	1/1	0.85	0.18	50,50,50,50	0
56	MG	2A	3637	1/1	0.85	0.19	57,57,57,57	0
56	MG	25	106	1/1	0.85	0.13	53,53,53,53	0
56	MG	1a	1657	1/1	0.85	0.57	56,56,56,56	0
56	MG	1A	3188	1/1	0.85	0.26	49,49,49,49	0
56	MG	2A	3208	1/1	0.85	0.25	68,68,68,68	0
56	MG	2a	1608	1/1	0.85	0.13	68,68,68,68	0
56	MG	1A	3195	1/1	0.85	0.10	46,46,46,46	0
56	MG	2A	3214	1/1	0.85	0.66	47,47,47,47	0
56	MG	1a	1665	1/1	0.85	0.10	60,60,60,60	0
56	MG	1A	3885	1/1	0.85	0.14	66,66,66,66	0
56	MG	2A	3016	1/1	0.85	0.17	62,62,62,62	0
56	MG	1B	224	1/1	0.85	0.22	64,64,64,64	0
56	MG	2a	1621	1/1	0.85	0.23	65,65,65,65	0
56	MG	1a	1677	1/1	0.85	0.16	68,68,68,68	0
56	MG	1A	3713	1/1	0.85	0.12	68,68,68,68	0
56	MG	2A	3361	1/1	0.85	0.20	63,63,63,63	0
56	MG	1A	3503	1/1	0.85	0.10	62,62,62,62	0
56	MG	2a	1655	1/1	0.85	0.18	64,64,64,64	0
56	MG	1A	3144	1/1	0.85	0.32	49,49,49,49	0
56	MG	2a	1659	1/1	0.85	0.13	63,63,63,63	0
56	MG	2A	3686	1/1	0.85	0.17	73,73,73,73	0
56	MG	2A	3240	1/1	0.85	0.41	61,61,61,61	0
56	MG	1A	3449	1/1	0.85	0.32	53,53,53,53	0
56	MG	1A	3124	1/1	0.85	0.14	47,47,47,47	0
56	MG	1A	3047	1/1	0.85	0.21	53,53,53,53	0
56	MG	2A	3256	1/1	0.85	0.23	58,58,58,58	0
56	MG	2A	3257	1/1	0.85	0.22	79,79,79,79	0
56	MG	2A	3720	1/1	0.85	0.11	54,54,54,54	0
56	MG	1A	3247	1/1	0.85	0.28	38,38,38,38	0
56	MG	2A	3263	1/1	0.85	0.56	63,63,63,63	0
56	MG	1a	1692	1/1	0.85	0.14	55,55,55,55	0
56	MG	1A	3529	1/1	0.85	0.13	76,76,76,76	0
56	MG	1A	3642	1/1	0.85	0.10	53,53,53,53	0
56	MG	2A	3421	1/1	0.85	0.21	55,55,55,55	0
56	MG	2A	3737	1/1	0.85	0.11	63,63,63,63	0
56	MG	2a	1714	1/1	0.85	0.10	66,66,66,66	0
56	MG	1A	4010	1/1	0.85	0.16	59,59,59,59	0
56	MG	2A	3270	1/1	0.85	0.28	70,70,70,70	0
56	MG	1a	1718	1/1	0.85	0.16	56,56,56,56	0
56	MG	2A	3751	1/1	0.85	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1727	1/1	0.85	0.41	70,70,70,70	0
56	MG	2a	1750	1/1	0.85	0.08	79,79,79,79	0
56	MG	2A	3758	1/1	0.85	0.19	60,60,60,60	0
56	MG	1A	3209	1/1	0.85	0.37	41,41,41,41	0
56	MG	1R	204	1/1	0.85	0.19	59,59,59,59	0
56	MG	1T	201	1/1	0.85	0.19	54,54,54,54	0
56	MG	2A	3473	1/1	0.85	0.14	63,63,63,63	0
56	MG	2A	3095	1/1	0.85	0.08	58,58,58,58	0
56	MG	1A	4016	1/1	0.85	0.07	53,53,53,53	0
56	MG	1A	3211	1/1	0.85	0.50	49,49,49,49	0
56	MG	1A	3308	1/1	0.85	0.26	65,65,65,65	0
56	MG	1A	3100	1/1	0.85	0.53	40,40,40,40	0
56	MG	2A	3290	1/1	0.85	0.49	61,61,61,61	0
56	MG	10	106	1/1	0.85	0.06	56,56,56,56	0
56	MG	1A	3550	1/1	0.85	0.20	67,67,67,67	0
56	MG	1A	3367	1/1	0.85	0.11	59,59,59,59	0
56	MG	1a	1604	1/1	0.85	0.21	64,64,64,64	0
56	MG	1A	3219	1/1	0.85	0.21	52,52,52,52	0
56	MG	2A	3306	1/1	0.85	0.19	70,70,70,70	0
56	MG	1A	3672	1/1	0.85	0.11	48,48,48,48	0
56	MG	2A	3571	1/1	0.85	0.25	46,46,46,46	0
56	MG	1A	3083	1/1	0.85	0.22	48,48,48,48	0
56	MG	1A	3949	1/1	0.85	0.19	44,44,44,44	0
56	MG	2w	101	1/1	0.85	0.15	69,69,69,69	0
56	MG	2w	102	1/1	0.85	0.11	86,86,86,86	0
56	MG	1a	1805	1/1	0.85	0.17	61,61,61,61	0
56	MG	1a	1630	1/1	0.85	0.20	65,65,65,65	0
56	MG	1a	1635	1/1	0.85	0.12	62,62,62,62	0
56	MG	1A	3319	1/1	0.85	0.13	65,65,65,65	0
56	MG	2A	3601	1/1	0.85	0.15	65,65,65,65	0
56	MG	2A	3602	1/1	0.85	0.14	67,67,67,67	0
56	MG	1A	3687	1/1	0.85	0.15	52,52,52,52	0
56	MG	1A	3259	1/1	0.85	0.16	39,39,39,39	0
56	MG	2T	202	1/1	0.86	0.16	66,66,66,66	0
56	MG	1B	236	1/1	0.86	0.14	49,49,49,49	0
56	MG	1A	3428	1/1	0.86	0.23	51,51,51,51	0
56	MG	1A	3467	1/1	0.86	0.49	63,63,63,63	0
56	MG	25	101	1/1	0.86	0.24	67,67,67,67	0
56	MG	1E	303	1/1	0.86	0.21	33,33,33,33	0
56	MG	2A	3639	1/1	0.86	0.08	72,72,72,72	0
56	MG	25	107	1/1	0.86	0.17	69,69,69,69	0
56	MG	2A	3212	1/1	0.86	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1E	307	1/1	0.86	0.31	59,59,59,59	0
56	MG	1E	313	1/1	0.86	0.08	62,62,62,62	0
56	MG	1A	3389	1/1	0.86	0.19	56,56,56,56	0
56	MG	1A	3157	1/1	0.86	0.19	37,37,37,37	0
56	MG	1A	3535	1/1	0.86	0.36	39,39,39,39	0
56	MG	1A	3476	1/1	0.86	0.27	52,52,52,52	0
56	MG	1I	201	1/1	0.86	0.14	59,59,59,59	0
56	MG	2A	3658	1/1	0.86	0.22	66,66,66,66	0
56	MG	1O	203	1/1	0.86	0.15	70,70,70,70	0
56	MG	1a	1683	1/1	0.86	0.18	45,45,45,45	0
56	MG	2a	1626	1/1	0.86	0.41	58,58,58,58	0
56	MG	2A	3376	1/1	0.86	0.31	62,62,62,62	0
56	MG	2a	1631	1/1	0.86	0.12	62,62,62,62	0
56	MG	2A	3034	1/1	0.86	0.25	55,55,55,55	0
56	MG	1A	3164	1/1	0.86	0.28	51,51,51,51	0
56	MG	1A	3292	1/1	0.86	0.18	53,53,53,53	0
56	MG	2a	1648	1/1	0.86	0.21	63,63,63,63	0
56	MG	2A	3251	1/1	0.86	0.42	80,80,80,80	0
56	MG	1A	4045	1/1	0.86	0.12	70,70,70,70	0
56	MG	1A	3445	1/1	0.86	0.15	51,51,51,51	0
56	MG	1A	3730	1/1	0.86	0.16	51,51,51,51	0
56	MG	2A	3701	1/1	0.86	0.12	64,64,64,64	0
56	MG	2A	3704	1/1	0.86	0.35	66,66,66,66	0
56	MG	2A	3708	1/1	0.86	0.20	45,45,45,45	0
56	MG	1A	3971	1/1	0.86	0.09	32,32,32,32	0
56	MG	1U	211	1/1	0.86	0.14	42,42,42,42	0
56	MG	1A	3120	1/1	0.86	0.28	56,56,56,56	0
56	MG	1A	3554	1/1	0.86	0.40	63,63,63,63	0
56	MG	2A	3069	1/1	0.86	0.14	57,57,57,57	0
56	MG	2a	1689	1/1	0.86	0.11	58,58,58,58	0
56	MG	2A	3426	1/1	0.86	0.27	49,49,49,49	0
56	MG	2A	3427	1/1	0.86	0.41	79,79,79,79	0
56	MG	1A	4076	1/1	0.86	0.14	66,66,66,66	0
56	MG	2a	1701	1/1	0.86	0.12	66,66,66,66	0
56	MG	10	108	1/1	0.86	0.16	51,51,51,51	0
56	MG	2a	1704	1/1	0.86	0.21	75,75,75,75	0
56	MG	1A	4079	1/1	0.86	0.10	65,65,65,65	0
56	MG	12	101	1/1	0.86	0.15	59,59,59,59	0
56	MG	2A	3087	1/1	0.86	0.12	82,82,82,82	0
56	MG	2A	3275	1/1	0.86	0.25	67,67,67,67	0
56	MG	2a	1727	1/1	0.86	0.29	81,81,81,81	0
56	MG	15	106	1/1	0.86	0.29	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	1750	1/1	0.86	0.12	54,54,54,54	0
56	MG	1A	3318	1/1	0.86	0.22	58,58,58,58	0
56	MG	1A	3251	1/1	0.86	0.18	57,57,57,57	0
56	MG	2A	3499	1/1	0.86	0.25	45,45,45,45	0
56	MG	2A	3503	1/1	0.86	0.25	49,49,49,49	0
56	MG	1a	1757	1/1	0.86	0.14	52,52,52,52	0
56	MG	1A	3320	1/1	0.86	0.17	51,51,51,51	0
56	MG	2A	3511	1/1	0.86	0.13	52,52,52,52	0
56	MG	1A	3458	1/1	0.86	0.28	56,56,56,56	0
56	MG	2a	1773	1/1	0.86	0.12	68,68,68,68	0
56	MG	1a	1763	1/1	0.86	0.09	67,67,67,67	0
56	MG	2A	3148	1/1	0.86	0.22	64,64,64,64	0
56	MG	1A	3052	1/1	0.86	0.27	50,50,50,50	0
56	MG	1a	1771	1/1	0.86	0.20	65,65,65,65	0
56	MG	1A	3590	1/1	0.86	0.27	61,61,61,61	0
56	MG	1A	3676	1/1	0.86	0.09	62,62,62,62	0
56	MG	1a	1632	1/1	0.86	0.15	64,64,64,64	0
56	MG	2A	3549	1/1	0.86	0.11	60,60,60,60	0
56	MG	1A	3283	1/1	0.86	0.12	65,65,65,65	0
56	MG	2A	3562	1/1	0.86	0.09	64,64,64,64	0
56	MG	1a	1637	1/1	0.86	0.11	61,61,61,61	0
56	MG	2j	3200	1/1	0.86	0.07	75,75,75,75	0
56	MG	2A	3316	1/1	0.86	0.18	73,73,73,73	0
56	MG	1a	1802	1/1	0.86	0.20	78,78,78,78	0
56	MG	1a	1639	1/1	0.86	0.26	67,67,67,67	0
56	MG	2A	3174	1/1	0.86	0.27	63,63,63,63	0
56	MG	2A	3590	1/1	0.86	0.14	74,74,74,74	0
56	MG	1A	3809	1/1	0.86	0.12	59,59,59,59	0
56	MG	2B	217	1/1	0.86	0.09	77,77,77,77	0
56	MG	1n	102	1/1	0.86	0.08	69,69,69,69	0
56	MG	1A	3814	1/1	0.86	0.20	23,23,23,23	0
56	MG	1A	3513	1/1	0.86	0.29	57,57,57,57	0
56	MG	1a	1652	1/1	0.86	0.11	49,49,49,49	0
56	MG	2A	3193	1/1	0.86	0.18	63,63,63,63	0
56	MG	1B	235	1/1	0.86	0.18	74,74,74,74	0
56	MG	2A	3195	1/1	0.86	0.30	61,61,61,61	0
56	MG	2A	3614	1/1	0.86	0.23	58,58,58,58	0
56	MG	2A	3175	1/1	0.87	0.28	58,58,58,58	0
56	MG	2A	3451	1/1	0.87	0.30	50,50,50,50	0
56	MG	1A	3617	1/1	0.87	0.22	38,38,38,38	0
56	MG	2A	3689	1/1	0.87	0.44	76,76,76,76	0
56	MG	1A	3423	1/1	0.87	0.21	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	1A	3847	1/1	0.87	0.15	26,26,26,26	0
56	MG	2a	1612	1/1	0.87	0.18	62,62,62,62	0
56	MG	1A	3056	1/1	0.87	0.27	45,45,45,45	0
56	MG	2A	3190	1/1	0.87	0.33	55,55,55,55	0
56	MG	2A	3702	1/1	0.87	0.15	58,58,58,58	0
56	MG	2A	3191	1/1	0.87	0.23	72,72,72,72	0
56	MG	1A	3942	1/1	0.87	0.28	65,65,65,65	0
56	MG	1A	3851	1/1	0.87	0.13	47,47,47,47	0
56	MG	2A	3038	1/1	0.87	0.21	58,58,58,58	0
56	MG	2A	3500	1/1	0.87	0.24	44,44,44,44	0
56	MG	1A	3745	1/1	0.87	0.19	25,25,25,25	0
56	MG	2A	3196	1/1	0.87	0.28	69,69,69,69	0
56	MG	1A	3254	1/1	0.87	0.41	68,68,68,68	0
56	MG	2a	1653	1/1	0.87	0.13	68,68,68,68	0
56	MG	2A	3510	1/1	0.87	0.14	36,36,36,36	0
56	MG	2A	3728	1/1	0.87	0.11	43,43,43,43	0
56	MG	2A	3203	1/1	0.87	0.20	66,66,66,66	0
56	MG	1G	3602	1/1	0.87	0.22	57,57,57,57	0
56	MG	2A	3321	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3736	1/1	0.87	0.12	44,44,44,44	0
56	MG	2a	1678	1/1	0.87	0.19	67,67,67,67	0
56	MG	1A	3880	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3055	1/1	0.87	0.15	65,65,65,65	0
56	MG	1A	3315	1/1	0.87	0.28	48,48,48,48	0
56	MG	1A	4065	1/1	0.87	0.16	78,78,78,78	0
56	MG	1A	3760	1/1	0.87	0.17	22,22,22,22	0
56	MG	2A	3542	1/1	0.87	0.28	73,73,73,73	0
56	MG	1A	3761	1/1	0.87	0.20	38,38,38,38	0
56	MG	1A	3552	1/1	0.87	0.14	70,70,70,70	0
56	MG	2A	3551	1/1	0.87	0.11	54,54,54,54	0
56	MG	1A	3898	1/1	0.87	0.10	58,58,58,58	0
56	MG	1A	3225	1/1	0.87	0.55	45,45,45,45	0
56	MG	1A	3190	1/1	0.87	0.25	47,47,47,47	0
56	MG	2A	3774	1/1	0.87	0.17	65,65,65,65	0
56	MG	1a	1794	1/1	0.87	0.06	55,55,55,55	0
56	MG	1a	1674	1/1	0.87	0.14	40,40,40,40	0
56	MG	1A	3340	1/1	0.87	0.16	55,55,55,55	0
56	MG	2a	1716	1/1	0.87	0.11	70,70,70,70	0
56	MG	1A	3402	1/1	0.87	0.28	69,69,69,69	0
56	MG	2A	3793	1/1	0.87	0.23	50,50,50,50	0
56	MG	2A	3349	1/1	0.87	0.21	65,65,65,65	0
56	MG	2A	3350	1/1	0.87	0.48	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3808	1/1	0.87	0.41	78,78,78,78	0
56	MG	2A	3596	1/1	0.87	0.09	76,76,76,76	0
56	MG	2A	3812	1/1	0.87	0.34	79,79,79,79	0
56	MG	2A	3248	1/1	0.87	0.43	65,65,65,65	0
56	MG	2A	3814	1/1	0.87	0.11	68,68,68,68	0
56	MG	2A	3091	1/1	0.87	0.18	44,44,44,44	0
56	MG	1A	3288	1/1	0.87	0.17	50,50,50,50	0
56	MG	2A	3254	1/1	0.87	0.17	82,82,82,82	0
56	MG	2B	201	1/1	0.87	0.25	73,73,73,73	0
56	MG	1m	3002	1/1	0.87	0.16	63,63,63,63	0
56	MG	10	103	1/1	0.87	0.50	45,45,45,45	0
56	MG	1B	209	1/1	0.87	0.13	45,45,45,45	0
56	MG	2A	3260	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3260	1/1	0.87	0.40	44,44,44,44	0
56	MG	1A	3718	1/1	0.87	0.26	58,58,58,58	0
56	MG	2B	215	1/1	0.87	0.21	71,71,71,71	0
56	MG	2A	3626	1/1	0.87	0.29	61,61,61,61	0
56	MG	1A	3448	1/1	0.87	0.26	51,51,51,51	0
56	MG	2A	3381	1/1	0.87	0.18	58,58,58,58	0
56	MG	1x	105	1/1	0.87	0.28	65,65,65,65	0
56	MG	1A	3916	1/1	0.87	0.11	59,59,59,59	0
56	MG	2l	203	1/1	0.87	0.11	68,68,68,68	0
56	MG	1x	107	1/1	0.87	0.15	62,62,62,62	0
56	MG	15	108	1/1	0.87	0.08	55,55,55,55	0
56	MG	1A	3325	1/1	0.87	0.17	66,66,66,66	0
56	MG	2A	3160	1/1	0.87	0.17	58,58,58,58	0
56	MG	1A	3925	1/1	0.87	0.29	49,49,49,49	0
56	MG	1B	234	1/1	0.87	0.16	64,64,64,64	0
56	MG	1A	3727	1/1	0.87	0.18	38,38,38,38	0
56	MG	1A	3352	1/1	0.87	0.21	48,48,48,48	0
56	MG	2Z	301	1/1	0.87	0.10	74,74,74,74	0
56	MG	2A	3423	1/1	0.87	0.13	74,74,74,74	0
56	MG	1a	1729	1/1	0.87	0.11	84,84,84,84	0
56	MG	2A	3171	1/1	0.87	0.11	58,58,58,58	0
56	MG	2A	3012	1/1	0.87	0.23	56,56,56,56	0
56	MG	2A	3676	1/1	0.87	0.16	60,60,60,60	0
56	MG	2A	3681	1/1	0.87	0.08	60,60,60,60	0
56	MG	1B	215	1/1	0.88	0.18	60,60,60,60	0
56	MG	2A	3679	1/1	0.88	0.08	67,67,67,67	0
56	MG	2A	3443	1/1	0.88	0.31	55,55,55,55	0
56	MG	1a	1703	1/1	0.88	0.18	64,64,64,64	0
56	MG	27	101	1/1	0.88	0.29	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	2A	3449	1/1	0.88	0.17	60,60,60,60	0
56	MG	1B	218	1/1	0.88	0.15	54,54,54,54	0
56	MG	13	103	1/1	0.88	0.21	51,51,51,51	0
56	MG	2A	3691	1/1	0.88	0.15	43,43,43,43	0
56	MG	1A	3553	1/1	0.88	0.30	43,43,43,43	0
56	MG	2A	3180	1/1	0.88	0.26	64,64,64,64	0
56	MG	1B	223	1/1	0.88	0.25	64,64,64,64	0
56	MG	1A	3140	1/1	0.88	0.42	42,42,42,42	0
56	MG	1A	3055	1/1	0.88	0.25	44,44,44,44	0
56	MG	2a	1614	1/1	0.88	0.18	68,68,68,68	0
56	MG	2A	3477	1/1	0.88	0.10	80,80,80,80	0
56	MG	2A	3705	1/1	0.88	0.13	61,61,61,61	0
56	MG	2a	1618	1/1	0.88	0.18	67,67,67,67	0
56	MG	1A	3206	1/1	0.88	0.16	51,51,51,51	0
56	MG	2a	1622	1/1	0.88	0.17	78,78,78,78	0
56	MG	1a	1738	1/1	0.88	0.13	65,65,65,65	0
56	MG	1A	3720	1/1	0.88	0.16	58,58,58,58	0
56	MG	2A	3717	1/1	0.88	0.11	82,82,82,82	0
56	MG	2a	1633	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	3823	1/1	0.88	0.12	58,58,58,58	0
56	MG	2A	3502	1/1	0.88	0.23	43,43,43,43	0
56	MG	2a	1641	1/1	0.88	0.17	78,78,78,78	0
56	MG	2A	3039	1/1	0.88	0.52	64,64,64,64	0
56	MG	2A	3723	1/1	0.88	0.22	60,60,60,60	0
56	MG	2A	3041	1/1	0.88	0.28	67,67,67,67	0
56	MG	2A	3507	1/1	0.88	0.21	63,63,63,63	0
56	MG	1A	3405	1/1	0.88	0.16	52,52,52,52	0
56	MG	1A	3825	1/1	0.88	0.18	52,52,52,52	0
56	MG	2A	3198	1/1	0.88	0.36	53,53,53,53	0
56	MG	1A	3145	1/1	0.88	0.11	42,42,42,42	0
56	MG	2A	3322	1/1	0.88	0.59	57,57,57,57	0
56	MG	1D	312	1/1	0.88	0.13	59,59,59,59	0
56	MG	1A	3661	1/1	0.88	0.20	34,34,34,34	0
56	MG	1A	3573	1/1	0.88	0.19	61,61,61,61	0
56	MG	1A	4042	1/1	0.88	0.23	56,56,56,56	0
56	MG	1A	3521	1/1	0.88	0.17	58,58,58,58	0
