



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 07:28 PM EDT

PDB ID : 7RQ9
Title : Crystal structure of the A2058-dimethylated *Thermus thermophilus* 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNAs, and aminoacylated P-site tRNA at 2.60Å resolution
Authors : Mitcheltree, M.J.; Pisipati, A.; Syroegin, E.A.; Silvestre, K.J.; Klepacki, D.; Mason, J.D.; Terwilliger, D.W.; Testolin, G.; Pote, A.R.; Wu, K.J.Y.; Ladley, R.P.; Chatman, K.; Mankin, A.S.; Polikanov, Y.S.; Myers, A.G.
Deposited on : 2021-08-06
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

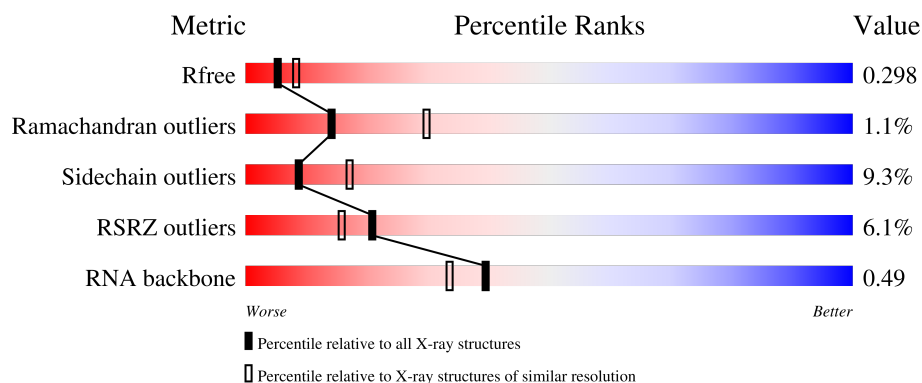
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



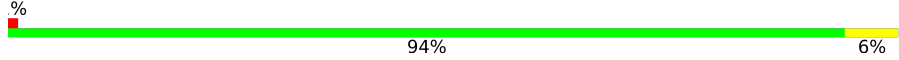
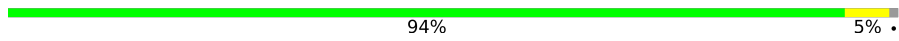
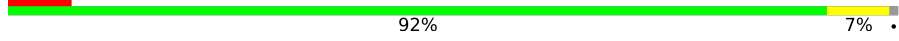
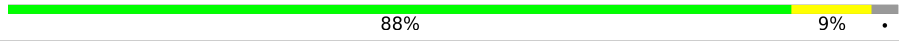
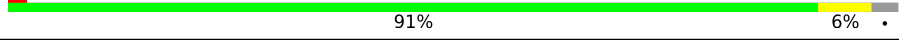




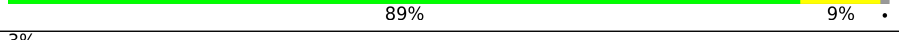

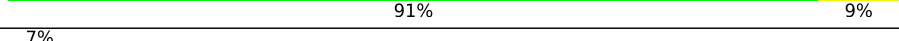
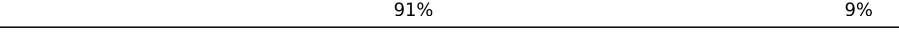
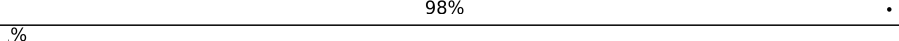
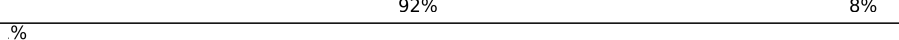


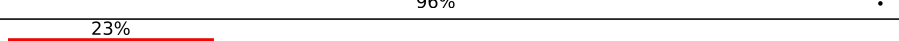
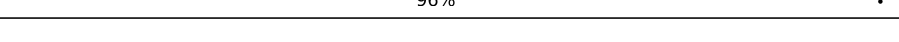
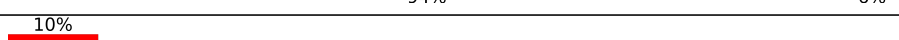
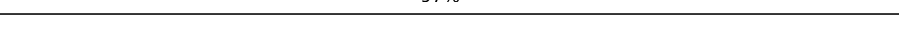




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 $\leq 5\%$. 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	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
2	2B	121	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>
3	1D	276	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

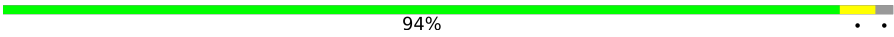
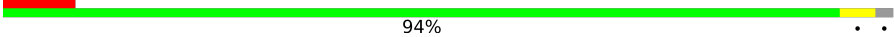