56	MG	2A	3753	1/1	0.88	0.22	47,47,47,47	0
56	MG	2A	3754	1/1	0.88	0.18	48,48,48,48	0
56	MG	1E	314	1/1	0.88	0.08	40,40,40,40	0
56	MG	2A	3757	1/1	0.88	0.24	41,41,41,41	0
56	MG	1A	3732	1/1	0.88	0.14	36,36,36,36	0
56	MG	2a	1693	1/1	0.88	0.15	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	1776	1/1	0.88	0.08	68,68,68,68	0
56	MG	1A	3191	1/1	0.88	0.20	50,50,50,50	0
56	MG	1A	3307	1/1	0.88	0.32	56,56,56,56	0
56	MG	2A	3557	1/1	0.88	0.23	62,62,62,62	0
56	MG	2A	3334	1/1	0.88	0.12	62,62,62,62	0
56	MG	2a	1706	1/1	0.88	0.24	66,66,66,66	0
56	MG	2A	3565	1/1	0.88	0.17	44,44,44,44	0
56	MG	1A	3875	1/1	0.88	0.17	27,27,27,27	0
56	MG	2A	3783	1/1	0.88	0.22	76,76,76,76	0
56	MG	2a	1717	1/1	0.88	0.13	72,72,72,72	0
56	MG	2A	3339	1/1	0.88	0.52	67,67,67,67	0
56	MG	2a	1726	1/1	0.88	0.28	68,68,68,68	0
56	MG	1A	3671	1/1	0.88	0.30	40,40,40,40	0
56	MG	2A	3086	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3788	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3236	1/1	0.88	0.15	72,72,72,72	0
56	MG	2A	3794	1/1	0.88	0.18	59,59,59,59	0
56	MG	2A	3237	1/1	0.88	0.20	59,59,59,59	0
56	MG	1A	4056	1/1	0.88	0.14	67,67,67,67	0
56	MG	1A	3353	1/1	0.88	0.60	47,47,47,47	0
56	MG	1A	3193	1/1	0.88	0.19	43,43,43,43	0
56	MG	2A	3092	1/1	0.88	0.20	46,46,46,46	0
56	MG	1A	3457	1/1	0.88	0.12	40,40,40,40	0
56	MG	2A	3097	1/1	0.88	0.12	68,68,68,68	0
56	MG	1A	3894	1/1	0.88	0.12	71,71,71,71	0
56	MG	2A	3362	1/1	0.88	0.11	71,71,71,71	0
56	MG	2A	3364	1/1	0.88	0.18	60,60,60,60	0
56	MG	2a	1787	1/1	0.88	0.38	70,70,70,70	0
56	MG	1R	205	1/1	0.88	0.29	40,40,40,40	0
56	MG	1n	101	1/1	0.88	0.09	56,56,56,56	0
56	MG	2a	1797	1/1	0.88	0.15	72,72,72,72	0
56	MG	2A	3618	1/1	0.88	0.16	64,64,64,64	0
56	MG	2A	3110	1/1	0.88	0.19	67,67,67,67	0
56	MG	2B	209	1/1	0.88	0.14	69,69,69,69	0
56	MG	2A	3625	1/1	0.88	0.14	62,62,62,62	0
56	MG	1A	3115	1/1	0.88	0.33	46,46,46,46	0
56	MG	2a	1810	1/1	0.88	0.14	78,78,78,78	0
56	MG	1A	3494	1/1	0.88	0.09	61,61,61,61	0
56	MG	2A	3122	1/1	0.88	0.14	68,68,68,68	0
56	MG	1A	3625	1/1	0.88	0.22	27,27,27,27	0
56	MG	2A	3386	1/1	0.88	0.45	58,58,58,58	0
56	MG	1A	3698	1/1	0.88	0.09	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	1A	3702	1/1	0.88	0.29	71,71,71,71	0
56	MG	2F	301	1/1	0.88	0.27	47,47,47,47	0
56	MG	1A	3989	1/1	0.88	0.07	45,45,45,45	0
56	MG	1a	1689	1/1	0.88	0.40	62,62,62,62	0
56	MG	1A	3311	1/1	0.88	0.18	42,42,42,42	0
56	MG	2A	3653	1/1	0.88	0.22	37,37,37,37	0
56	MG	2A	3272	1/1	0.88	0.35	59,59,59,59	0
56	MG	2A	3159	1/1	0.88	0.17	72,72,72,72	0
56	MG	1A	3214	1/1	0.88	0.58	65,65,65,65	0
56	MG	1x	110	1/1	0.88	0.19	45,45,45,45	0
56	MG	2A	3278	1/1	0.88	0.17	68,68,68,68	0
56	MG	1B	212	1/1	0.88	0.22	63,63,63,63	0
56	MG	1a	1694	1/1	0.88	0.18	72,72,72,72	0
56	MG	1A	3998	1/1	0.89	0.14	60,60,60,60	0
56	MG	1A	3441	1/1	0.89	0.38	58,58,58,58	0
56	MG	1A	3250	1/1	0.89	0.19	68,68,68,68	0
56	MG	2A	3353	1/1	0.89	0.27	53,53,53,53	0
56	MG	1A	3216	1/1	0.89	0.20	55,55,55,55	0
56	MG	2W	202	1/1	0.89	0.17	67,67,67,67	0
56	MG	1A	3163	1/1	0.89	0.33	57,57,57,57	0
56	MG	1A	3735	1/1	0.89	0.18	19,19,19,19	0
56	MG	1A	3515	1/1	0.89	0.54	56,56,56,56	0
56	MG	21	101	1/1	0.89	1.10	53,53,53,53	0
56	MG	1A	4018	1/1	0.89	0.29	58,58,58,58	0
56	MG	1A	3516	1/1	0.89	0.37	58,58,58,58	0
56	MG	25	105	1/1	0.89	0.31	60,60,60,60	0
56	MG	1A	3136	1/1	0.89	0.14	37,37,37,37	0
56	MG	2A	3363	1/1	0.89	0.12	72,72,72,72	0
56	MG	1A	3080	1/1	0.89	0.47	53,53,53,53	0
56	MG	1A	3451	1/1	0.89	0.13	43,43,43,43	0
56	MG	2A	3222	1/1	0.89	0.40	46,46,46,46	0
56	MG	1A	3004	1/1	0.89	0.12	28,28,28,28	0
56	MG	1A	3769	1/1	0.89	0.11	35,35,35,35	0
56	MG	2A	3659	1/1	0.89	0.14	64,64,64,64	0
56	MG	1A	3234	1/1	0.89	0.21	50,50,50,50	0
56	MG	1a	1698	1/1	0.89	0.09	46,46,46,46	0
56	MG	2A	3665	1/1	0.89	0.22	72,72,72,72	0
56	MG	2A	3235	1/1	0.89	0.18	61,61,61,61	0
56	MG	1A	3530	1/1	0.89	0.13	48,48,48,48	0
56	MG	2A	3387	1/1	0.89	0.30	60,60,60,60	0
56	MG	2A	3388	1/1	0.89	0.33	56,56,56,56	0
56	MG	2A	3391	1/1	0.89	0.37	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	3048	1/1	0.89	0.36	70,70,70,70	0
56	MG	1A	3919	1/1	0.89	0.07	47,47,47,47	0
56	MG	1A	4050	1/1	0.89	0.19	70,70,70,70	0
56	MG	2A	3400	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3244	1/1	0.89	0.13	55,55,55,55	0
56	MG	1A	3456	1/1	0.89	0.15	54,54,54,54	0
56	MG	1a	1707	1/1	0.89	0.25	58,58,58,58	0
56	MG	2a	1636	1/1	0.89	0.10	61,61,61,61	0
56	MG	1a	1708	1/1	0.89	0.19	48,48,48,48	0
56	MG	2a	1639	1/1	0.89	0.55	67,67,67,67	0
56	MG	2A	3700	1/1	0.89	0.19	66,66,66,66	0
56	MG	1a	1716	1/1	0.89	0.21	66,66,66,66	0
56	MG	1V	206	1/1	0.89	0.15	55,55,55,55	0
56	MG	2A	3422	1/1	0.89	0.59	60,60,60,60	0
56	MG	1A	3930	1/1	0.89	0.23	51,51,51,51	0
56	MG	2A	3425	1/1	0.89	0.27	64,64,64,64	0
56	MG	1A	3932	1/1	0.89	0.20	67,67,67,67	0
56	MG	1A	4069	1/1	0.89	0.19	54,54,54,54	0
56	MG	2A	3428	1/1	0.89	0.16	68,68,68,68	0
56	MG	2A	3259	1/1	0.89	0.19	55,55,55,55	0
56	MG	10	104	1/1	0.89	0.25	66,66,66,66	0
56	MG	2A	3078	1/1	0.89	0.44	58,58,58,58	0
56	MG	2A	3448	1/1	0.89	0.17	70,70,70,70	0
56	MG	1A	3349	1/1	0.89	0.48	65,65,65,65	0
56	MG	10	107	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	4073	1/1	0.89	0.20	57,57,57,57	0
56	MG	2a	1686	1/1	0.89	0.09	71,71,71,71	0
56	MG	11	101	1/1	0.89	0.75	47,47,47,47	0
56	MG	11	103	1/1	0.89	0.11	50,50,50,50	0
56	MG	2a	1690	1/1	0.89	0.07	71,71,71,71	0
56	MG	2A	3467	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3734	1/1	0.89	0.13	59,59,59,59	0
56	MG	2A	3090	1/1	0.89	0.57	61,61,61,61	0
56	MG	1A	4074	1/1	0.89	0.20	66,66,66,66	0
56	MG	1A	3073	1/1	0.89	0.16	34,34,34,34	0
56	MG	2A	3093	1/1	0.89	0.29	66,66,66,66	0
56	MG	1a	1754	1/1	0.89	0.10	52,52,52,52	0
56	MG	2A	3491	1/1	0.89	0.14	44,44,44,44	0
56	MG	2A	3497	1/1	0.89	0.11	76,76,76,76	0
56	MG	1A	3459	1/1	0.89	0.12	54,54,54,54	0
56	MG	15	103	1/1	0.89	0.34	42,42,42,42	0
56	MG	2A	3280	1/1	0.89	0.28	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	1A	3181	1/1	0.89	0.33	47,47,47,47	0
56	MG	1A	3812	1/1	0.89	0.11	50,50,50,50	0
56	MG	17	103	1/1	0.89	0.19	45,45,45,45	0
56	MG	17	106	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3314	1/1	0.89	0.15	64,64,64,64	0
56	MG	1a	1603	1/1	0.89	0.11	66,66,66,66	0
56	MG	2A	3125	1/1	0.89	0.22	49,49,49,49	0
56	MG	2A	3130	1/1	0.89	0.13	50,50,50,50	0
56	MG	1a	1780	1/1	0.89	0.08	78,78,78,78	0
56	MG	2A	3525	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3145	1/1	0.89	0.41	50,50,50,50	0
56	MG	1A	3407	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3300	1/1	0.89	0.20	67,67,67,67	0
56	MG	1A	3185	1/1	0.89	0.50	40,40,40,40	0
56	MG	1a	1791	1/1	0.89	0.15	75,75,75,75	0
56	MG	1A	3469	1/1	0.89	0.15	34,34,34,34	0
56	MG	1A	3074	1/1	0.89	0.17	39,39,39,39	0
56	MG	2A	3805	1/1	0.89	0.15	72,72,72,72	0
56	MG	2A	3544	1/1	0.89	0.30	70,70,70,70	0
56	MG	1A	3697	1/1	0.89	0.17	50,50,50,50	0
56	MG	1a	1800	1/1	0.89	0.28	58,58,58,58	0
56	MG	1A	3420	1/1	0.89	0.16	43,43,43,43	0
56	MG	1A	3831	1/1	0.89	0.13	42,42,42,42	0
56	MG	2a	1799	1/1	0.89	0.22	59,59,59,59	0
56	MG	1a	1811	1/1	0.89	0.06	61,61,61,61	0
56	MG	2A	3820	1/1	0.89	0.27	68,68,68,68	0
56	MG	1A	3244	1/1	0.89	0.20	38,38,38,38	0
56	MG	2A	3823	1/1	0.89	0.07	72,72,72,72	0
56	MG	2a	1805	1/1	0.89	0.12	65,65,65,65	0
56	MG	2A	3826	1/1	0.89	0.20	62,62,62,62	0
56	MG	1m	3001	1/1	0.89	0.12	57,57,57,57	0
56	MG	2A	3575	1/1	0.89	0.18	68,68,68,68	0
56	MG	1A	3972	1/1	0.89	0.24	42,42,42,42	0
56	MG	1A	3287	1/1	0.89	0.15	37,37,37,37	0
56	MG	1A	3108	1/1	0.89	0.26	39,39,39,39	0
56	MG	1a	1645	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3849	1/1	0.89	0.21	35,35,35,35	0
56	MG	1A	3370	1/1	0.89	0.42	42,42,42,42	0
56	MG	1A	3322	1/1	0.89	0.20	52,52,52,52	0
56	MG	1A	3213	1/1	0.89	0.11	44,44,44,44	0
56	MG	2A	3189	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3112	1/1	0.89	0.17	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	3610	1/1	0.89	0.12	31,31,31,31	0
56	MG	1A	3492	1/1	0.89	0.31	48,48,48,48	0
56	MG	1A	3380	1/1	0.89	0.35	47,47,47,47	0
56	MG	2A	3342	1/1	0.89	0.14	69,69,69,69	0
56	MG	1x	111	1/1	0.89	0.18	73,73,73,73	0
56	MG	1A	3437	1/1	0.89	0.33	41,41,41,41	0
56	MG	1A	3280	1/1	0.90	0.16	45,45,45,45	0
56	MG	1A	3123	1/1	0.90	0.22	37,37,37,37	0
56	MG	1A	3857	1/1	0.90	0.13	25,25,25,25	0
56	MG	1A	3576	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3436	1/1	0.90	0.18	69,69,69,69	0
56	MG	2A	3606	1/1	0.90	0.13	71,71,71,71	0
56	MG	1A	3104	1/1	0.90	0.23	42,42,42,42	0
56	MG	1A	3084	1/1	0.90	0.14	55,55,55,55	0
56	MG	2A	3352	1/1	0.90	0.11	74,74,74,74	0
56	MG	1a	1684	1/1	0.90	0.15	55,55,55,55	0
56	MG	2O	201	1/1	0.90	0.19	68,68,68,68	0
56	MG	1A	3719	1/1	0.90	0.21	54,54,54,54	0
56	MG	1A	4014	1/1	0.90	0.14	19,19,19,19	0
56	MG	2R	201	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3619	1/1	0.90	0.21	71,71,71,71	0
56	MG	1A	3442	1/1	0.90	0.25	67,67,67,67	0
56	MG	2A	3623	1/1	0.90	0.17	48,48,48,48	0
56	MG	2A	3026	1/1	0.90	0.78	58,58,58,58	0
56	MG	1Q	203	1/1	0.90	0.19	52,52,52,52	0
56	MG	2A	3632	1/1	0.90	0.12	58,58,58,58	0
56	MG	2A	3029	1/1	0.90	0.26	58,58,58,58	0
56	MG	2A	3030	1/1	0.90	0.29	45,45,45,45	0
56	MG	1A	3887	1/1	0.90	0.19	32,32,32,32	0
56	MG	1A	3607	1/1	0.90	0.21	61,61,61,61	0
56	MG	1A	3150	1/1	0.90	0.15	48,48,48,48	0
56	MG	1A	3156	1/1	0.90	0.19	52,52,52,52	0
56	MG	1a	1702	1/1	0.90	0.20	59,59,59,59	0
56	MG	2A	3378	1/1	0.90	0.36	66,66,66,66	0
56	MG	1A	3896	1/1	0.90	0.08	40,40,40,40	0
56	MG	2A	3649	1/1	0.90	0.36	60,60,60,60	0
56	MG	1U	207	1/1	0.90	0.65	42,42,42,42	0
56	MG	1A	3391	1/1	0.90	0.25	59,59,59,59	0
56	MG	2A	3231	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3233	1/1	0.90	0.37	68,68,68,68	0
56	MG	1A	3394	1/1	0.90	0.08	48,48,48,48	0
56	MG	2A	3051	1/1	0.90	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3389	1/1	0.90	0.28	63,63,63,63	0
56	MG	2a	1615	1/1	0.90	0.12	73,73,73,73	0
56	MG	1W	209	1/1	0.90	0.25	44,44,44,44	0
56	MG	2A	3394	1/1	0.90	0.37	52,52,52,52	0
56	MG	1A	3514	1/1	0.90	0.17	56,56,56,56	0
56	MG	2A	3673	1/1	0.90	0.37	77,77,77,77	0
56	MG	2A	3675	1/1	0.90	0.32	65,65,65,65	0
56	MG	1A	3046	1/1	0.90	0.19	56,56,56,56	0
56	MG	10	101	1/1	0.90	0.26	44,44,44,44	0
56	MG	2a	1629	1/1	0.90	0.11	75,75,75,75	0
56	MG	2A	3246	1/1	0.90	0.47	63,63,63,63	0
56	MG	2A	3061	1/1	0.90	0.06	70,70,70,70	0
56	MG	10	102	1/1	0.90	0.41	54,54,54,54	0
56	MG	1A	3398	1/1	0.90	0.16	48,48,48,48	0
56	MG	2A	3412	1/1	0.90	0.18	72,72,72,72	0
56	MG	1A	3738	1/1	0.90	0.14	78,78,78,78	0
56	MG	2A	3253	1/1	0.90	0.24	69,69,69,69	0
56	MG	2A	3067	1/1	0.90	0.34	58,58,58,58	0
56	MG	1A	3909	1/1	0.90	0.10	61,61,61,61	0
56	MG	2a	1652	1/1	0.90	0.21	41,41,41,41	0
56	MG	1A	3095	1/1	0.90	0.15	33,33,33,33	0
56	MG	1A	3258	1/1	0.90	0.13	41,41,41,41	0
56	MG	2A	3074	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3703	1/1	0.90	0.35	50,50,50,50	0
56	MG	2A	3076	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3635	1/1	0.90	0.17	27,27,27,27	0
56	MG	1a	1747	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3438	1/1	0.90	0.12	39,39,39,39	0
56	MG	2A	3714	1/1	0.90	0.12	60,60,60,60	0
56	MG	1A	4070	1/1	0.90	0.07	73,73,73,73	0
56	MG	1A	3096	1/1	0.90	0.31	43,43,43,43	0
56	MG	2a	1683	1/1	0.90	0.13	70,70,70,70	0
56	MG	1A	3754	1/1	0.90	0.25	60,60,60,60	0
56	MG	1A	3755	1/1	0.90	0.18	57,57,57,57	0
56	MG	1A	3756	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3072	1/1	0.90	0.24	41,41,41,41	0
56	MG	1A	3326	1/1	0.90	0.30	59,59,59,59	0
56	MG	2A	3460	1/1	0.90	0.14	61,61,61,61	0
56	MG	1A	3303	1/1	0.90	0.21	51,51,51,51	0
56	MG	2A	3730	1/1	0.90	0.11	68,68,68,68	0
56	MG	1A	3771	1/1	0.90	0.18	59,59,59,59	0
56	MG	2a	1695	1/1	0.90	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1696	1/1	0.90	0.12	60,60,60,60	0
56	MG	1a	1766	1/1	0.90	0.08	49,49,49,49	0
56	MG	2A	3277	1/1	0.90	0.22	63,63,63,63	0
56	MG	1a	1767	1/1	0.90	0.10	55,55,55,55	0
56	MG	2a	1703	1/1	0.90	0.29	61,61,61,61	0
56	MG	1A	3332	1/1	0.90	0.12	55,55,55,55	0
56	MG	2A	3480	1/1	0.90	0.51	60,60,60,60	0
56	MG	2A	3489	1/1	0.90	0.08	63,63,63,63	0
56	MG	2A	3102	1/1	0.90	0.12	82,82,82,82	0
56	MG	1a	1775	1/1	0.90	0.21	45,45,45,45	0
56	MG	2A	3107	1/1	0.90	0.09	46,46,46,46	0
56	MG	1A	3653	1/1	0.90	0.19	32,32,32,32	0
56	MG	1A	3413	1/1	0.90	0.29	57,57,57,57	0
56	MG	2A	3114	1/1	0.90	0.21	61,61,61,61	0
56	MG	2A	3756	1/1	0.90	0.24	43,43,43,43	0
56	MG	2A	3501	1/1	0.90	0.09	55,55,55,55	0
56	MG	1a	1779	1/1	0.90	0.10	64,64,64,64	0
56	MG	1A	3542	1/1	0.90	0.22	46,46,46,46	0
56	MG	1A	3414	1/1	0.90	0.21	47,47,47,47	0
56	MG	2a	1743	1/1	0.90	0.10	67,67,67,67	0
56	MG	2a	1744	1/1	0.90	0.26	49,49,49,49	0
56	MG	2A	3767	1/1	0.90	0.17	61,61,61,61	0
56	MG	1A	3372	1/1	0.90	0.48	45,45,45,45	0
56	MG	1a	1621	1/1	0.90	0.16	56,56,56,56	0
56	MG	2A	3140	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1626	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3775	1/1	0.90	0.26	58,58,58,58	0
56	MG	2A	3302	1/1	0.90	0.36	59,59,59,59	0
56	MG	2a	1776	1/1	0.90	0.15	65,65,65,65	0
56	MG	1B	213	1/1	0.90	0.29	63,63,63,63	0
56	MG	2A	3523	1/1	0.90	0.34	73,73,73,73	0
56	MG	1A	3141	1/1	0.90	0.23	32,32,32,32	0
56	MG	2a	1781	1/1	0.90	0.16	77,77,77,77	0
56	MG	2a	1783	1/1	0.90	0.31	71,71,71,71	0
56	MG	2A	3528	1/1	0.90	0.15	58,58,58,58	0
56	MG	1A	3272	1/1	0.90	0.24	46,46,46,46	0
56	MG	2A	3313	1/1	0.90	0.09	85,85,85,85	0
56	MG	2a	1796	1/1	0.90	0.11	71,71,71,71	0
56	MG	1A	3471	1/1	0.90	0.21	41,41,41,41	0
56	MG	2A	3795	1/1	0.90	0.14	56,56,56,56	0
56	MG	1A	3815	1/1	0.90	0.17	43,43,43,43	0
56	MG	2A	3802	1/1	0.90	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3539	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3376	1/1	0.90	0.09	51,51,51,51	0
56	MG	1f	201	1/1	0.90	0.22	50,50,50,50	0
56	MG	2A	3319	1/1	0.90	0.32	54,54,54,54	0
56	MG	2A	3161	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3548	1/1	0.90	0.21	71,71,71,71	0
56	MG	1A	3970	1/1	0.90	0.20	25,25,25,25	0
56	MG	1a	1644	1/1	0.90	0.10	53,53,53,53	0
56	MG	1A	3336	1/1	0.90	0.16	68,68,68,68	0
56	MG	1A	3555	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3556	1/1	0.90	0.24	62,62,62,62	0
56	MG	2A	3564	1/1	0.90	0.16	77,77,77,77	0
56	MG	1A	3688	1/1	0.90	0.16	61,61,61,61	0
56	MG	2v	103	1/1	0.90	0.18	59,59,59,59	0
56	MG	1A	3689	1/1	0.90	0.10	63,63,63,63	0
56	MG	1A	3560	1/1	0.90	0.22	43,43,43,43	0
56	MG	1A	3427	1/1	0.90	0.20	57,57,57,57	0
56	MG	2B	207	1/1	0.90	0.15	67,67,67,67	0
56	MG	1A	3379	1/1	0.90	0.32	44,44,44,44	0
56	MG	1A	3699	1/1	0.90	0.15	49,49,49,49	0
56	MG	2x	107	1/1	0.90	0.21	61,61,61,61	0
56	MG	1A	3848	1/1	0.90	0.14	31,31,31,31	0
56	MG	2y	101	1/1	0.90	0.12	62,62,62,62	0
56	MG	1E	308	1/1	0.90	0.21	66,66,66,66	0
56	MG	2B	213	1/1	0.90	0.23	54,54,54,54	0
56	MG	1A	3279	1/1	0.90	0.19	28,28,28,28	0
58	ZN	14	102	1/1	0.90	0.07	95,95,95,95	0
56	MG	2A	3822	1/1	0.91	0.10	71,71,71,71	0
56	MG	2A	3537	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3618	1/1	0.91	0.18	41,41,41,41	0
56	MG	14	101	1/1	0.91	0.21	71,71,71,71	0
56	MG	2A	3117	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3119	1/1	0.91	0.09	76,76,76,76	0
56	MG	1A	3933	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3803	1/1	0.91	0.08	42,42,42,42	0
56	MG	2A	3546	1/1	0.91	0.22	67,67,67,67	0
56	MG	2A	3311	1/1	0.91	0.23	74,74,74,74	0
56	MG	1a	1778	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3297	1/1	0.91	0.21	51,51,51,51	0
56	MG	2A	3555	1/1	0.91	0.18	39,39,39,39	0
56	MG	1A	4077	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3135	1/1	0.91	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3559	1/1	0.91	0.24	52,52,52,52	0
56	MG	1a	1782	1/1	0.91	0.10	74,74,74,74	0
56	MG	2B	219	1/1	0.91	0.08	75,75,75,75	0
56	MG	1A	3299	1/1	0.91	0.20	49,49,49,49	0
56	MG	1a	1785	1/1	0.91	0.21	66,66,66,66	0
56	MG	2A	3150	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3038	1/1	0.91	0.12	36,36,36,36	0
56	MG	1A	4082	1/1	0.91	0.16	65,65,65,65	0
56	MG	1A	3043	1/1	0.91	0.20	34,34,34,34	0
56	MG	2A	3585	1/1	0.91	0.11	58,58,58,58	0
56	MG	1B	202	1/1	0.91	0.32	57,57,57,57	0
56	MG	2A	3158	1/1	0.91	0.33	48,48,48,48	0
56	MG	1a	1606	1/1	0.91	0.22	53,53,53,53	0
56	MG	1A	3626	1/1	0.91	0.14	62,62,62,62	0
56	MG	1a	1617	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3264	1/1	0.91	0.25	55,55,55,55	0
56	MG	1A	3217	1/1	0.91	0.18	54,54,54,54	0
56	MG	1A	3717	1/1	0.91	0.10	49,49,49,49	0
56	MG	2A	3603	1/1	0.91	0.14	70,70,70,70	0
56	MG	1A	3275	1/1	0.91	0.22	46,46,46,46	0
56	MG	1A	3218	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3957	1/1	0.91	0.24	47,47,47,47	0
56	MG	2A	3172	1/1	0.91	0.27	59,59,59,59	0
56	MG	2A	3612	1/1	0.91	0.16	64,64,64,64	0
56	MG	2A	3340	1/1	0.91	0.24	72,72,72,72	0
56	MG	1a	1634	1/1	0.91	0.13	54,54,54,54	0
56	MG	26	101	1/1	0.91	0.07	69,69,69,69	0
56	MG	2A	3615	1/1	0.91	0.15	65,65,65,65	0
56	MG	1A	3489	1/1	0.91	0.56	41,41,41,41	0
56	MG	27	103	1/1	0.91	0.73	58,58,58,58	0
56	MG	2A	3179	1/1	0.91	0.15	50,50,50,50	0
56	MG	29	101	1/1	0.91	0.61	71,71,71,71	0
56	MG	1a	1636	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3959	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3960	1/1	0.91	0.25	44,44,44,44	0
56	MG	1a	1640	1/1	0.91	0.10	67,67,67,67	0
56	MG	1A	3638	1/1	0.91	0.15	31,31,31,31	0
56	MG	2A	3630	1/1	0.91	0.14	52,52,52,52	0
56	MG	1A	3834	1/1	0.91	0.41	36,36,36,36	0
56	MG	2A	3356	1/1	0.91	0.08	67,67,67,67	0
56	MG	2A	3635	1/1	0.91	0.15	69,69,69,69	0
56	MG	1A	3640	1/1	0.91	0.16	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	3107	1/1	0.91	0.22	49,49,49,49	0
56	MG	1A	3450	1/1	0.91	0.11	54,54,54,54	0
56	MG	1B	232	1/1	0.91	0.23	64,64,64,64	0
56	MG	1A	3978	1/1	0.91	0.19	51,51,51,51	0
56	MG	2A	3644	1/1	0.91	0.12	62,62,62,62	0
56	MG	1A	3201	1/1	0.91	0.25	61,61,61,61	0
56	MG	1A	3498	1/1	0.91	0.18	53,53,53,53	0
56	MG	1A	3418	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3365	1/1	0.91	0.34	65,65,65,65	0
56	MG	2A	3199	1/1	0.91	0.26	66,66,66,66	0
56	MG	2A	3200	1/1	0.91	0.17	52,52,52,52	0
56	MG	1A	3656	1/1	0.91	0.11	66,66,66,66	0
56	MG	2A	3656	1/1	0.91	0.28	67,67,67,67	0
56	MG	2A	3657	1/1	0.91	0.17	58,58,58,58	0
56	MG	2a	1642	1/1	0.91	0.07	80,80,80,80	0
56	MG	2a	1643	1/1	0.91	0.10	79,79,79,79	0
56	MG	2a	1645	1/1	0.91	0.26	47,47,47,47	0
56	MG	2A	3377	1/1	0.91	0.29	63,63,63,63	0
56	MG	1D	313	1/1	0.91	0.26	39,39,39,39	0
56	MG	2A	3009	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	3419	1/1	0.91	0.14	59,59,59,59	0
56	MG	2A	3209	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3743	1/1	0.91	0.10	51,51,51,51	0
56	MG	2A	3385	1/1	0.91	0.24	58,58,58,58	0
56	MG	2a	1664	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3211	1/1	0.91	0.20	63,63,63,63	0
56	MG	2a	1670	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3871	1/1	0.91	0.12	45,45,45,45	0
56	MG	1A	3872	1/1	0.91	0.20	43,43,43,43	0
56	MG	2A	3677	1/1	0.91	0.15	64,64,64,64	0
56	MG	2a	1679	1/1	0.91	0.09	56,56,56,56	0
56	MG	1A	3455	1/1	0.91	0.24	56,56,56,56	0
56	MG	2A	3390	1/1	0.91	0.36	78,78,78,78	0
56	MG	1a	1679	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3392	1/1	0.91	0.25	45,45,45,45	0
56	MG	1A	3876	1/1	0.91	0.14	32,32,32,32	0
56	MG	2A	3221	1/1	0.91	0.49	52,52,52,52	0
56	MG	1A	3997	1/1	0.91	0.08	44,44,44,44	0
56	MG	2A	3397	1/1	0.91	0.38	68,68,68,68	0
56	MG	1F	305	1/1	0.91	0.14	35,35,35,35	0
56	MG	1A	3878	1/1	0.91	0.13	37,37,37,37	0
56	MG	1A	3665	1/1	0.91	0.08	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	3227	1/1	0.91	0.13	42,42,42,42	0
56	MG	1A	4003	1/1	0.91	0.14	58,58,58,58	0
56	MG	1A	3746	1/1	0.91	0.09	76,76,76,76	0
56	MG	1A	3748	1/1	0.91	0.13	34,34,34,34	0
56	MG	1N	201	1/1	0.91	0.17	63,63,63,63	0
56	MG	2a	1700	1/1	0.91	0.13	79,79,79,79	0
56	MG	2A	3420	1/1	0.91	0.27	68,68,68,68	0
56	MG	2A	3044	1/1	0.91	0.29	65,65,65,65	0
56	MG	1N	202	1/1	0.91	0.39	52,52,52,52	0
56	MG	1N	203	1/1	0.91	0.20	48,48,48,48	0
56	MG	1A	3045	1/1	0.91	0.18	45,45,45,45	0
56	MG	1A	3511	1/1	0.91	0.14	22,22,22,22	0
56	MG	2a	1710	1/1	0.91	0.35	69,69,69,69	0
56	MG	2A	3054	1/1	0.91	0.13	67,67,67,67	0
56	MG	2a	1713	1/1	0.91	0.17	66,66,66,66	0
56	MG	1A	3132	1/1	0.91	0.22	34,34,34,34	0
56	MG	1A	3383	1/1	0.91	0.15	63,63,63,63	0
56	MG	2A	3058	1/1	0.91	0.16	58,58,58,58	0
56	MG	2A	3441	1/1	0.91	0.40	63,63,63,63	0
56	MG	2a	1719	1/1	0.91	0.21	71,71,71,71	0
56	MG	2A	3442	1/1	0.91	0.10	67,67,67,67	0
56	MG	1Q	204	1/1	0.91	0.11	57,57,57,57	0
56	MG	1A	3578	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3759	1/1	0.91	0.17	32,32,32,32	0
56	MG	1A	4021	1/1	0.91	0.11	45,45,45,45	0
56	MG	1a	1713	1/1	0.91	0.13	72,72,72,72	0
56	MG	2a	1740	1/1	0.91	0.10	77,77,77,77	0
56	MG	1A	3899	1/1	0.91	0.12	41,41,41,41	0
56	MG	2A	3258	1/1	0.91	0.23	59,59,59,59	0
56	MG	2A	3739	1/1	0.91	0.14	70,70,70,70	0
56	MG	2A	3457	1/1	0.91	0.34	52,52,52,52	0
56	MG	2A	3068	1/1	0.91	0.29	48,48,48,48	0
56	MG	2A	3461	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3750	1/1	0.91	0.12	66,66,66,66	0
56	MG	2a	1767	1/1	0.91	0.15	71,71,71,71	0
56	MG	2a	1769	1/1	0.91	0.07	76,76,76,76	0
56	MG	2A	3462	1/1	0.91	0.16	75,75,75,75	0
56	MG	2a	1772	1/1	0.91	0.28	56,56,56,56	0
56	MG	1A	4026	1/1	0.91	0.20	38,38,38,38	0
56	MG	1A	3229	1/1	0.91	0.16	52,52,52,52	0
56	MG	1A	3110	1/1	0.91	0.19	41,41,41,41	0
56	MG	2a	1778	1/1	0.91	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3072	1/1	0.91	0.21	47,47,47,47	0
56	MG	2A	3471	1/1	0.91	0.13	45,45,45,45	0
56	MG	2A	3265	1/1	0.91	0.15	58,58,58,58	0
56	MG	1A	3763	1/1	0.91	0.07	62,62,62,62	0
56	MG	2A	3761	1/1	0.91	0.30	51,51,51,51	0
56	MG	2A	3763	1/1	0.91	0.14	41,41,41,41	0
56	MG	1W	203	1/1	0.91	0.27	46,46,46,46	0
56	MG	2A	3485	1/1	0.91	0.15	37,37,37,37	0
56	MG	1W	204	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3764	1/1	0.91	0.09	51,51,51,51	0
56	MG	2A	3084	1/1	0.91	0.26	56,56,56,56	0
56	MG	2A	3494	1/1	0.91	0.21	40,40,40,40	0
56	MG	1X	102	1/1	0.91	0.15	37,37,37,37	0
56	MG	1A	3677	1/1	0.91	0.45	61,61,61,61	0
56	MG	1A	4046	1/1	0.91	0.19	63,63,63,63	0
56	MG	1a	1748	1/1	0.91	0.19	67,67,67,67	0
56	MG	2a	1809	1/1	0.91	0.17	82,82,82,82	0
56	MG	2A	3785	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3007	1/1	0.91	0.13	41,41,41,41	0
56	MG	1A	3008	1/1	0.91	0.16	33,33,33,33	0
56	MG	1A	3604	1/1	0.91	0.15	25,25,25,25	0
56	MG	1A	3778	1/1	0.91	0.12	29,29,29,29	0
56	MG	2q	202	1/1	0.91	0.11	73,73,73,73	0
56	MG	1A	3779	1/1	0.91	0.21	54,54,54,54	0
56	MG	1A	4059	1/1	0.91	0.18	52,52,52,52	0
56	MG	1A	3793	1/1	0.91	0.16	63,63,63,63	0
56	MG	2A	3801	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3005	1/1	0.91	0.28	48,48,48,48	0
56	MG	1A	3321	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3804	1/1	0.91	0.24	45,45,45,45	0
56	MG	2A	3518	1/1	0.91	0.29	49,49,49,49	0
56	MG	1a	1765	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3809	1/1	0.91	0.25	54,54,54,54	0
56	MG	1A	3294	1/1	0.91	0.23	50,50,50,50	0
56	MG	2A	3108	1/1	0.91	0.12	63,63,63,63	0
56	MG	2A	3295	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3296	1/1	0.91	0.36	65,65,65,65	0
56	MG	2A	3815	1/1	0.91	0.17	65,65,65,65	0
56	MG	2A	3530	1/1	0.91	0.11	43,43,43,43	0
56	MG	2A	3297	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	4072	1/1	0.91	0.30	54,54,54,54	0
58	ZN	24	501	1/1	0.91	0.06	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3213	1/1	0.92	0.15	68,68,68,68	0
56	MG	1A	3660	1/1	0.92	0.19	37,37,37,37	0
56	MG	1A	3019	1/1	0.92	0.18	36,36,36,36	0
56	MG	20	103	1/1	0.92	0.21	64,64,64,64	0
56	MG	20	104	1/1	0.92	0.11	60,60,60,60	0
56	MG	20	105	1/1	0.92	0.16	70,70,70,70	0
56	MG	2A	3638	1/1	0.92	0.19	60,60,60,60	0
56	MG	1N	205	1/1	0.92	0.33	49,49,49,49	0
56	MG	2A	3218	1/1	0.92	0.28	49,49,49,49	0
56	MG	1A	3316	1/1	0.92	0.23	53,53,53,53	0
56	MG	1A	3044	1/1	0.92	0.22	35,35,35,35	0
56	MG	1A	3446	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	4034	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	4038	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	3111	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3567	1/1	0.92	0.13	31,31,31,31	0
56	MG	2A	3228	1/1	0.92	0.28	49,49,49,49	0
56	MG	1a	1693	1/1	0.92	0.23	62,62,62,62	0
56	MG	2a	1601	1/1	0.92	0.13	63,63,63,63	0
56	MG	1S	202	1/1	0.92	0.11	59,59,59,59	0
56	MG	2a	1605	1/1	0.92	0.12	78,78,78,78	0
56	MG	2a	1607	1/1	0.92	0.15	65,65,65,65	0
56	MG	1A	3162	1/1	0.92	0.66	51,51,51,51	0
56	MG	1a	1699	1/1	0.92	0.25	60,60,60,60	0
56	MG	1T	202	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3906	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3057	1/1	0.92	0.23	60,60,60,60	0
56	MG	1A	3496	1/1	0.92	0.18	62,62,62,62	0
56	MG	1U	206	1/1	0.92	0.33	40,40,40,40	0
56	MG	2A	3669	1/1	0.92	0.12	42,42,42,42	0
56	MG	1A	3773	1/1	0.92	0.13	36,36,36,36	0
56	MG	2A	3419	1/1	0.92	0.16	77,77,77,77	0
56	MG	1A	4048	1/1	0.92	0.15	63,63,63,63	0
56	MG	1V	202	1/1	0.92	0.32	39,39,39,39	0
56	MG	1A	3571	1/1	0.92	0.16	46,46,46,46	0
56	MG	2A	3065	1/1	0.92	0.30	61,61,61,61	0
56	MG	2A	3678	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3066	1/1	0.92	0.23	38,38,38,38	0
56	MG	2A	3680	1/1	0.92	0.22	60,60,60,60	0
56	MG	1W	202	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3911	1/1	0.92	0.12	71,71,71,71	0
56	MG	1A	3777	1/1	0.92	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1637	1/1	0.92	0.12	79,79,79,79	0