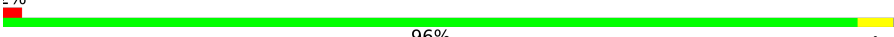
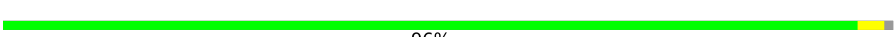



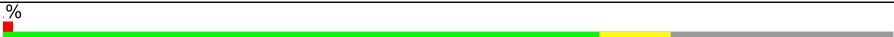


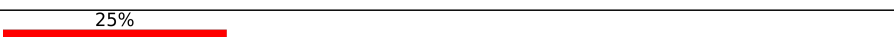
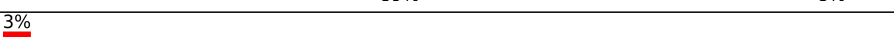
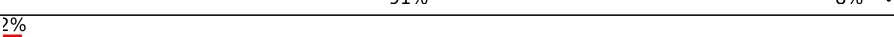
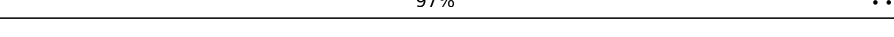
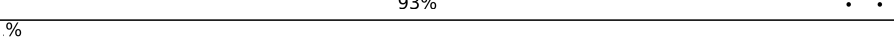
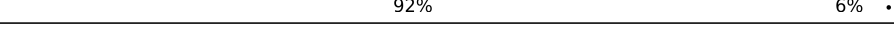
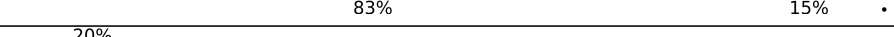
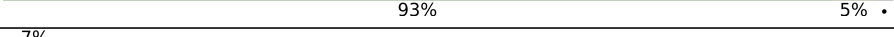




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Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	

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Mol	Chain	Length	Quality of chain
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	
27	25	60	
28	16	54	

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Mol	Chain	Length	Quality of chain
28	26	54	
29	17	49	
29	27	49	
30	18	65	
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	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	

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Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	

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Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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
57	MG	1A	3951	-	-	-	X
57	MG	1B	227	-	-	-	X
57	MG	1a	1680	-	-	-	X
57	MG	2w	106	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299665 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
			61854	27533	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60324	26850	11284	19390	2800			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			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	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	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 tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	72	Total	C	N	O	P	S	0	0
			1550	694	277	505	72	2		
54	2w	70	Total	C	N	O	P	S	0	0
			1502	671	270	489	70	2		

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

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

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1087	Total	Mg	0	0
			1087	1087		
57	1B	34	Total	Mg	0	0
			34	34		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	15	Total	Mg	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	4	Total 4	Mg 4	0	0
57	1P	5	Total 5	Mg 5	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	6	Total 6	Mg 6	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	5	Total 5	Mg 5	0	0
57	1U	9	Total 9	Mg 9	0	0
57	1V	6	Total 6	Mg 6	0	0
57	1W	10	Total 10	Mg 10	0	0
57	1X	7	Total 7	Mg 7	0	0
57	1Y	3	Total 3	Mg 3	0	0
57	1Z	5	Total 5	Mg 5	0	0
57	10	9	Total 9	Mg 9	0	0
57	11	6	Total 6	Mg 6	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	8	Total 8	Mg 8	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	1	Total 1	Mg 1	0	0
57	17	8	Total 8	Mg 8	0	0
57	18	5	Total 5	Mg 5	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	211	Total 211	Mg 211	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1e	1	Total 1	Mg 1	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1h	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1p	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	2	Total 2	Mg 2	0	0
57	1w	9	Total 9	Mg 9	0	0
57	1x	15	Total 15	Mg 15	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	855	Total 855	Mg 855	0	0
57	2B	19	Total 19	Mg 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2D	5	Total 5 Mg 5	0	0
57	2E	8	Total 8 Mg 8	0	0
57	2F	8	Total 8 Mg 8	0	0
57	2G	1	Total 1 Mg 1	0	0
57	2N	1	Total 1 Mg 1	0	0
57	2O	1	Total 1 Mg 1	0	0
57	2P	3	Total 3 Mg 3	0	0
57	2Q	2	Total 2 Mg 2	0	0
57	2R	2	Total 2 Mg 2	0	0
57	2T	5	Total 5 Mg 5	0	0
57	2U	2	Total 2 Mg 2	0	0
57	2V	2	Total 2 Mg 2	0	0
57	2X	3	Total 3 Mg 3	0	0
57	2Z	1	Total 1 Mg 1	0	0
57	20	2	Total 2 Mg 2	0	0
57	21	2	Total 2 Mg 2	0	0
57	23	2	Total 2 Mg 2	0	0
57	25	4	Total 4 Mg 4	0	0
57	26	1	Total 1 Mg 1	0	0
57	27	2	Total 2 Mg 2	0	0
57	28	3	Total 3 Mg 3	0	0