56	MG	2A	3435	1/1	0.92	0.17	65,65,65,65	0
56	MG	1A	3572	1/1	0.92	0.17	29,29,29,29	0
56	MG	1A	4058	1/1	0.92	0.10	34,34,34,34	0
56	MG	2A	3440	1/1	0.92	0.15	53,53,53,53	0
56	MG	1X	103	1/1	0.92	0.20	48,48,48,48	0
56	MG	2a	1644	1/1	0.92	0.14	68,68,68,68	0
56	MG	2A	3073	1/1	0.92	0.48	45,45,45,45	0
56	MG	1X	106	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	3010	1/1	0.92	0.14	38,38,38,38	0
56	MG	2a	1651	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	4061	1/1	0.92	0.26	68,68,68,68	0
56	MG	1A	3790	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3918	1/1	0.92	0.14	59,59,59,59	0
56	MG	2A	3267	1/1	0.92	0.29	68,68,68,68	0
56	MG	2a	1658	1/1	0.92	0.09	62,62,62,62	0
56	MG	1A	3065	1/1	0.92	0.41	55,55,55,55	0
56	MG	2a	1663	1/1	0.92	0.12	69,69,69,69	0
56	MG	1A	3682	1/1	0.92	0.28	47,47,47,47	0
56	MG	2a	1665	1/1	0.92	0.19	53,53,53,53	0
56	MG	2A	3458	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3117	1/1	0.92	0.22	34,34,34,34	0
56	MG	1A	3021	1/1	0.92	0.09	69,69,69,69	0
56	MG	1A	3231	1/1	0.92	0.19	37,37,37,37	0
56	MG	2A	3463	1/1	0.92	0.17	47,47,47,47	0
56	MG	1A	3593	1/1	0.92	0.06	36,36,36,36	0
56	MG	1A	3805	1/1	0.92	0.17	39,39,39,39	0
56	MG	11	104	1/1	0.92	0.20	63,63,63,63	0
56	MG	2A	3276	1/1	0.92	0.38	65,65,65,65	0
56	MG	1A	3510	1/1	0.92	0.25	51,51,51,51	0
56	MG	1A	4078	1/1	0.92	0.21	44,44,44,44	0
56	MG	13	102	1/1	0.92	0.18	47,47,47,47	0
56	MG	2A	3478	1/1	0.92	0.19	55,55,55,55	0
56	MG	2A	3479	1/1	0.92	0.09	53,53,53,53	0
56	MG	1A	3600	1/1	0.92	0.14	27,27,27,27	0
56	MG	2A	3484	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3327	1/1	0.92	0.23	38,38,38,38	0
56	MG	2A	3487	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3298	1/1	0.92	0.17	46,46,46,46	0
56	MG	2a	1694	1/1	0.92	0.26	56,56,56,56	0
56	MG	2A	3743	1/1	0.92	0.18	74,74,74,74	0
56	MG	2A	3105	1/1	0.92	0.31	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3106	1/1	0.92	0.14	68,68,68,68	0
56	MG	2A	3748	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3493	1/1	0.92	0.11	53,53,53,53	0
56	MG	1a	1772	1/1	0.92	0.11	76,76,76,76	0
56	MG	1A	3143	1/1	0.92	0.24	40,40,40,40	0
56	MG	2A	3289	1/1	0.92	0.12	77,77,77,77	0
56	MG	2A	3109	1/1	0.92	0.22	68,68,68,68	0
56	MG	1A	3945	1/1	0.92	0.12	67,67,67,67	0
56	MG	2a	1707	1/1	0.92	0.12	67,67,67,67	0
56	MG	2a	1709	1/1	0.92	0.21	58,58,58,58	0
56	MG	2A	3294	1/1	0.92	0.32	69,69,69,69	0
56	MG	16	101	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3609	1/1	0.92	0.17	37,37,37,37	0
56	MG	1A	3378	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3613	1/1	0.92	0.14	65,65,65,65	0
56	MG	1A	3208	1/1	0.92	0.28	44,44,44,44	0
56	MG	1A	3517	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3123	1/1	0.92	0.21	73,73,73,73	0
56	MG	1a	1784	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3828	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3305	1/1	0.92	0.20	62,62,62,62	0
56	MG	1A	3460	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	1788	1/1	0.92	0.12	69,69,69,69	0
56	MG	2A	3137	1/1	0.92	0.29	53,53,53,53	0
56	MG	1a	1607	1/1	0.92	0.16	52,52,52,52	0
56	MG	1a	1608	1/1	0.92	0.23	58,58,58,58	0
56	MG	2A	3531	1/1	0.92	0.07	70,70,70,70	0
56	MG	2a	1747	1/1	0.92	0.10	62,62,62,62	0
56	MG	2a	1748	1/1	0.92	0.20	63,63,63,63	0
56	MG	2A	3315	1/1	0.92	0.26	61,61,61,61	0
56	MG	1A	3621	1/1	0.92	0.20	41,41,41,41	0
56	MG	1a	1796	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3236	1/1	0.92	0.23	62,62,62,62	0
56	MG	2a	1757	1/1	0.92	0.17	68,68,68,68	0
56	MG	1A	3520	1/1	0.92	0.09	69,69,69,69	0
56	MG	2a	1762	1/1	0.92	0.18	68,68,68,68	0
56	MG	2a	1764	1/1	0.92	0.23	69,69,69,69	0
56	MG	2A	3798	1/1	0.92	0.41	70,70,70,70	0
56	MG	1A	3463	1/1	0.92	0.31	47,47,47,47	0
56	MG	1A	3263	1/1	0.92	0.37	41,41,41,41	0
56	MG	1a	1627	1/1	0.92	0.20	68,68,68,68	0
56	MG	1B	226	1/1	0.92	0.27	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	3728	1/1	0.92	0.15	30,30,30,30	0
56	MG	1l	202	1/1	0.92	0.16	69,69,69,69	0
56	MG	1A	3023	1/1	0.92	0.15	30,30,30,30	0
56	MG	2A	3550	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3426	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3854	1/1	0.92	0.14	26,26,26,26	0
56	MG	1B	233	1/1	0.92	0.15	64,64,64,64	0
56	MG	2a	1784	1/1	0.92	0.09	69,69,69,69	0
56	MG	2a	1785	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	3855	1/1	0.92	0.15	28,28,28,28	0
56	MG	2a	1789	1/1	0.92	0.26	64,64,64,64	0
56	MG	1w	101	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3051	1/1	0.92	0.20	55,55,55,55	0
56	MG	2A	3333	1/1	0.92	0.05	74,74,74,74	0
56	MG	2A	3173	1/1	0.92	0.20	63,63,63,63	0
56	MG	1A	3187	1/1	0.92	0.35	41,41,41,41	0
56	MG	2A	3573	1/1	0.92	0.19	46,46,46,46	0
56	MG	1A	3341	1/1	0.92	0.17	51,51,51,51	0
56	MG	2A	3178	1/1	0.92	0.11	60,60,60,60	0
56	MG	1x	103	1/1	0.92	0.26	71,71,71,71	0
56	MG	1A	3866	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3869	1/1	0.92	0.10	41,41,41,41	0
56	MG	2B	206	1/1	0.92	0.22	73,73,73,73	0
56	MG	1A	3472	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	3388	1/1	0.92	0.19	57,57,57,57	0
56	MG	2d	301	1/1	0.92	0.07	70,70,70,70	0
56	MG	2f	202	1/1	0.92	0.24	74,74,74,74	0
56	MG	2g	201	1/1	0.92	0.11	69,69,69,69	0
56	MG	1a	1649	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3873	1/1	0.92	0.29	43,43,43,43	0
56	MG	1A	3474	1/1	0.92	0.33	73,73,73,73	0
56	MG	1x	114	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3355	1/1	0.92	0.23	61,61,61,61	0
56	MG	1E	311	1/1	0.92	0.08	62,62,62,62	0
56	MG	1A	3276	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3001	1/1	0.92	0.34	65,65,65,65	0
56	MG	1A	3645	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3551	1/1	0.92	0.38	34,34,34,34	0
56	MG	1A	3750	1/1	0.92	0.11	41,41,41,41	0
56	MG	1a	1666	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	3884	1/1	0.92	0.08	42,42,42,42	0
56	MG	2A	3013	1/1	0.92	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3648	1/1	0.92	0.17	35,35,35,35	0
56	MG	2A	3371	1/1	0.92	0.22	57,57,57,57	0
56	MG	1a	1671	1/1	0.92	0.27	66,66,66,66	0
56	MG	2A	3374	1/1	0.92	0.29	46,46,46,46	0
56	MG	1A	4013	1/1	0.92	0.30	74,74,74,74	0
56	MG	1A	3243	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3014	1/1	0.92	0.14	33,33,33,33	0
56	MG	2A	3028	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3189	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3659	1/1	0.93	0.09	41,41,41,41	0
56	MG	1B	220	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3508	1/1	0.93	0.20	57,57,57,57	0
56	MG	1A	3509	1/1	0.93	0.19	63,63,63,63	0
56	MG	1A	3277	1/1	0.93	0.17	57,57,57,57	0
56	MG	2A	3662	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	3462	1/1	0.93	0.23	42,42,42,42	0
56	MG	2A	3430	1/1	0.93	0.15	62,62,62,62	0
56	MG	2A	3668	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3434	1/1	0.93	0.45	73,73,73,73	0
56	MG	1A	3574	1/1	0.93	0.15	35,35,35,35	0
56	MG	1A	3246	1/1	0.93	0.12	66,66,66,66	0
56	MG	1A	3082	1/1	0.93	0.28	56,56,56,56	0
56	MG	1A	3050	1/1	0.93	0.18	45,45,45,45	0
56	MG	1A	3588	1/1	0.93	0.17	47,47,47,47	0
56	MG	1a	1773	1/1	0.93	0.13	60,60,60,60	0
56	MG	1A	3011	1/1	0.93	0.20	40,40,40,40	0
56	MG	1A	3999	1/1	0.93	0.20	53,53,53,53	0
56	MG	1A	4000	1/1	0.93	0.14	26,26,26,26	0
56	MG	1B	237	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3100	1/1	0.93	0.12	28,28,28,28	0
56	MG	1a	1619	1/1	0.93	0.14	49,49,49,49	0
56	MG	2a	1620	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3888	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3456	1/1	0.93	0.16	27,27,27,27	0
56	MG	1a	1781	1/1	0.93	0.10	50,50,50,50	0
56	MG	1a	1624	1/1	0.93	0.13	56,56,56,56	0
56	MG	1D	303	1/1	0.93	0.25	43,43,43,43	0
56	MG	1A	3591	1/1	0.93	0.18	27,27,27,27	0
56	MG	1A	3202	1/1	0.93	0.17	36,36,36,36	0
56	MG	2a	1634	1/1	0.93	0.24	79,79,79,79	0
56	MG	1a	1786	1/1	0.93	0.11	62,62,62,62	0
56	MG	1A	3203	1/1	0.93	0.23	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	3227	1/1	0.93	0.51	38,38,38,38	0
56	MG	1a	1789	1/1	0.93	0.20	80,80,80,80	0
56	MG	1a	1790	1/1	0.93	0.12	67,67,67,67	0
56	MG	2a	1640	1/1	0.93	0.07	71,71,71,71	0
56	MG	1a	1633	1/1	0.93	0.19	65,65,65,65	0
56	MG	2A	3709	1/1	0.93	0.22	67,67,67,67	0
56	MG	1A	3601	1/1	0.93	0.13	42,42,42,42	0
56	MG	2A	3121	1/1	0.93	0.10	52,52,52,52	0
56	MG	1a	1793	1/1	0.93	0.06	71,71,71,71	0
56	MG	2A	3293	1/1	0.93	0.22	69,69,69,69	0
56	MG	1A	3354	1/1	0.93	0.21	50,50,50,50	0
56	MG	1A	3792	1/1	0.93	0.30	43,43,43,43	0
56	MG	2A	3127	1/1	0.93	0.14	73,73,73,73	0
56	MG	2A	3722	1/1	0.93	0.14	75,75,75,75	0
56	MG	1A	3901	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	1656	1/1	0.93	0.26	60,60,60,60	0
56	MG	2A	3132	1/1	0.93	0.25	51,51,51,51	0
56	MG	2A	3133	1/1	0.93	0.15	42,42,42,42	0
56	MG	2A	3726	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	1662	1/1	0.93	0.23	59,59,59,59	0
56	MG	1A	3228	1/1	0.93	0.30	33,33,33,33	0
56	MG	2A	3729	1/1	0.93	0.12	59,59,59,59	0
56	MG	2A	3492	1/1	0.93	0.16	40,40,40,40	0
56	MG	1A	3795	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3522	1/1	0.93	0.33	41,41,41,41	0
56	MG	1A	3357	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3087	1/1	0.93	0.16	72,72,72,72	0
56	MG	2a	1677	1/1	0.93	0.20	69,69,69,69	0
56	MG	1A	3612	1/1	0.93	0.14	28,28,28,28	0
56	MG	2A	3309	1/1	0.93	0.13	74,74,74,74	0
56	MG	2A	3738	1/1	0.93	0.13	66,66,66,66	0
56	MG	1A	4033	1/1	0.93	0.06	55,55,55,55	0
56	MG	1A	3477	1/1	0.93	0.19	44,44,44,44	0
56	MG	1A	4036	1/1	0.93	0.26	35,35,35,35	0
56	MG	1A	3804	1/1	0.93	0.30	54,54,54,54	0
56	MG	1A	3616	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3531	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3810	1/1	0.93	0.30	71,71,71,71	0
56	MG	1A	3532	1/1	0.93	0.19	26,26,26,26	0
56	MG	1w	104	1/1	0.93	0.12	69,69,69,69	0
56	MG	1P	202	1/1	0.93	0.25	37,37,37,37	0
56	MG	1w	106	1/1	0.93	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1P	203	1/1	0.93	0.19	28,28,28,28	0
56	MG	1P	205	1/1	0.93	0.11	36,36,36,36	0
56	MG	2A	3526	1/1	0.93	0.23	56,56,56,56	0
56	MG	1x	104	1/1	0.93	0.19	52,52,52,52	0
56	MG	2a	1697	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3168	1/1	0.93	0.35	67,67,67,67	0
56	MG	2a	1699	1/1	0.93	0.22	57,57,57,57	0
56	MG	2A	3762	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3359	1/1	0.93	0.34	29,29,29,29	0
56	MG	1A	3537	1/1	0.93	0.34	44,44,44,44	0
56	MG	1a	1672	1/1	0.93	0.16	62,62,62,62	0
56	MG	1A	3182	1/1	0.93	0.21	34,34,34,34	0
56	MG	2A	3771	1/1	0.93	0.24	47,47,47,47	0
56	MG	1Q	206	1/1	0.93	0.29	44,44,44,44	0
56	MG	2A	3176	1/1	0.93	0.26	59,59,59,59	0
56	MG	1A	3926	1/1	0.93	0.17	31,31,31,31	0
56	MG	1A	3233	1/1	0.93	0.95	51,51,51,51	0
56	MG	1A	4051	1/1	0.93	0.26	53,53,53,53	0
56	MG	1A	3931	1/1	0.93	0.21	60,60,60,60	0
56	MG	1A	3818	1/1	0.93	0.20	22,22,22,22	0
56	MG	2A	3545	1/1	0.93	0.34	56,56,56,56	0
56	MG	2A	3186	1/1	0.93	0.26	61,61,61,61	0
56	MG	1A	3324	1/1	0.93	0.28	39,39,39,39	0
56	MG	1A	3057	1/1	0.93	0.26	58,58,58,58	0
56	MG	2a	1720	1/1	0.93	0.16	77,77,77,77	0
56	MG	2A	3789	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	4060	1/1	0.93	0.21	56,56,56,56	0
56	MG	2A	3005	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3553	1/1	0.93	0.19	68,68,68,68	0
56	MG	2a	1733	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3348	1/1	0.93	0.34	62,62,62,62	0
56	MG	1A	3487	1/1	0.93	0.45	39,39,39,39	0
56	MG	1A	3628	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3351	1/1	0.93	0.25	73,73,73,73	0
56	MG	2A	3561	1/1	0.93	0.21	47,47,47,47	0
56	MG	1A	4067	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3826	1/1	0.93	0.16	48,48,48,48	0
56	MG	2a	1749	1/1	0.93	0.16	68,68,68,68	0
56	MG	2A	3806	1/1	0.93	0.18	48,48,48,48	0
56	MG	2A	3807	1/1	0.93	0.18	68,68,68,68	0
56	MG	2A	3014	1/1	0.93	0.22	69,69,69,69	0
56	MG	2A	3566	1/1	0.93	0.22	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1V	207	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3725	1/1	0.93	0.15	42,42,42,42	0
56	MG	1a	1696	1/1	0.93	0.10	64,64,64,64	0
56	MG	1A	3829	1/1	0.93	0.13	36,36,36,36	0
56	MG	2a	1765	1/1	0.93	0.15	64,64,64,64	0
56	MG	2a	1766	1/1	0.93	0.27	61,61,61,61	0
56	MG	2A	3582	1/1	0.93	0.28	59,59,59,59	0
56	MG	2a	1768	1/1	0.93	0.14	78,78,78,78	0
56	MG	2A	3201	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3488	1/1	0.93	0.21	40,40,40,40	0
56	MG	1A	3943	1/1	0.93	0.15	60,60,60,60	0
56	MG	1a	1701	1/1	0.93	0.28	50,50,50,50	0
56	MG	2a	1774	1/1	0.93	0.13	63,63,63,63	0
56	MG	1A	3944	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3032	1/1	0.93	0.22	47,47,47,47	0
56	MG	1A	3155	1/1	0.93	0.22	50,50,50,50	0
56	MG	1A	3947	1/1	0.93	0.23	24,24,24,24	0
56	MG	2A	3600	1/1	0.93	0.16	60,60,60,60	0
56	MG	1A	3049	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3077	1/1	0.93	0.38	31,31,31,31	0
56	MG	2A	3040	1/1	0.93	0.29	60,60,60,60	0
56	MG	1A	3840	1/1	0.93	0.16	48,48,48,48	0
56	MG	2a	1786	1/1	0.93	0.11	52,52,52,52	0
56	MG	1a	1709	1/1	0.93	0.32	40,40,40,40	0
56	MG	2B	210	1/1	0.93	0.17	78,78,78,78	0
56	MG	1a	1710	1/1	0.93	0.34	70,70,70,70	0
56	MG	1a	1712	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3159	1/1	0.93	0.55	46,46,46,46	0
56	MG	1a	1714	1/1	0.93	0.09	68,68,68,68	0
56	MG	1a	1715	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3079	1/1	0.93	0.29	38,38,38,38	0
56	MG	2A	3053	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3304	1/1	0.93	0.22	34,34,34,34	0
56	MG	1a	1721	1/1	0.93	0.14	50,50,50,50	0
56	MG	1a	1722	1/1	0.93	0.15	40,40,40,40	0
56	MG	2E	308	1/1	0.93	0.20	56,56,56,56	0
56	MG	2a	1808	1/1	0.93	0.10	86,86,86,86	0
56	MG	1A	3557	1/1	0.93	0.21	55,55,55,55	0
56	MG	2A	3232	1/1	0.93	0.39	60,60,60,60	0
56	MG	1a	1728	1/1	0.93	0.19	64,64,64,64	0
56	MG	2F	306	1/1	0.93	0.49	53,53,53,53	0
56	MG	2f	201	1/1	0.93	0.19	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	1A	3274	1/1	0.93	0.22	45,45,45,45	0
56	MG	1A	3422	1/1	0.93	0.15	50,50,50,50	0
56	MG	1a	1734	1/1	0.93	0.11	64,64,64,64	0
56	MG	1B	206	1/1	0.93	0.46	50,50,50,50	0
56	MG	2P	202	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3636	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3062	1/1	0.93	0.23	36,36,36,36	0
56	MG	2T	201	1/1	0.93	0.20	57,57,57,57	0
56	MG	1a	1741	1/1	0.93	0.13	56,56,56,56	0
56	MG	2T	203	1/1	0.93	0.08	67,67,67,67	0
56	MG	2V	202	1/1	0.93	0.18	57,57,57,57	0
56	MG	1B	208	1/1	0.93	0.08	60,60,60,60	0
56	MG	2A	3403	1/1	0.93	0.39	64,64,64,64	0
56	MG	2A	3404	1/1	0.93	0.27	63,63,63,63	0
56	MG	2A	3405	1/1	0.93	0.29	49,49,49,49	0
56	MG	2x	102	1/1	0.93	0.26	75,75,75,75	0
56	MG	1A	3566	1/1	0.93	0.17	52,52,52,52	0
56	MG	1A	3142	1/1	0.93	0.30	36,36,36,36	0
56	MG	2A	3646	1/1	0.93	0.14	31,31,31,31	0
56	MG	1B	211	1/1	0.93	0.21	55,55,55,55	0
56	MG	1A	3654	1/1	0.93	0.17	28,28,28,28	0
56	MG	2A	3252	1/1	0.93	0.23	53,53,53,53	0
56	MG	25	102	1/1	0.93	0.22	43,43,43,43	0
56	MG	1A	3655	1/1	0.93	0.19	21,21,21,21	0
56	MG	15	101	1/1	0.93	0.28	37,37,37,37	0
56	MG	1A	3506	1/1	0.93	0.20	39,39,39,39	0
56	MG	2A	3115	1/1	0.94	0.15	44,44,44,44	0
56	MG	2D	306	1/1	0.94	0.25	68,68,68,68	0
56	MG	2D	307	1/1	0.94	0.20	62,62,62,62	0
56	MG	2E	302	1/1	0.94	0.18	62,62,62,62	0
56	MG	2A	3116	1/1	0.94	0.17	47,47,47,47	0
56	MG	2E	306	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	3923	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3118	1/1	0.94	0.22	58,58,58,58	0
56	MG	2A	3574	1/1	0.94	0.23	60,60,60,60	0
56	MG	12	102	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3586	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3581	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3085	1/1	0.94	0.20	27,27,27,27	0
56	MG	2N	201	1/1	0.94	0.21	76,76,76,76	0
56	MG	2A	3583	1/1	0.94	0.18	41,41,41,41	0
56	MG	1a	1774	1/1	0.94	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	104	1/1	0.94	0.13	48,48,48,48	0
56	MG	2Q	202	1/1	0.94	0.28	47,47,47,47	0
56	MG	2A	3124	1/1	0.94	0.12	55,55,55,55	0
56	MG	1A	3152	1/1	0.94	0.17	30,30,30,30	0
56	MG	2R	202	1/1	0.94	0.38	55,55,55,55	0
56	MG	2A	3126	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3591	1/1	0.94	0.23	49,49,49,49	0
56	MG	1A	3130	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3086	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3131	1/1	0.94	0.37	58,58,58,58	0
56	MG	2A	3599	1/1	0.94	0.08	68,68,68,68	0
56	MG	1A	3686	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3384	1/1	0.94	0.15	51,51,51,51	0
56	MG	1A	3385	1/1	0.94	0.14	35,35,35,35	0
56	MG	20	102	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3806	1/1	0.94	0.18	64,64,64,64	0
56	MG	2A	3337	1/1	0.94	0.11	68,68,68,68	0
56	MG	2A	3136	1/1	0.94	0.34	61,61,61,61	0
56	MG	1A	3598	1/1	0.94	0.14	52,52,52,52	0
56	MG	21	102	1/1	0.94	0.15	60,60,60,60	0
56	MG	18	103	1/1	0.94	0.53	58,58,58,58	0
56	MG	2A	3611	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3144	1/1	0.94	0.33	62,62,62,62	0
56	MG	1A	3692	1/1	0.94	0.09	42,42,42,42	0
56	MG	1a	1601	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3149	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3599	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3037	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3092	1/1	0.94	0.23	66,66,66,66	0
56	MG	2A	3155	1/1	0.94	0.20	62,62,62,62	0
56	MG	2A	3622	1/1	0.94	0.11	70,70,70,70	0
56	MG	1A	3160	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3700	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3701	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3629	1/1	0.94	0.39	60,60,60,60	0
56	MG	1A	3256	1/1	0.94	0.31	47,47,47,47	0
56	MG	2A	3631	1/1	0.94	0.16	55,55,55,55	0
56	MG	1a	1616	1/1	0.94	0.10	48,48,48,48	0
56	MG	1a	1795	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3822	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	3951	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3703	1/1	0.94	0.14	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	1a	1620	1/1	0.94	0.14	54,54,54,54	0
56	MG	1a	1803	1/1	0.94	0.08	65,65,65,65	0
56	MG	2A	3640	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3015	1/1	0.94	0.24	45,45,45,45	0
56	MG	2A	3169	1/1	0.94	0.12	51,51,51,51	0
56	MG	1a	1806	1/1	0.94	0.10	59,59,59,59	0
56	MG	2A	3372	1/1	0.94	0.39	48,48,48,48	0
56	MG	1a	1810	1/1	0.94	0.10	64,64,64,64	0
56	MG	1A	3956	1/1	0.94	0.07	57,57,57,57	0
56	MG	1a	1625	1/1	0.94	0.23	58,58,58,58	0
56	MG	1A	3705	1/1	0.94	0.13	29,29,29,29	0
56	MG	1A	3113	1/1	0.94	0.64	53,53,53,53	0
56	MG	2A	3650	1/1	0.94	0.09	61,61,61,61	0
56	MG	2A	3177	1/1	0.94	0.12	41,41,41,41	0
56	MG	1A	3827	1/1	0.94	0.22	49,49,49,49	0
56	MG	1A	3707	1/1	0.94	0.13	19,19,19,19	0
56	MG	1a	1631	1/1	0.94	0.23	26,26,26,26	0
56	MG	1A	3966	1/1	0.94	0.28	68,68,68,68	0
56	MG	2A	3183	1/1	0.94	0.12	68,68,68,68	0
56	MG	1t	201	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3114	1/1	0.94	0.49	45,45,45,45	0
56	MG	1v	102	1/1	0.94	0.06	50,50,50,50	0
56	MG	1A	3712	1/1	0.94	0.24	37,37,37,37	0
56	MG	2A	3664	1/1	0.94	0.22	43,43,43,43	0
56	MG	1A	3832	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3666	1/1	0.94	0.19	39,39,39,39	0
56	MG	2a	1647	1/1	0.94	0.25	69,69,69,69	0
56	MG	1w	103	1/1	0.94	0.12	60,60,60,60	0
56	MG	1A	3302	1/1	0.94	0.37	35,35,35,35	0
56	MG	1A	3342	1/1	0.94	0.12	46,46,46,46	0
56	MG	1a	1638	1/1	0.94	0.11	74,74,74,74	0
56	MG	1w	107	1/1	0.94	0.07	64,64,64,64	0
56	MG	1A	3835	1/1	0.94	0.09	28,28,28,28	0
56	MG	2A	3398	1/1	0.94	0.29	58,58,58,58	0
56	MG	1A	3399	1/1	0.94	0.23	51,51,51,51	0
56	MG	2A	3197	1/1	0.94	0.15	67,67,67,67	0
56	MG	1A	3165	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3846	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3344	1/1	0.94	0.52	49,49,49,49	0
56	MG	1A	3345	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3407	1/1	0.94	0.38	50,50,50,50	0
56	MG	2A	3684	1/1	0.94	0.26	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	2A	3685	1/1	0.94	0.33	46,46,46,46	0
56	MG	2A	3408	1/1	0.94	0.19	64,64,64,64	0
56	MG	2A	3687	1/1	0.94	0.21	43,43,43,43	0
56	MG	2A	3688	1/1	0.94	0.09	73,73,73,73	0
56	MG	1A	3988	1/1	0.94	0.11	43,43,43,43	0
56	MG	1A	3346	1/1	0.94	0.25	42,42,42,42	0
56	MG	2A	3692	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3204	1/1	0.94	0.15	63,63,63,63	0
56	MG	1A	3534	1/1	0.94	0.32	37,37,37,37	0
56	MG	1A	3724	1/1	0.94	0.16	25,25,25,25	0
56	MG	2A	3697	1/1	0.94	0.21	57,57,57,57	0
56	MG	2A	3698	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3699	1/1	0.94	0.16	50,50,50,50	0
56	MG	1x	113	1/1	0.94	0.28	73,73,73,73	0
56	MG	1A	3993	1/1	0.94	0.19	45,45,45,45	0
56	MG	1x	115	1/1	0.94	0.15	49,49,49,49	0
56	MG	1E	312	1/1	0.94	0.24	43,43,43,43	0
56	MG	1A	3205	1/1	0.94	0.21	52,52,52,52	0
56	MG	1a	1659	1/1	0.94	0.14	57,57,57,57	0
56	MG	1a	1661	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3348	1/1	0.94	0.26	40,40,40,40	0
56	MG	1A	3305	1/1	0.94	0.23	47,47,47,47	0
56	MG	2A	3712	1/1	0.94	0.15	70,70,70,70	0
56	MG	2A	3429	1/1	0.94	0.17	37,37,37,37	0
56	MG	1A	3066	1/1	0.94	0.14	33,33,33,33	0
56	MG	2A	3431	1/1	0.94	0.14	75,75,75,75	0
56	MG	1A	3862	1/1	0.94	0.18	45,45,45,45	0
56	MG	1a	1669	1/1	0.94	0.16	64,64,64,64	0
56	MG	1F	310	1/1	0.94	0.12	49,49,49,49	0
56	MG	1F	311	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3116	1/1	0.94	0.28	31,31,31,31	0
56	MG	2A	3226	1/1	0.94	0.12	58,58,58,58	0
56	MG	2A	3017	1/1	0.94	0.22	47,47,47,47	0
56	MG	2A	3018	1/1	0.94	0.27	58,58,58,58	0
56	MG	2A	3446	1/1	0.94	0.19	63,63,63,63	0
56	MG	1G	3601	1/1	0.94	0.24	37,37,37,37	0
56	MG	1A	4001	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	3865	1/1	0.94	0.21	47,47,47,47	0
56	MG	1A	3629	1/1	0.94	0.21	32,32,32,32	0
56	MG	1A	3867	1/1	0.94	0.25	38,38,38,38	0
56	MG	1A	3265	1/1	0.94	0.38	41,41,41,41	0
56	MG	1A	3870	1/1	0.94	0.11	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	2a	1721	1/1	0.94	0.17	73,73,73,73	0
56	MG	2a	1724	1/1	0.94	0.09	71,71,71,71	0
56	MG	2a	1725	1/1	0.94	0.20	81,81,81,81	0
56	MG	1A	3547	1/1	0.94	0.36	42,42,42,42	0
56	MG	2A	3239	1/1	0.94	0.38	71,71,71,71	0
56	MG	1N	206	1/1	0.94	0.22	44,44,44,44	0
56	MG	2a	1731	1/1	0.94	0.07	67,67,67,67	0
56	MG	2A	3242	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3742	1/1	0.94	0.09	82,82,82,82	0
56	MG	2a	1736	1/1	0.94	0.14	68,68,68,68	0
56	MG	2A	3243	1/1	0.94	0.13	61,61,61,61	0
56	MG	1A	3736	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3634	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3466	1/1	0.94	0.13	62,62,62,62	0
56	MG	1A	4015	1/1	0.94	0.17	59,59,59,59	0
56	MG	2a	1745	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3309	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3752	1/1	0.94	0.08	82,82,82,82	0
56	MG	1P	204	1/1	0.94	0.43	32,32,32,32	0
56	MG	1A	3268	1/1	0.94	0.38	41,41,41,41	0
56	MG	1A	3017	1/1	0.94	0.23	53,53,53,53	0
56	MG	2a	1753	1/1	0.94	0.14	71,71,71,71	0
56	MG	1A	4020	1/1	0.94	0.14	27,27,27,27	0
56	MG	2A	3047	1/1	0.94	0.20	37,37,37,37	0
56	MG	1A	3312	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3641	1/1	0.94	0.17	36,36,36,36	0
56	MG	2a	1761	1/1	0.94	0.10	64,64,64,64	0
56	MG	1R	201	1/1	0.94	0.14	59,59,59,59	0
56	MG	1R	203	1/1	0.94	0.15	32,32,32,32	0
56	MG	2A	3486	1/1	0.94	0.23	48,48,48,48	0
56	MG	1A	3238	1/1	0.94	0.25	34,34,34,34	0
56	MG	1A	3240	1/1	0.94	0.31	45,45,45,45	0
56	MG	1A	3364	1/1	0.94	0.57	30,30,30,30	0
56	MG	1A	3365	1/1	0.94	0.27	27,27,27,27	0
56	MG	2a	1770	1/1	0.94	0.07	67,67,67,67	0
56	MG	1A	3889	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3486	1/1	0.94	0.21	30,30,30,30	0
56	MG	1A	4040	1/1	0.94	0.36	65,65,65,65	0
56	MG	1U	204	1/1	0.94	0.21	37,37,37,37	0
56	MG	2a	1775	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3893	1/1	0.94	0.08	38,38,38,38	0
56	MG	1A	3177	1/1	0.94	0.30	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1U	210	1/1	0.94	0.34	52,52,52,52	0
56	MG	1A	3758	1/1	0.94	0.19	24,24,24,24	0
56	MG	1A	3651	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3561	1/1	0.94	0.18	32,32,32,32	0
56	MG	2A	3504	1/1	0.94	0.27	61,61,61,61	0
56	MG	1a	1719	1/1	0.94	0.13	55,55,55,55	0
56	MG	1a	1720	1/1	0.94	0.11	69,69,69,69	0
56	MG	1A	3098	1/1	0.94	0.12	25,25,25,25	0
56	MG	1W	201	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3797	1/1	0.94	0.17	62,62,62,62	0
56	MG	1a	1724	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3514	1/1	0.94	0.22	80,80,80,80	0
56	MG	2A	3516	1/1	0.94	0.10	72,72,72,72	0
56	MG	2A	3279	1/1	0.94	0.20	61,61,61,61	0
56	MG	1a	1726	1/1	0.94	0.09	61,61,61,61	0
56	MG	1A	3762	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3563	1/1	0.94	0.15	40,40,40,40	0
56	MG	1A	3013	1/1	0.94	0.34	35,35,35,35	0
56	MG	1a	1732	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3184	1/1	0.94	0.10	50,50,50,50	0
56	MG	1X	101	1/1	0.94	0.44	44,44,44,44	0
56	MG	1A	3432	1/1	0.94	0.18	58,58,58,58	0
56	MG	1a	1737	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3245	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	4057	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3495	1/1	0.94	0.11	82,82,82,82	0
56	MG	2A	3816	1/1	0.94	0.26	55,55,55,55	0
56	MG	1Y	204	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3819	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3282	1/1	0.94	0.07	55,55,55,55	0
56	MG	2l	201	1/1	0.94	0.24	68,68,68,68	0
56	MG	1Z	302	1/1	0.94	0.14	76,76,76,76	0
56	MG	2p	101	1/1	0.94	0.09	64,64,64,64	0
56	MG	1A	3148	1/1	0.94	0.43	35,35,35,35	0
56	MG	1A	3668	1/1	0.94	0.16	31,31,31,31	0
56	MG	2A	3099	1/1	0.94	0.14	60,60,60,60	0
56	MG	2r	101	1/1	0.94	0.27	69,69,69,69	0
56	MG	2A	3828	1/1	0.94	0.14	66,66,66,66	0
56	MG	1A	3913	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	4066	1/1	0.94	0.08	50,50,50,50	0
56	MG	10	105	1/1	0.94	0.14	53,53,53,53	0
56	MG	2B	203	1/1	0.94	0.24	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1755	1/1	0.94	0.17	71,71,71,71	0
56	MG	2A	3304	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3440	1/1	0.94	0.27	46,46,46,46	0
56	MG	2A	3552	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	4068	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3554	1/1	0.94	0.18	68,68,68,68	0
56	MG	2x	106	1/1	0.94	0.12	71,71,71,71	0
56	MG	1a	1760	1/1	0.94	0.16	73,73,73,73	0
56	MG	1A	3787	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3024	1/1	0.94	0.25	28,28,28,28	0
56	MG	2y	102	1/1	0.94	0.17	80,80,80,80	0
56	MG	1A	3323	1/1	0.94	0.34	39,39,39,39	0
56	MG	2A	3112	1/1	0.94	0.16	57,57,57,57	0
56	MG	1A	3285	1/1	0.94	0.19	33,33,33,33	0
56	MG	2A	3563	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3794	1/1	0.94	0.32	62,62,62,62	0
58	ZN	29	102	1/1	0.94	0.07	74,74,74,74	0
56	MG	1A	3415	1/1	0.95	0.25	34,34,34,34	0
56	MG	1A	4023	1/1	0.95	0.17	46,46,46,46	0
56	MG	1a	1801	1/1	0.95	0.10	67,67,67,67	0
56	MG	2A	3476	1/1	0.95	0.12	67,67,67,67	0
56	MG	1A	3606	1/1	0.95	0.29	59,59,59,59	0
56	MG	2A	3690	1/1	0.95	0.24	61,61,61,61	0
56	MG	1A	3416	1/1	0.95	0.27	40,40,40,40	0
56	MG	1a	1804	1/1	0.95	0.18	64,64,64,64	0
56	MG	2A	3291	1/1	0.95	0.13	70,70,70,70	0
56	MG	2A	3483	1/1	0.95	0.20	56,56,56,56	0
56	MG	1a	1648	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	4030	1/1	0.95	0.18	40,40,40,40	0
56	MG	1a	1651	1/1	0.95	0.19	65,65,65,65	0
56	MG	2a	1619	1/1	0.95	0.19	55,55,55,55	0
56	MG	2A	3129	1/1	0.95	0.39	48,48,48,48	0
56	MG	1O	201	1/1	0.95	0.13	54,54,54,54	0
56	MG	1O	202	1/1	0.95	0.14	56,56,56,56	0
56	MG	2a	1624	1/1	0.95	0.24	51,51,51,51	0
56	MG	1A	3063	1/1	0.95	0.28	34,34,34,34	0
56	MG	1A	3468	1/1	0.95	0.26	36,36,36,36	0
56	MG	1A	3374	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3802	1/1	0.95	0.09	63,63,63,63	0
56	MG	2A	3707	1/1	0.95	0.19	45,45,45,45	0
56	MG	1a	1660	1/1	0.95	0.12	65,65,65,65	0
56	MG	1A	3075	1/1	0.95	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	1r	101	1/1	0.95	0.28	56,56,56,56	0
56	MG	2A	3141	1/1	0.95	0.21	60,60,60,60	0
56	MG	1a	1662	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3614	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3310	1/1	0.95	0.13	61,61,61,61	0
56	MG	2A	3718	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	3615	1/1	0.95	0.20	42,42,42,42	0
56	MG	2A	3505	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3220	1/1	0.95	0.31	37,37,37,37	0
56	MG	1A	3536	1/1	0.95	0.23	42,42,42,42	0
56	MG	2A	3152	1/1	0.95	0.19	53,53,53,53	0
56	MG	2A	3509	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3171	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	3009	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3146	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3922	1/1	0.95	0.14	29,29,29,29	0
56	MG	1a	1673	1/1	0.95	0.18	52,52,52,52	0
56	MG	1A	3708	1/1	0.95	0.32	59,59,59,59	0
56	MG	1a	1676	1/1	0.95	0.10	69,69,69,69	0
56	MG	1A	3924	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3543	1/1	0.95	0.10	39,39,39,39	0
56	MG	2a	1661	1/1	0.95	0.16	71,71,71,71	0
56	MG	1A	3174	1/1	0.95	0.27	50,50,50,50	0
56	MG	2A	3527	1/1	0.95	0.21	55,55,55,55	0
56	MG	1A	3928	1/1	0.95	0.32	46,46,46,46	0
56	MG	1x	108	1/1	0.95	0.19	64,64,64,64	0
56	MG	2A	3740	1/1	0.95	0.29	75,75,75,75	0
56	MG	1A	3127	1/1	0.95	0.13	49,49,49,49	0
56	MG	2a	1672	1/1	0.95	0.22	59,59,59,59	0
56	MG	1A	3176	1/1	0.95	0.17	75,75,75,75	0
56	MG	2a	1674	1/1	0.95	0.08	72,72,72,72	0
56	MG	2A	3532	1/1	0.95	0.10	68,68,68,68	0
56	MG	2A	3745	1/1	0.95	0.09	78,78,78,78	0
56	MG	1A	3230	1/1	0.95	0.28	38,38,38,38	0
56	MG	1A	3089	1/1	0.95	0.18	34,34,34,34	0
56	MG	2A	3535	1/1	0.95	0.27	69,69,69,69	0
56	MG	2A	3749	1/1	0.95	0.12	50,50,50,50	0
56	MG	1U	208	1/1	0.95	0.33	36,36,36,36	0
56	MG	1A	4062	1/1	0.95	0.17	43,43,43,43	0
56	MG	1A	3001	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3935	1/1	0.95	0.09	66,66,66,66	0
56	MG	1A	3067	1/1	0.95	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3632	1/1	0.95	0.17	25,25,25,25	0
56	MG	1A	3290	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3435	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3004	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3547	1/1	0.95	0.23	57,57,57,57	0
56	MG	2A	3760	1/1	0.95	0.12	37,37,37,37	0
56	MG	1a	1697	1/1	0.95	0.18	53,53,53,53	0
56	MG	2A	3344	1/1	0.95	0.17	66,66,66,66	0
56	MG	1A	3081	1/1	0.95	0.22	44,44,44,44	0
56	MG	1A	3941	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3830	1/1	0.95	0.23	44,44,44,44	0
56	MG	1A	3726	1/1	0.95	0.16	31,31,31,31	0
56	MG	2A	3769	1/1	0.95	0.07	62,62,62,62	0
56	MG	2A	3770	1/1	0.95	0.12	70,70,70,70	0
56	MG	1A	3210	1/1	0.95	0.24	44,44,44,44	0
56	MG	1A	3438	1/1	0.95	0.19	48,48,48,48	0
56	MG	1X	105	1/1	0.95	0.12	52,52,52,52	0
56	MG	1a	1705	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3135	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3071	1/1	0.95	0.28	46,46,46,46	0
56	MG	2a	1708	1/1	0.95	0.16	73,73,73,73	0
56	MG	2A	3782	1/1	0.95	0.14	31,31,31,31	0
56	MG	2A	3024	1/1	0.95	0.32	47,47,47,47	0
56	MG	1Y	203	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3731	1/1	0.95	0.18	35,35,35,35	0
56	MG	1A	3837	1/1	0.95	0.13	37,37,37,37	0
56	MG	2a	1715	1/1	0.95	0.16	67,67,67,67	0
56	MG	1A	3392	1/1	0.95	0.15	49,49,49,49	0
56	MG	2A	3568	1/1	0.95	0.23	54,54,54,54	0
56	MG	2A	3570	1/1	0.95	0.09	63,63,63,63	0
56	MG	2A	3790	1/1	0.95	0.24	50,50,50,50	0
56	MG	1A	3443	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3572	1/1	0.95	0.13	66,66,66,66	0
56	MG	2A	3031	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	3954	1/1	0.95	0.40	40,40,40,40	0
56	MG	1A	3393	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3577	1/1	0.95	0.26	47,47,47,47	0
56	MG	1A	3646	1/1	0.95	0.16	29,29,29,29	0
56	MG	2A	3368	1/1	0.95	0.27	50,50,50,50	0
56	MG	2A	3369	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3035	1/1	0.95	0.12	53,53,53,53	0
56	MG	2a	1735	1/1	0.95	0.11	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1717	1/1	0.95	0.15	60,60,60,60	0
56	MG	2A	3205	1/1	0.95	0.39	46,46,46,46	0
56	MG	2A	3206	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3295	1/1	0.95	0.15	59,59,59,59	0
56	MG	2a	1741	1/1	0.95	0.14	63,63,63,63	0
56	MG	2A	3589	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3739	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3740	1/1	0.95	0.14	33,33,33,33	0
56	MG	2a	1746	1/1	0.95	0.29	59,59,59,59	0
56	MG	1A	3962	1/1	0.95	0.14	34,34,34,34	0
56	MG	2A	3595	1/1	0.95	0.31	49,49,49,49	0
56	MG	1A	3853	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3239	1/1	0.95	0.21	58,58,58,58	0
56	MG	2a	1751	1/1	0.95	0.19	51,51,51,51	0
56	MG	1A	3396	1/1	0.95	0.35	43,43,43,43	0
56	MG	2A	3382	1/1	0.95	0.13	61,61,61,61	0
56	MG	1A	3397	1/1	0.95	0.24	38,38,38,38	0
56	MG	2A	3215	1/1	0.95	0.12	53,53,53,53	0
56	MG	2a	1756	1/1	0.95	0.13	73,73,73,73	0
56	MG	1A	3652	1/1	0.95	0.21	38,38,38,38	0
56	MG	1A	3974	1/1	0.95	0.10	41,41,41,41	0
56	MG	2a	1760	1/1	0.95	0.12	66,66,66,66	0
56	MG	2A	3605	1/1	0.95	0.25	65,65,65,65	0
56	MG	2A	3827	1/1	0.95	0.08	60,60,60,60	0
56	MG	2a	1763	1/1	0.95	0.28	77,77,77,77	0
56	MG	1a	1731	1/1	0.95	0.14	38,38,38,38	0
56	MG	1B	219	1/1	0.95	0.32	51,51,51,51	0
56	MG	2A	3830	1/1	0.95	0.11	65,65,65,65	0
56	MG	2A	3609	1/1	0.95	0.25	61,61,61,61	0
56	MG	2A	3220	1/1	0.95	0.33	51,51,51,51	0
56	MG	1A	3975	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3054	1/1	0.95	0.21	50,50,50,50	0
56	MG	1B	222	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3099	1/1	0.95	0.29	41,41,41,41	0
56	MG	1A	3361	1/1	0.95	0.12	55,55,55,55	0
56	MG	1a	1740	1/1	0.95	0.17	43,43,43,43	0
56	MG	15	104	1/1	0.95	0.22	40,40,40,40	0
56	MG	15	105	1/1	0.95	0.51	32,32,32,32	0
56	MG	2A	3229	1/1	0.95	0.16	57,57,57,57	0
56	MG	1A	3266	1/1	0.95	0.19	29,29,29,29	0
56	MG	1A	3575	1/1	0.95	0.19	45,45,45,45	0
56	MG	1A	3328	1/1	0.95	0.69	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	17	101	1/1	0.95	0.10	35,35,35,35	0
56	MG	2a	1782	1/1	0.95	0.15	75,75,75,75	0
56	MG	2A	3406	1/1	0.95	0.17	68,68,68,68	0
56	MG	1A	3512	1/1	0.95	0.38	48,48,48,48	0
56	MG	2D	301	1/1	0.95	0.47	56,56,56,56	0
56	MG	17	105	1/1	0.95	0.22	62,62,62,62	0
56	MG	1A	3662	1/1	0.95	0.19	28,28,28,28	0
56	MG	1A	3663	1/1	0.95	0.22	58,58,58,58	0
56	MG	2A	3634	1/1	0.95	0.24	42,42,42,42	0
56	MG	18	104	1/1	0.95	0.19	41,41,41,41	0
56	MG	2E	304	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3579	1/1	0.95	0.17	26,26,26,26	0
56	MG	1A	3874	1/1	0.95	0.14	34,34,34,34	0
56	MG	2A	3417	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	3580	1/1	0.95	0.18	36,36,36,36	0
56	MG	1A	3404	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3077	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3366	1/1	0.95	0.17	27,27,27,27	0
56	MG	2A	3080	1/1	0.95	0.31	52,52,52,52	0
56	MG	2A	3424	1/1	0.95	0.27	58,58,58,58	0
56	MG	1A	3879	1/1	0.95	0.29	38,38,38,38	0
56	MG	2A	3083	1/1	0.95	0.23	56,56,56,56	0
56	MG	1D	304	1/1	0.95	0.17	36,36,36,36	0
56	MG	1D	310	1/1	0.95	0.18	45,45,45,45	0
56	MG	2e	201	1/1	0.95	0.06	75,75,75,75	0
56	MG	1A	3029	1/1	0.95	0.14	47,47,47,47	0
56	MG	1a	1769	1/1	0.95	0.09	64,64,64,64	0
56	MG	1a	1614	1/1	0.95	0.07	65,65,65,65	0
56	MG	2A	3089	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3408	1/1	0.95	0.29	52,52,52,52	0
56	MG	2l	202	1/1	0.95	0.11	68,68,68,68	0
56	MG	1E	301	1/1	0.95	0.34	32,32,32,32	0
56	MG	1A	3883	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3271	1/1	0.95	0.79	43,43,43,43	0
56	MG	1A	3102	1/1	0.95	0.23	36,36,36,36	0
56	MG	1A	3673	1/1	0.95	0.11	55,55,55,55	0
56	MG	1a	1622	1/1	0.95	0.22	52,52,52,52	0
56	MG	1E	309	1/1	0.95	0.14	24,24,24,24	0
56	MG	1E	310	1/1	0.95	0.20	31,31,31,31	0
56	MG	1A	4005	1/1	0.95	0.27	44,44,44,44	0
56	MG	1A	3411	1/1	0.95	0.18	44,44,44,44	0
56	MG	2A	3667	1/1	0.95	0.24	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	3597	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	3371	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3273	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3455	1/1	0.95	0.29	58,58,58,58	0
56	MG	2A	3672	1/1	0.95	0.18	60,60,60,60	0
56	MG	1A	3781	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3785	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3786	1/1	0.95	0.17	38,38,38,38	0
56	MG	1A	3464	1/1	0.95	0.18	47,47,47,47	0
56	MG	1A	4017	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3524	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3602	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3527	1/1	0.95	0.29	44,44,44,44	0
56	MG	1G	3604	1/1	0.95	0.20	63,63,63,63	0
57	6IF	2A	3831	32/32	0.95	0.25	38,44,50,53	0
58	ZN	1Y	205	1/1	0.95	0.13	72,72,72,72	0
56	MG	1a	1641	1/1	0.95	0.11	59,59,59,59	0
56	MG	2a	1603	1/1	0.95	0.18	70,70,70,70	0
56	MG	1A	3902	1/1	0.95	0.09	40,40,40,40	0
58	ZN	2n	501	1/1	0.95	0.08	85,85,85,85	0
56	MG	1D	309	1/1	0.96	0.26	55,55,55,55	0
56	MG	1A	3137	1/1	0.96	0.35	31,31,31,31	0
56	MG	1A	3643	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3807	1/1	0.96	0.06	58,58,58,58	0
56	MG	2a	1630	1/1	0.96	0.20	69,69,69,69	0
56	MG	2A	3727	1/1	0.96	0.18	64,64,64,64	0
56	MG	2A	3345	1/1	0.96	0.08	74,74,74,74	0
56	MG	17	104	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3808	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3536	1/1	0.96	0.17	41,41,41,41	0
56	MG	1a	1730	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3478	1/1	0.96	0.28	62,62,62,62	0
56	MG	18	101	1/1	0.96	0.54	51,51,51,51	0
56	MG	18	102	1/1	0.96	0.18	44,44,44,44	0
56	MG	2A	3036	1/1	0.96	0.20	27,27,27,27	0
56	MG	2A	3037	1/1	0.96	0.10	68,68,68,68	0
56	MG	1A	3105	1/1	0.96	0.32	37,37,37,37	0
56	MG	1a	1735	1/1	0.96	0.10	59,59,59,59	0
56	MG	1A	3121	1/1	0.96	0.22	36,36,36,36	0
56	MG	1A	3908	1/1	0.96	0.07	46,46,46,46	0
56	MG	19	101	1/1	0.96	0.14	49,49,49,49	0
56	MG	1a	1739	1/1	0.96	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1649	1/1	0.96	0.10	65,65,65,65	0
56	MG	2a	1650	1/1	0.96	0.15	59,59,59,59	0
56	MG	1A	3584	1/1	0.96	0.14	57,57,57,57	0
56	MG	1A	3091	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3222	1/1	0.96	0.20	31,31,31,31	0
56	MG	2a	1654	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3912	1/1	0.96	0.17	52,52,52,52	0
56	MG	2A	3050	1/1	0.96	0.22	60,60,60,60	0
56	MG	1A	3223	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3367	1/1	0.96	0.16	60,60,60,60	0
56	MG	1A	3485	1/1	0.96	0.31	30,30,30,30	0
56	MG	2a	1660	1/1	0.96	0.17	62,62,62,62	0
56	MG	2A	3558	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	4024	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3560	1/1	0.96	0.14	47,47,47,47	0
56	MG	1a	1749	1/1	0.96	0.08	60,60,60,60	0
56	MG	1a	1612	1/1	0.96	0.20	58,58,58,58	0
56	MG	1A	3070	1/1	0.96	0.12	35,35,35,35	0
56	MG	1F	306	1/1	0.96	0.11	42,42,42,42	0
56	MG	2a	1671	1/1	0.96	0.32	43,43,43,43	0
56	MG	1a	1753	1/1	0.96	0.05	72,72,72,72	0
56	MG	1a	1615	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3059	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3595	1/1	0.96	0.12	22,22,22,22	0
56	MG	2a	1676	1/1	0.96	0.23	67,67,67,67	0
56	MG	1A	4032	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3168	1/1	0.96	0.18	29,29,29,29	0
56	MG	1A	3169	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3490	1/1	0.96	0.37	32,32,32,32	0
56	MG	1A	3541	1/1	0.96	0.20	73,73,73,73	0
56	MG	1A	3125	1/1	0.96	0.17	40,40,40,40	0
56	MG	1H	201	1/1	0.96	0.31	48,48,48,48	0
56	MG	2A	3580	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	4041	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3452	1/1	0.96	0.35	56,56,56,56	0
56	MG	2A	3780	1/1	0.96	0.16	60,60,60,60	0
56	MG	2A	3781	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3126	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3742	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3545	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3075	1/1	0.96	0.24	34,34,34,34	0
56	MG	1A	3035	1/1	0.96	0.43	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	3147	1/1	0.96	0.23	43,43,43,43	0
56	MG	1A	3497	1/1	0.96	0.23	57,57,57,57	0
56	MG	2A	3079	1/1	0.96	0.14	68,68,68,68	0
56	MG	2A	3234	1/1	0.96	0.14	65,65,65,65	0
56	MG	2A	3593	1/1	0.96	0.34	63,63,63,63	0
56	MG	2A	3594	1/1	0.96	0.31	57,57,57,57	0
56	MG	1A	3608	1/1	0.96	0.23	28,28,28,28	0
56	MG	2A	3796	1/1	0.96	0.10	62,62,62,62	0
56	MG	2A	3081	1/1	0.96	0.33	51,51,51,51	0
56	MG	1A	3749	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3402	1/1	0.96	0.35	53,53,53,53	0
56	MG	1A	3839	1/1	0.96	0.30	38,38,38,38	0
56	MG	1A	3549	1/1	0.96	0.31	50,50,50,50	0
56	MG	1A	4055	1/1	0.96	0.40	49,49,49,49	0
56	MG	1A	3129	1/1	0.96	0.44	38,38,38,38	0
56	MG	1A	3611	1/1	0.96	0.14	31,31,31,31	0
56	MG	2a	1711	1/1	0.96	0.34	53,53,53,53	0
56	MG	1Q	202	1/1	0.96	0.20	42,42,42,42	0
56	MG	2A	3245	1/1	0.96	0.18	63,63,63,63	0
56	MG	1A	3351	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3501	1/1	0.96	0.33	33,33,33,33	0
56	MG	1Q	205	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3502	1/1	0.96	0.26	43,43,43,43	0
56	MG	1A	3679	1/1	0.96	0.11	65,65,65,65	0
56	MG	2A	3094	1/1	0.96	0.13	71,71,71,71	0
56	MG	1A	3680	1/1	0.96	0.07	29,29,29,29	0
56	MG	2A	3096	1/1	0.96	0.24	53,53,53,53	0
56	MG	2a	1722	1/1	0.96	0.15	75,75,75,75	0
56	MG	2a	1723	1/1	0.96	0.20	78,78,78,78	0
56	MG	2A	3817	1/1	0.96	0.11	60,60,60,60	0
56	MG	1a	1650	1/1	0.96	0.13	51,51,51,51	0
56	MG	1A	3289	1/1	0.96	0.22	41,41,41,41	0
56	MG	1A	3946	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3036	1/1	0.96	0.27	36,36,36,36	0
56	MG	1A	3016	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	3858	1/1	0.96	0.18	27,27,27,27	0
56	MG	2A	3624	1/1	0.96	0.29	58,58,58,58	0
56	MG	1U	201	1/1	0.96	0.26	33,33,33,33	0
56	MG	2A	3104	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3950	1/1	0.96	0.14	25,25,25,25	0
56	MG	2a	1738	1/1	0.96	0.09	70,70,70,70	0
56	MG	1A	3859	1/1	0.96	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3860	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	3261	1/1	0.96	0.27	32,32,32,32	0
56	MG	1A	3558	1/1	0.96	0.21	64,64,64,64	0
56	MG	2A	3437	1/1	0.96	0.18	61,61,61,61	0
56	MG	2B	205	1/1	0.96	0.22	61,61,61,61	0
56	MG	1a	1664	1/1	0.96	0.06	66,66,66,66	0
56	MG	2A	3439	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3766	1/1	0.96	0.14	27,27,27,27	0
56	MG	1a	1807	1/1	0.96	0.23	61,61,61,61	0
56	MG	1A	3768	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3559	1/1	0.96	0.35	43,43,43,43	0
56	MG	2A	3445	1/1	0.96	0.13	58,58,58,58	0
56	MG	1e	201	1/1	0.96	0.12	69,69,69,69	0
56	MG	1A	3690	1/1	0.96	0.16	59,59,59,59	0
56	MG	1k	201	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3622	1/1	0.96	0.19	29,29,29,29	0
56	MG	2A	3450	1/1	0.96	0.15	51,51,51,51	0
56	MG	2a	1758	1/1	0.96	0.15	69,69,69,69	0
56	MG	2B	218	1/1	0.96	0.16	71,71,71,71	0
56	MG	1A	3693	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3964	1/1	0.96	0.10	36,36,36,36	0
56	MG	2D	303	1/1	0.96	0.21	28,28,28,28	0
56	MG	2D	304	1/1	0.96	0.84	49,49,49,49	0
56	MG	1A	3775	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3179	1/1	0.96	0.35	42,42,42,42	0
56	MG	1A	3180	1/1	0.96	0.11	59,59,59,59	0
56	MG	2E	301	1/1	0.96	0.08	69,69,69,69	0
56	MG	1W	207	1/1	0.96	0.23	40,40,40,40	0
56	MG	1A	3151	1/1	0.96	0.24	35,35,35,35	0
56	MG	1B	205	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3296	1/1	0.96	0.23	59,59,59,59	0
56	MG	1A	3973	1/1	0.96	0.15	25,25,25,25	0
56	MG	2E	309	1/1	0.96	0.20	43,43,43,43	0
56	MG	1X	104	1/1	0.96	0.29	47,47,47,47	0
56	MG	2F	302	1/1	0.96	0.18	62,62,62,62	0
56	MG	2A	3660	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3430	1/1	0.96	0.28	57,57,57,57	0
56	MG	2F	305	1/1	0.96	0.16	41,41,41,41	0
56	MG	1A	3877	1/1	0.96	0.21	30,30,30,30	0
56	MG	1a	1685	1/1	0.96	0.28	54,54,54,54	0
56	MG	1A	3783	1/1	0.96	0.12	30,30,30,30	0
56	MG	1a	1687	1/1	0.96	0.34	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	1Y	202	1/1	0.96	0.39	47,47,47,47	0
56	MG	2A	3472	1/1	0.96	0.30	70,70,70,70	0
56	MG	2A	3138	1/1	0.96	0.22	44,44,44,44	0
56	MG	2A	3139	1/1	0.96	0.21	49,49,49,49	0
56	MG	1A	3565	1/1	0.96	0.08	58,58,58,58	0
56	MG	2a	1788	1/1	0.96	0.27	56,56,56,56	0
56	MG	1A	3028	1/1	0.96	0.58	34,34,34,34	0
56	MG	2a	1790	1/1	0.96	0.11	60,60,60,60	0
56	MG	2A	3143	1/1	0.96	0.19	41,41,41,41	0
56	MG	2R	203	1/1	0.96	0.20	50,50,50,50	0
56	MG	2a	1793	1/1	0.96	0.27	50,50,50,50	0
56	MG	2a	1794	1/1	0.96	0.08	70,70,70,70	0
56	MG	1A	3881	1/1	0.96	0.13	46,46,46,46	0
56	MG	2A	3674	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3362	1/1	0.96	0.26	55,55,55,55	0
56	MG	2U	201	1/1	0.96	0.36	53,53,53,53	0
56	MG	2A	3146	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3147	1/1	0.96	0.30	65,65,65,65	0
56	MG	1Z	303	1/1	0.96	0.27	51,51,51,51	0
56	MG	1A	3982	1/1	0.96	0.27	55,55,55,55	0
56	MG	2Y	201	1/1	0.96	0.30	63,63,63,63	0
56	MG	2a	1807	1/1	0.96	0.06	68,68,68,68	0
56	MG	2A	3488	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3307	1/1	0.96	0.19	63,63,63,63	0
56	MG	1A	3631	1/1	0.96	0.11	24,24,24,24	0
56	MG	1A	3791	1/1	0.96	0.34	55,55,55,55	0
56	MG	1A	3987	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3363	1/1	0.96	0.40	45,45,45,45	0
56	MG	1A	3886	1/1	0.96	0.12	59,59,59,59	0
56	MG	1A	3076	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3570	1/1	0.96	0.17	29,29,29,29	0
56	MG	1B	227	1/1	0.96	0.20	40,40,40,40	0
56	MG	11	102	1/1	0.96	0.75	57,57,57,57	0
56	MG	1A	3267	1/1	0.96	0.27	32,32,32,32	0
56	MG	1A	3890	1/1	0.96	0.16	41,41,41,41	0
56	MG	2A	3162	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3709	1/1	0.96	0.19	53,53,53,53	0
56	MG	1A	3892	1/1	0.96	0.11	14,14,14,14	0
56	MG	1A	3042	1/1	0.96	0.11	24,24,24,24	0
56	MG	1a	1711	1/1	0.96	0.16	45,45,45,45	0
56	MG	2A	3008	1/1	0.96	0.17	65,65,65,65	0
56	MG	1A	3269	1/1	0.96	0.32	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	3011	1/1	0.96	0.09	55,55,55,55	0
56	MG	2a	1602	1/1	0.96	0.22	75,75,75,75	0
56	MG	1A	3639	1/1	0.96	0.18	24,24,24,24	0
56	MG	2A	3512	1/1	0.96	0.17	40,40,40,40	0
56	MG	2A	3513	1/1	0.96	0.12	64,64,64,64	0
56	MG	2a	1606	1/1	0.96	0.11	60,60,60,60	0
56	MG	1A	3801	1/1	0.96	0.34	58,58,58,58	0
56	MG	2A	3706	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3515	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3897	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3015	1/1	0.96	0.28	51,51,51,51	0
56	MG	1A	3714	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3711	1/1	0.96	0.04	64,64,64,64	0
56	MG	2A	3519	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3520	1/1	0.96	0.12	43,43,43,43	0
56	MG	2A	3521	1/1	0.96	0.11	59,59,59,59	0
56	MG	1A	3439	1/1	0.96	0.18	49,49,49,49	0
57	6IF	1A	4084	32/32	0.96	0.22	25,32,37,38	0
56	MG	1A	3018	1/1	0.96	0.15	19,19,19,19	0
56	MG	1D	306	1/1	0.96	0.28	41,41,41,41	0
56	MG	2A	3336	1/1	0.96	0.14	67,67,67,67	0
58	ZN	1n	103	1/1	0.96	0.14	63,63,63,63	0
56	MG	1D	308	1/1	0.96	0.19	42,42,42,42	0
56	MG	15	107	1/1	0.96	0.45	38,38,38,38	0
56	MG	2a	1623	1/1	0.96	0.08	64,64,64,64	0
60	K	1x	101	1/1	0.96	0.36	66,66,66,66	0
56	MG	2A	3621	1/1	0.97	0.16	75,75,75,75	0
56	MG	2A	3151	1/1	0.97	0.30	46,46,46,46	0
56	MG	2a	1668	1/1	0.97	0.19	59,59,59,59	0
56	MG	1F	308	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3454	1/1	0.97	0.23	38,38,38,38	0
56	MG	1a	1723	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3533	1/1	0.97	0.33	40,40,40,40	0
56	MG	2A	3627	1/1	0.97	0.14	63,63,63,63	0
56	MG	1A	3034	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3955	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3734	1/1	0.97	0.08	59,59,59,59	0
56	MG	1A	3674	1/1	0.97	0.18	50,50,50,50	0
56	MG	2A	3810	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	4053	1/1	0.97	0.20	42,42,42,42	0
56	MG	1a	1602	1/1	0.97	0.05	58,58,58,58	0
56	MG	2A	3464	1/1	0.97	0.16	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	3330	1/1	0.97	0.33	31,31,31,31	0
56	MG	2A	3020	1/1	0.97	0.27	56,56,56,56	0
56	MG	2A	3308	1/1	0.97	0.18	56,56,56,56	0
56	MG	2A	3468	1/1	0.97	0.19	51,51,51,51	0
56	MG	2a	1687	1/1	0.97	0.15	68,68,68,68	0
56	MG	1A	3737	1/1	0.97	0.06	39,39,39,39	0
56	MG	1G	3605	1/1	0.97	0.13	48,48,48,48	0
56	MG	1A	3199	1/1	0.97	0.25	38,38,38,38	0
56	MG	1A	3027	1/1	0.97	0.35	28,28,28,28	0
56	MG	1A	3963	1/1	0.97	0.17	25,25,25,25	0
56	MG	1a	1609	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3824	1/1	0.97	0.31	65,65,65,65	0
56	MG	1a	1610	1/1	0.97	0.12	65,65,65,65	0
56	MG	2A	3170	1/1	0.97	0.21	38,38,38,38	0
56	MG	1A	3538	1/1	0.97	0.39	36,36,36,36	0
56	MG	1A	3811	1/1	0.97	0.16	54,54,54,54	0
56	MG	2A	3481	1/1	0.97	0.16	49,49,49,49	0
56	MG	2A	3651	1/1	0.97	0.21	54,54,54,54	0
56	MG	2A	3652	1/1	0.97	0.15	33,33,33,33	0
56	MG	2A	3482	1/1	0.97	0.12	49,49,49,49	0
56	MG	1a	1742	1/1	0.97	0.17	57,57,57,57	0
56	MG	1A	3967	1/1	0.97	0.27	67,67,67,67	0
56	MG	1A	3278	1/1	0.97	0.25	49,49,49,49	0
56	MG	1A	4064	1/1	0.97	0.22	53,53,53,53	0
56	MG	1a	1746	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3969	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	3540	1/1	0.97	0.30	35,35,35,35	0
56	MG	1A	3582	1/1	0.97	0.19	37,37,37,37	0
56	MG	2A	3181	1/1	0.97	0.14	57,57,57,57	0
56	MG	1P	201	1/1	0.97	0.41	34,34,34,34	0
56	MG	1A	3683	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	3684	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3747	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3819	1/1	0.97	0.20	28,28,28,28	0
56	MG	2A	3045	1/1	0.97	0.29	57,57,57,57	0
56	MG	2A	3046	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3820	1/1	0.97	0.15	37,37,37,37	0
56	MG	1a	1756	1/1	0.97	0.14	54,54,54,54	0
56	MG	1Q	201	1/1	0.97	0.18	27,27,27,27	0
56	MG	1a	1758	1/1	0.97	0.05	67,67,67,67	0
56	MG	1a	1628	1/1	0.97	0.07	57,57,57,57	0
56	MG	2A	3341	1/1	0.97	0.17	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	1A	3977	1/1	0.97	0.11	44,44,44,44	0
56	MG	1a	1761	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3334	1/1	0.97	0.28	39,39,39,39	0
56	MG	2a	1728	1/1	0.97	0.15	45,45,45,45	0
56	MG	2a	1729	1/1	0.97	0.17	58,58,58,58	0
56	MG	1A	3585	1/1	0.97	0.27	30,30,30,30	0
56	MG	1A	3068	1/1	0.97	0.29	46,46,46,46	0
56	MG	2E	307	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3158	1/1	0.97	0.19	37,37,37,37	0
56	MG	2a	1734	1/1	0.97	0.21	46,46,46,46	0
56	MG	1A	3178	1/1	0.97	0.12	45,45,45,45	0
56	MG	1R	202	1/1	0.97	0.26	46,46,46,46	0
56	MG	1a	1768	1/1	0.97	0.06	64,64,64,64	0
56	MG	1A	3983	1/1	0.97	0.22	60,60,60,60	0
56	MG	1a	1770	1/1	0.97	0.15	52,52,52,52	0
56	MG	1A	3691	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3985	1/1	0.97	0.12	53,53,53,53	0
56	MG	1S	201	1/1	0.97	0.65	55,55,55,55	0
56	MG	1A	3589	1/1	0.97	0.11	53,53,53,53	0
56	MG	1S	203	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3636	1/1	0.97	0.21	29,29,29,29	0
56	MG	1a	1643	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3757	1/1	0.97	0.12	20,20,20,20	0
56	MG	2Q	201	1/1	0.97	0.13	67,67,67,67	0
56	MG	1A	3695	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3368	1/1	0.97	0.41	47,47,47,47	0
56	MG	2Q	204	1/1	0.97	0.29	60,60,60,60	0
56	MG	1A	3338	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3992	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3592	1/1	0.97	0.08	51,51,51,51	0
56	MG	1A	3434	1/1	0.97	0.11	56,56,56,56	0
56	MG	1A	3995	1/1	0.97	0.09	48,48,48,48	0
56	MG	1U	209	1/1	0.97	0.47	34,34,34,34	0
56	MG	1A	3594	1/1	0.97	0.13	40,40,40,40	0
56	MG	2V	201	1/1	0.97	0.43	49,49,49,49	0
56	MG	1A	3400	1/1	0.97	0.52	52,52,52,52	0
56	MG	1V	201	1/1	0.97	0.59	30,30,30,30	0
56	MG	1A	3255	1/1	0.97	0.30	49,49,49,49	0
56	MG	1V	203	1/1	0.97	0.22	34,34,34,34	0
56	MG	2X	101	1/1	0.97	0.13	62,62,62,62	0
56	MG	1V	204	1/1	0.97	0.25	26,26,26,26	0
56	MG	1B	214	1/1	0.97	0.19	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	3838	1/1	0.97	0.20	37,37,37,37	0
56	MG	1B	217	1/1	0.97	0.20	44,44,44,44	0
56	MG	2A	3713	1/1	0.97	0.20	58,58,58,58	0
56	MG	1A	3128	1/1	0.97	0.28	30,30,30,30	0
56	MG	1A	3078	1/1	0.97	0.46	36,36,36,36	0
56	MG	1a	1798	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3383	1/1	0.97	0.12	54,54,54,54	0
56	MG	23	101	1/1	0.97	0.15	58,58,58,58	0
56	MG	1a	1799	1/1	0.97	0.20	67,67,67,67	0
56	MG	1A	3843	1/1	0.97	0.10	71,71,71,71	0
56	MG	1W	205	1/1	0.97	0.37	39,39,39,39	0
56	MG	1A	3844	1/1	0.97	0.21	35,35,35,35	0
56	MG	1W	208	1/1	0.97	0.28	31,31,31,31	0
56	MG	1A	3845	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3069	1/1	0.97	0.28	48,48,48,48	0
56	MG	2A	3241	1/1	0.97	0.14	65,65,65,65	0
56	MG	1A	4008	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3393	1/1	0.97	0.24	52,52,52,52	0
56	MG	1B	225	1/1	0.97	0.15	60,60,60,60	0
56	MG	1a	1809	1/1	0.97	0.18	66,66,66,66	0
56	MG	1A	3118	1/1	0.97	0.25	38,38,38,38	0
56	MG	1A	3039	1/1	0.97	0.12	30,30,30,30	0
56	MG	1d	301	1/1	0.97	0.20	55,55,55,55	0
56	MG	1B	228	1/1	0.97	0.15	40,40,40,40	0
56	MG	1e	202	1/1	0.97	0.28	56,56,56,56	0
56	MG	2A	3250	1/1	0.97	0.20	63,63,63,63	0
56	MG	2A	3567	1/1	0.97	0.19	60,60,60,60	0
56	MG	2a	1795	1/1	0.97	0.14	71,71,71,71	0
56	MG	1A	4011	1/1	0.97	0.23	24,24,24,24	0
56	MG	2A	3569	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3774	1/1	0.97	0.33	45,45,45,45	0
56	MG	1A	3133	1/1	0.97	0.16	19,19,19,19	0
56	MG	1A	3650	1/1	0.97	0.12	26,26,26,26	0
56	MG	2A	3111	1/1	0.97	0.22	67,67,67,67	0
56	MG	1A	3927	1/1	0.97	0.19	45,45,45,45	0
56	MG	1A	3186	1/1	0.97	0.77	35,35,35,35	0
56	MG	2a	1804	1/1	0.97	0.08	75,75,75,75	0
56	MG	2A	3576	1/1	0.97	0.15	41,41,41,41	0
56	MG	2a	1806	1/1	0.97	0.15	77,77,77,77	0
56	MG	1A	3167	1/1	0.97	0.16	34,34,34,34	0
56	MG	2A	3578	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3605	1/1	0.97	0.11	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3411	1/1	0.97	0.26	24,24,24,24	0
56	MG	1A	3856	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3780	1/1	0.97	0.14	26,26,26,26	0
56	MG	2d	302	1/1	0.97	0.18	56,56,56,56	0
56	MG	2A	3414	1/1	0.97	0.28	61,61,61,61	0
56	MG	1D	301	1/1	0.97	0.21	46,46,46,46	0
56	MG	1D	302	1/1	0.97	0.19	37,37,37,37	0
56	MG	2A	3586	1/1	0.97	0.14	47,47,47,47	0
56	MG	2a	1628	1/1	0.97	0.31	67,67,67,67	0
56	MG	1A	3040	1/1	0.97	0.17	35,35,35,35	0
56	MG	1A	3782	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3412	1/1	0.97	0.35	43,43,43,43	0
56	MG	2a	1632	1/1	0.97	0.13	71,71,71,71	0
56	MG	1D	307	1/1	0.97	0.23	39,39,39,39	0
56	MG	1A	3053	1/1	0.97	0.05	61,61,61,61	0
56	MG	2A	3764	1/1	0.97	0.18	42,42,42,42	0
56	MG	1A	4025	1/1	0.97	0.22	18,18,18,18	0
56	MG	2A	3766	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3657	1/1	0.97	0.22	30,30,30,30	0
56	MG	1D	311	1/1	0.97	0.42	31,31,31,31	0
56	MG	2A	3128	1/1	0.97	0.32	52,52,52,52	0
56	MG	1A	3170	1/1	0.97	0.17	24,24,24,24	0
56	MG	1A	3789	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3033	1/1	0.97	0.28	32,32,32,32	0
56	MG	1A	3523	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3432	1/1	0.97	0.17	63,63,63,63	0
56	MG	1A	3868	1/1	0.97	0.18	57,57,57,57	0
56	MG	2A	3777	1/1	0.97	0.11	75,75,75,75	0
56	MG	2x	105	1/1	0.97	0.34	65,65,65,65	0
56	MG	1E	305	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3192	1/1	0.97	0.18	23,23,23,23	0
56	MG	15	102	1/1	0.97	0.24	29,29,29,29	0
56	MG	1A	4037	1/1	0.97	0.30	42,42,42,42	0
56	MG	2A	3607	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3526	1/1	0.97	0.46	39,39,39,39	0
56	MG	1A	4039	1/1	0.97	0.24	57,57,57,57	0
56	MG	1A	3417	1/1	0.97	0.38	36,36,36,36	0
56	MG	1A	3048	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	3194	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3221	1/1	0.97	0.27	40,40,40,40	0
56	MG	1F	301	1/1	0.97	0.27	39,39,39,39	0
56	MG	17	102	1/1	0.97	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	ZN	2Y	202	1/1	0.97	0.11	101,101,101,101	0
56	MG	1A	3138	1/1	0.97	0.21	34,34,34,34	0
58	ZN	26	102	1/1	0.97	0.14	63,63,63,63	0
56	MG	1A	3196	1/1	0.97	0.17	20,20,20,20	0
56	MG	1A	3620	1/1	0.97	0.14	48,48,48,48	0
56	MG	1F	307	1/1	0.97	0.29	30,30,30,30	0
56	MG	2A	3338	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3119	1/1	0.98	0.22	36,36,36,36	0
56	MG	1A	3965	1/1	0.98	0.15	52,52,52,52	0
56	MG	1F	302	1/1	0.98	0.27	35,35,35,35	0
56	MG	2A	3433	1/1	0.98	0.18	53,53,53,53	0
56	MG	1a	1611	1/1	0.98	0.08	67,67,67,67	0
56	MG	1A	3678	1/1	0.98	0.15	20,20,20,20	0
56	MG	1A	3475	1/1	0.98	0.22	64,64,64,64	0
56	MG	1A	3030	1/1	0.98	0.15	41,41,41,41	0
56	MG	1W	206	1/1	0.98	0.20	41,41,41,41	0
56	MG	1A	3813	1/1	0.98	0.20	34,34,34,34	0
56	MG	1a	1695	1/1	0.98	0.24	65,65,65,65	0
56	MG	2A	3540	1/1	0.98	0.06	60,60,60,60	0
56	MG	2D	302	1/1	0.98	0.30	52,52,52,52	0
56	MG	1A	3765	1/1	0.98	0.12	53,53,53,53	0
56	MG	2A	3744	1/1	0.98	0.21	60,60,60,60	0
56	MG	1A	3215	1/1	0.98	0.35	39,39,39,39	0
56	MG	1A	4029	1/1	0.98	0.30	53,53,53,53	0
56	MG	2A	3007	1/1	0.98	0.17	42,42,42,42	0
56	MG	1A	3723	1/1	0.98	0.19	42,42,42,42	0
56	MG	1F	312	1/1	0.98	0.10	51,51,51,51	0
56	MG	2A	3010	1/1	0.98	0.12	39,39,39,39	0
56	MG	1A	3153	1/1	0.98	0.41	34,34,34,34	0
56	MG	2E	305	1/1	0.98	0.08	57,57,57,57	0
56	MG	1a	1623	1/1	0.98	0.11	63,63,63,63	0
56	MG	1A	3770	1/1	0.98	0.51	32,32,32,32	0
56	MG	1A	3920	1/1	0.98	0.12	37,37,37,37	0
56	MG	1A	4035	1/1	0.98	0.10	41,41,41,41	0
56	MG	1A	3061	1/1	0.98	0.19	19,19,19,19	0
56	MG	1B	216	1/1	0.98	0.07	70,70,70,70	0
56	MG	1A	3480	1/1	0.98	0.24	32,32,32,32	0
56	MG	1A	3685	1/1	0.98	0.18	21,21,21,21	0
56	MG	1A	3577	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3459	1/1	0.98	0.13	53,53,53,53	0
56	MG	2a	1666	1/1	0.98	0.33	58,58,58,58	0
56	MG	2A	3366	1/1	0.98	0.35	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3106	1/1	0.98	0.08	34,34,34,34	0
56	MG	2a	1669	1/1	0.98	0.29	57,57,57,57	0
56	MG	2A	3023	1/1	0.98	0.30	60,60,60,60	0
56	MG	1A	3093	1/1	0.98	0.20	40,40,40,40	0
56	MG	2A	3370	1/1	0.98	0.30	40,40,40,40	0
56	MG	2A	3025	1/1	0.98	0.20	39,39,39,39	0
56	MG	1N	204	1/1	0.98	0.17	44,44,44,44	0
56	MG	1A	3197	1/1	0.98	0.18	36,36,36,36	0
56	MG	1A	3929	1/1	0.98	0.12	49,49,49,49	0
56	MG	1A	3581	1/1	0.98	0.18	12,12,12,12	0
56	MG	2A	3287	1/1	0.98	0.18	55,55,55,55	0
56	MG	1A	3032	1/1	0.98	0.25	33,33,33,33	0
56	MG	1A	3583	1/1	0.98	0.14	39,39,39,39	0
56	MG	1A	3109	1/1	0.98	0.26	30,30,30,30	0
56	MG	2A	3776	1/1	0.98	0.18	39,39,39,39	0
56	MG	2A	3475	1/1	0.98	0.08	49,49,49,49	0
56	MG	2A	3778	1/1	0.98	0.10	57,57,57,57	0
56	MG	1A	3694	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3041	1/1	0.98	0.46	34,34,34,34	0
56	MG	1A	3784	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	3161	1/1	0.98	0.39	58,58,58,58	0
56	MG	11	105	1/1	0.98	0.12	48,48,48,48	0
56	MG	1a	1725	1/1	0.98	0.10	60,60,60,60	0
56	MG	1A	3026	1/1	0.98	0.32	28,28,28,28	0
56	MG	1A	3658	1/1	0.98	0.14	45,45,45,45	0
56	MG	1A	3788	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3097	1/1	0.98	0.26	39,39,39,39	0
56	MG	1a	1808	1/1	0.98	0.21	62,62,62,62	0
56	MG	1A	3204	1/1	0.98	0.22	34,34,34,34	0
56	MG	2A	3791	1/1	0.98	0.19	49,49,49,49	0
56	MG	1A	3183	1/1	0.98	0.38	39,39,39,39	0
56	MG	1A	3058	1/1	0.98	0.21	33,33,33,33	0
56	MG	1b	301	1/1	0.98	0.07	71,71,71,71	0
56	MG	1A	3841	1/1	0.98	0.26	36,36,36,36	0
56	MG	1a	1654	1/1	0.98	0.19	67,67,67,67	0
56	MG	1A	3842	1/1	0.98	0.22	36,36,36,36	0
56	MG	2A	3799	1/1	0.98	0.09	71,71,71,71	0
56	MG	1a	1656	1/1	0.98	0.14	58,58,58,58	0
56	MG	2A	3693	1/1	0.98	0.17	56,56,56,56	0
56	MG	2A	3496	1/1	0.98	0.24	49,49,49,49	0
56	MG	1A	3525	1/1	0.98	0.22	38,38,38,38	0
56	MG	1A	4063	1/1	0.98	0.20	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1D	305	1/1	0.98	0.21	20,20,20,20	0
56	MG	1A	3493	1/1	0.98	0.20	62,62,62,62	0
56	MG	2A	3598	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3329	1/1	0.98	0.29	46,46,46,46	0
56	MG	2A	3142	1/1	0.98	0.31	47,47,47,47	0
56	MG	1A	4004	1/1	0.98	0.20	26,26,26,26	0
56	MG	1A	3356	1/1	0.98	0.08	35,35,35,35	0
56	MG	1A	3088	1/1	0.98	0.28	42,42,42,42	0
56	MG	1A	4007	1/1	0.98	0.19	33,33,33,33	0
56	MG	1A	3166	1/1	0.98	0.40	39,39,39,39	0
56	MG	1a	1667	1/1	0.98	0.12	50,50,50,50	0
56	MG	1A	3752	1/1	0.98	0.19	23,23,23,23	0
56	MG	1A	3232	1/1	0.98	0.25	33,33,33,33	0
56	MG	1A	3022	1/1	0.98	0.23	32,32,32,32	0
56	MG	1U	205	1/1	0.98	0.26	46,46,46,46	0
56	MG	1A	3852	1/1	0.98	0.22	52,52,52,52	0
56	MG	2A	3416	1/1	0.98	0.13	65,65,65,65	0
56	MG	1E	304	1/1	0.98	0.34	32,32,32,32	0
56	MG	2A	3715	1/1	0.98	0.10	79,79,79,79	0
56	MG	2A	3418	1/1	0.98	0.19	38,38,38,38	0
56	MG	2A	3825	1/1	0.98	0.05	70,70,70,70	0
56	MG	1A	3500	1/1	0.98	0.27	42,42,42,42	0
56	MG	2A	3616	1/1	0.98	0.33	47,47,47,47	0
56	MG	1E	306	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	3101	1/1	0.98	0.45	32,32,32,32	0
56	MG	1A	3090	1/1	0.98	0.16	26,26,26,26	0
56	MG	1A	3103	1/1	0.98	0.17	34,34,34,34	0
56	MG	2a	1625	1/1	0.98	0.29	54,54,54,54	0
56	MG	1A	3961	1/1	0.98	0.11	20,20,20,20	0
56	MG	1A	4080	1/1	0.98	0.19	54,54,54,54	0
56	MG	2A	3524	1/1	0.98	0.20	34,34,34,34	0
58	ZN	25	108	1/1	0.98	0.21	60,60,60,60	0
56	MG	1A	3716	1/1	0.98	0.12	25,25,25,25	0
56	MG	2a	1742	1/1	0.98	0.12	65,65,65,65	0
56	MG	1V	205	1/1	0.98	0.18	35,35,35,35	0
56	MG	1A	3286	1/1	0.98	0.23	27,27,27,27	0
56	MG	1A	3012	1/1	0.99	0.14	27,27,27,27	0
56	MG	1A	4028	1/1	0.99	0.12	21,21,21,21	0
56	MG	2A	3735	1/1	0.99	0.20	42,42,42,42	0
56	MG	1A	3741	1/1	0.99	0.19	26,26,26,26	0
56	MG	2A	3019	1/1	0.99	0.24	28,28,28,28	0
56	MG	1A	3711	1/1	0.99	0.11	43,43,43,43	0

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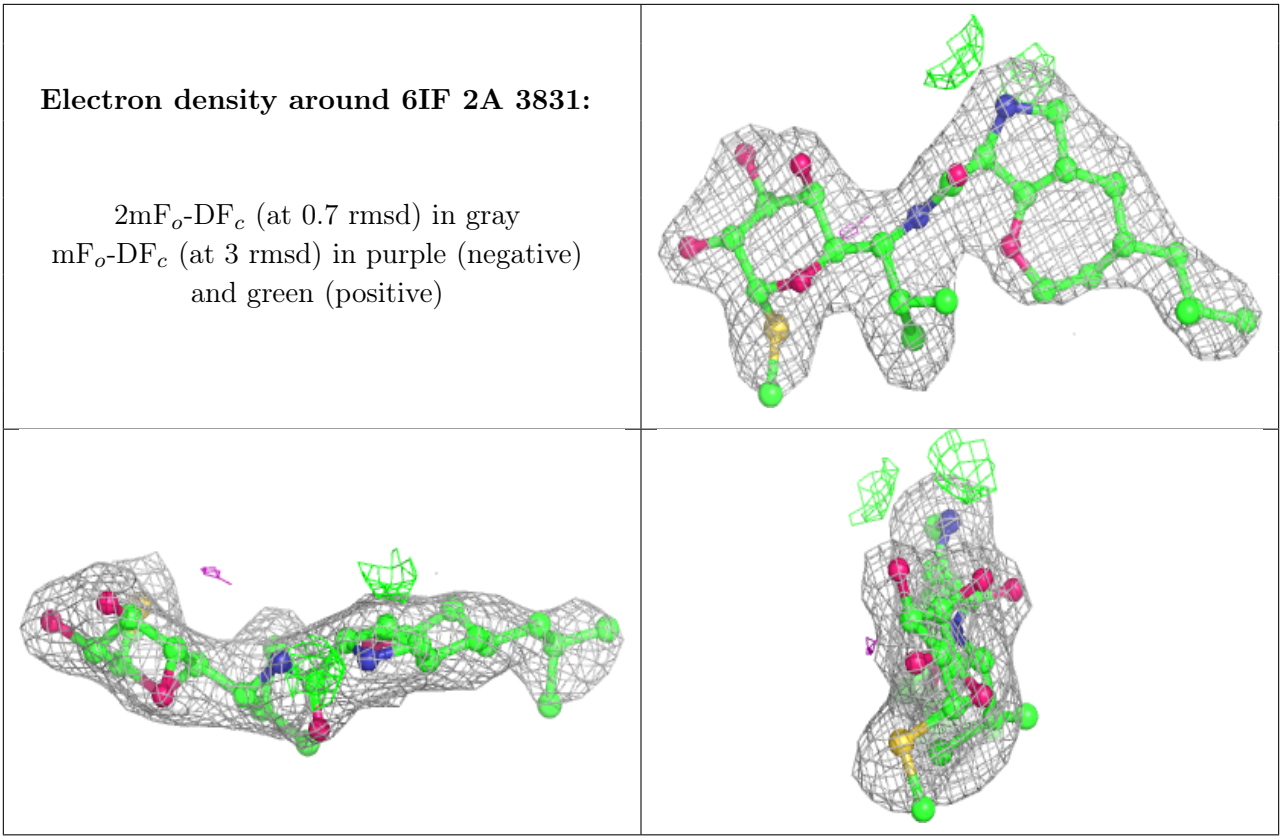
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	201	1/1	0.99	0.26	49,49,49,49	0
56	MG	2A	3495	1/1	0.99	0.24	32,32,32,32	0
56	MG	1A	4031	1/1	0.99	0.13	56,56,56,56	0
56	MG	1a	1688	1/1	0.99	0.23	51,51,51,51	0
56	MG	1A	3666	1/1	0.99	0.11	18,18,18,18	0
56	MG	25	104	1/1	0.99	0.11	46,46,46,46	0
56	MG	1A	3031	1/1	0.99	0.17	22,22,22,22	0
56	MG	1A	3767	1/1	0.99	0.19	28,28,28,28	0
56	MG	1A	4052	1/1	0.99	0.25	55,55,55,55	0
56	MG	2A	3444	1/1	0.99	0.14	65,65,65,65	0
56	MG	1A	3507	1/1	0.99	0.18	42,42,42,42	0
56	MG	2A	3474	1/1	0.99	0.16	35,35,35,35	0
56	MG	1A	3270	1/1	0.99	0.30	31,31,31,31	0
56	MG	28	101	1/1	0.99	0.17	57,57,57,57	0
56	MG	1A	3064	1/1	0.99	0.16	19,19,19,19	0
56	MG	1A	3025	1/1	0.99	0.19	24,24,24,24	0
56	MG	2A	3628	1/1	0.99	0.07	69,69,69,69	0
56	MG	1A	3003	1/1	0.99	0.13	30,30,30,30	0
56	MG	1a	1675	1/1	0.99	0.08	71,71,71,71	0
56	MG	1F	304	1/1	0.99	0.35	35,35,35,35	0
56	MG	2A	3262	1/1	0.99	0.20	50,50,50,50	0
58	ZN	15	109	1/1	0.99	0.19	44,44,44,44	0
58	ZN	16	102	1/1	0.99	0.20	47,47,47,47	0
58	ZN	19	102	1/1	0.99	0.18	48,48,48,48	0
56	MG	2A	3059	1/1	0.99	0.10	46,46,46,46	0
56	MG	2A	3185	1/1	0.99	0.14	57,57,57,57	0
56	MG	2A	3792	1/1	0.99	0.15	45,45,45,45	0
56	MG	1A	3406	1/1	0.99	0.69	37,37,37,37	0
56	MG	1A	3863	1/1	0.99	0.24	30,30,30,30	0
56	MG	1A	3798	1/1	0.99	0.13	34,34,34,34	0
56	MG	1A	3921	1/1	0.99	0.18	57,57,57,57	0
59	SF4	1d	302	8/8	0.99	0.18	59,63,68,73	0
59	SF4	2d	303	8/8	0.99	0.14	62,73,81,82	0
56	MG	13	101	1/1	0.99	0.11	39,39,39,39	0
60	K	2x	101	1/1	0.99	0.23	73,73,73,73	0
56	MG	1A	3154	1/1	1.00	0.48	35,35,35,35	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.

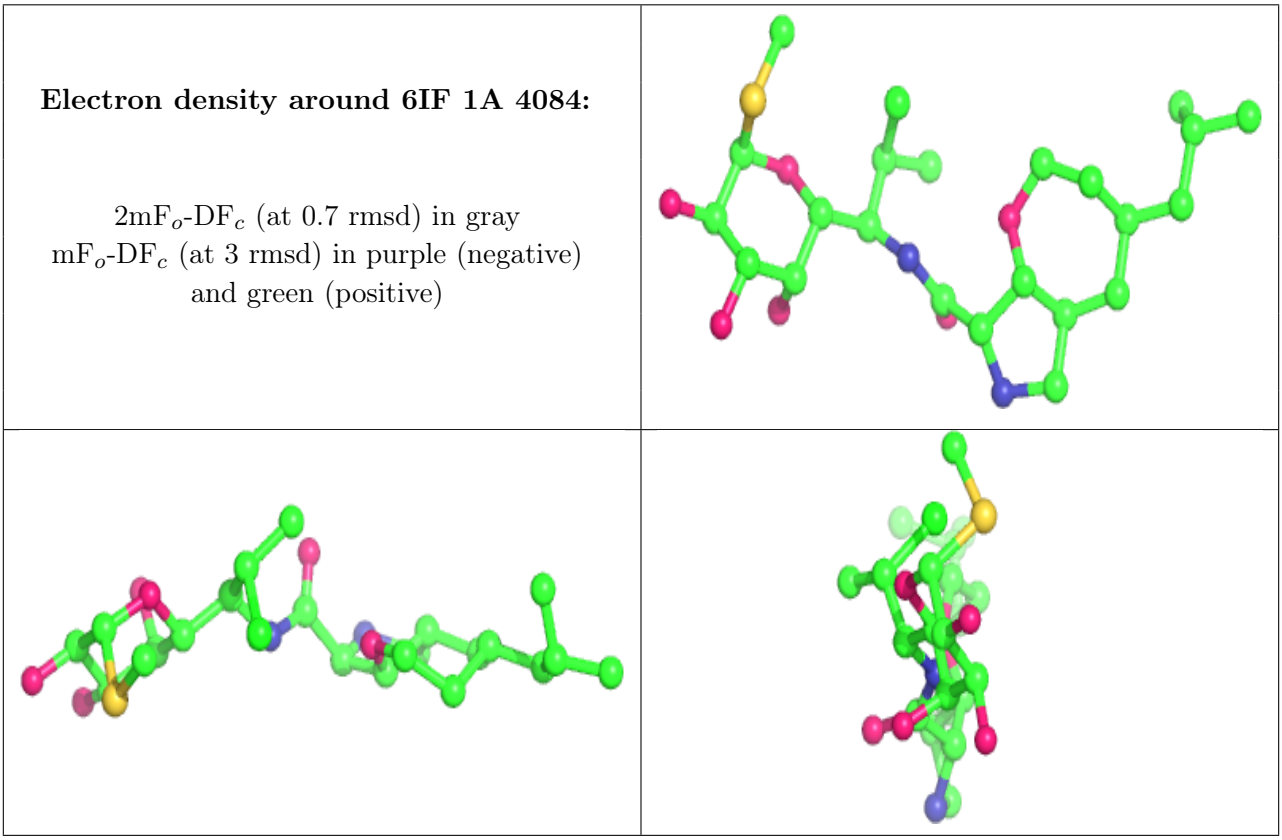
Electron density around 6IF 2A 3831:

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



Electron density around 6IF 1A 4084:

$2mF_o$-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.