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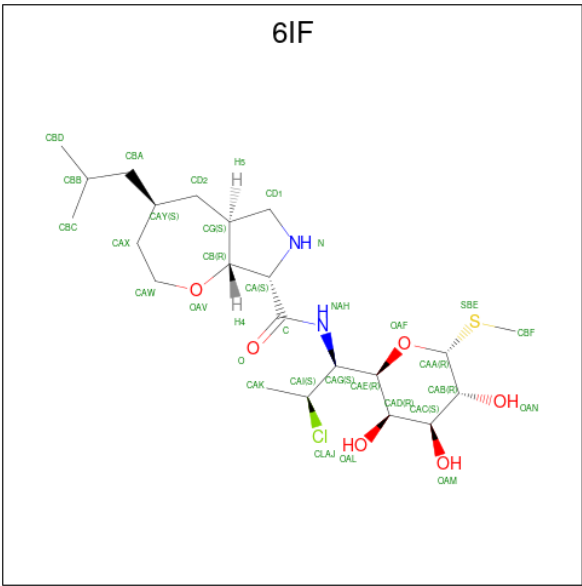
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2a	230	Total 230	Mg 230	0	0
57	2d	1	Total 1	Mg 1	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	4	Total 4	Mg 4	0	0
57	2m	1	Total 1	Mg 1	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r	1	Total 1	Mg 1	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2w	9	Total 9	Mg 9	0	0
57	2x	6	Total 6	Mg 6	0	0
57	2y	6	Total 6	Mg 6	0	0

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

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

- Molecule 59 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-α-D-galacto-octopyran

oside (three-letter code: 6IF) (formula: C₂₂H₃₉ClN₂O₆S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
59	1A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		
59	2A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

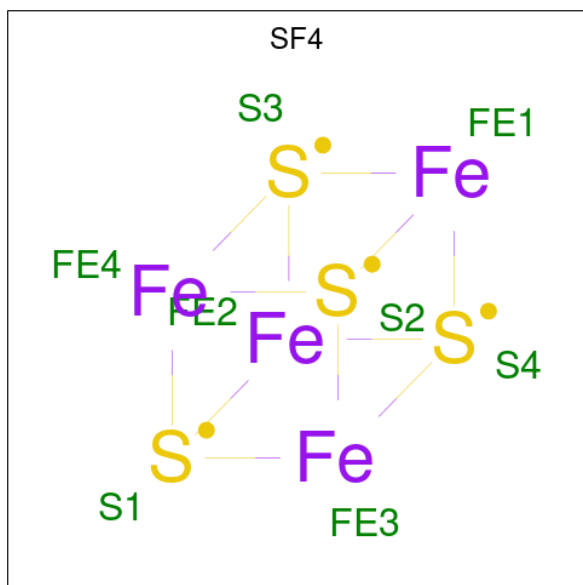
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1910	Total	O	0	0
			1910	1910		
62	1B	61	Total	O	0	0
			61	61		
62	1D	28	Total	O	0	0
			28	28		
62	1E	29	Total	O	0	0
			29	29		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1F	18	Total 18	O 18	0	0
62	1G	2	Total 2	O 2	0	0
62	1H	1	Total 1	O 1	0	0
62	1I	1	Total 1	O 1	0	0
62	1N	6	Total 6	O 6	0	0
62	1O	4	Total 4	O 4	0	0
62	1P	24	Total 24	O 24	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	11	Total 11	O 11	0	0
62	1S	6	Total 6	O 6	0	0
62	1T	7	Total 7	O 7	0	0
62	1U	13	Total 13	O 13	0	0
62	1V	8	Total 8	O 8	0	0
62	1W	7	Total 7	O 7	0	0
62	1X	6	Total 6	O 6	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	11	Total 11	O 11	0	0
62	11	13	Total 13	O 13	0	0
62	12	4	Total 4	O 4	0	0
62	13	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	14	1	Total 1	O 1	0	0
62	15	5	Total 5	O 5	0	0
62	16	3	Total 3	O 3	0	0
62	17	10	Total 10	O 10	0	0
62	18	9	Total 9	O 9	0	0
62	19	1	Total 1	O 1	0	0
62	1a	313	Total 313	O 313	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1j	1	Total 1	O 1	0	0
62	1l	5	Total 5	O 5	0	0
62	1m	2	Total 2	O 2	0	0
62	1n	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	4	Total 4	O 4	0	0
62	1w	9	Total 9	O 9	0	0
62	1x	12	Total 12	O 12	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1010	Total 1010	O 1010	0	0
62	2B	21	Total 21	O 21	0	0

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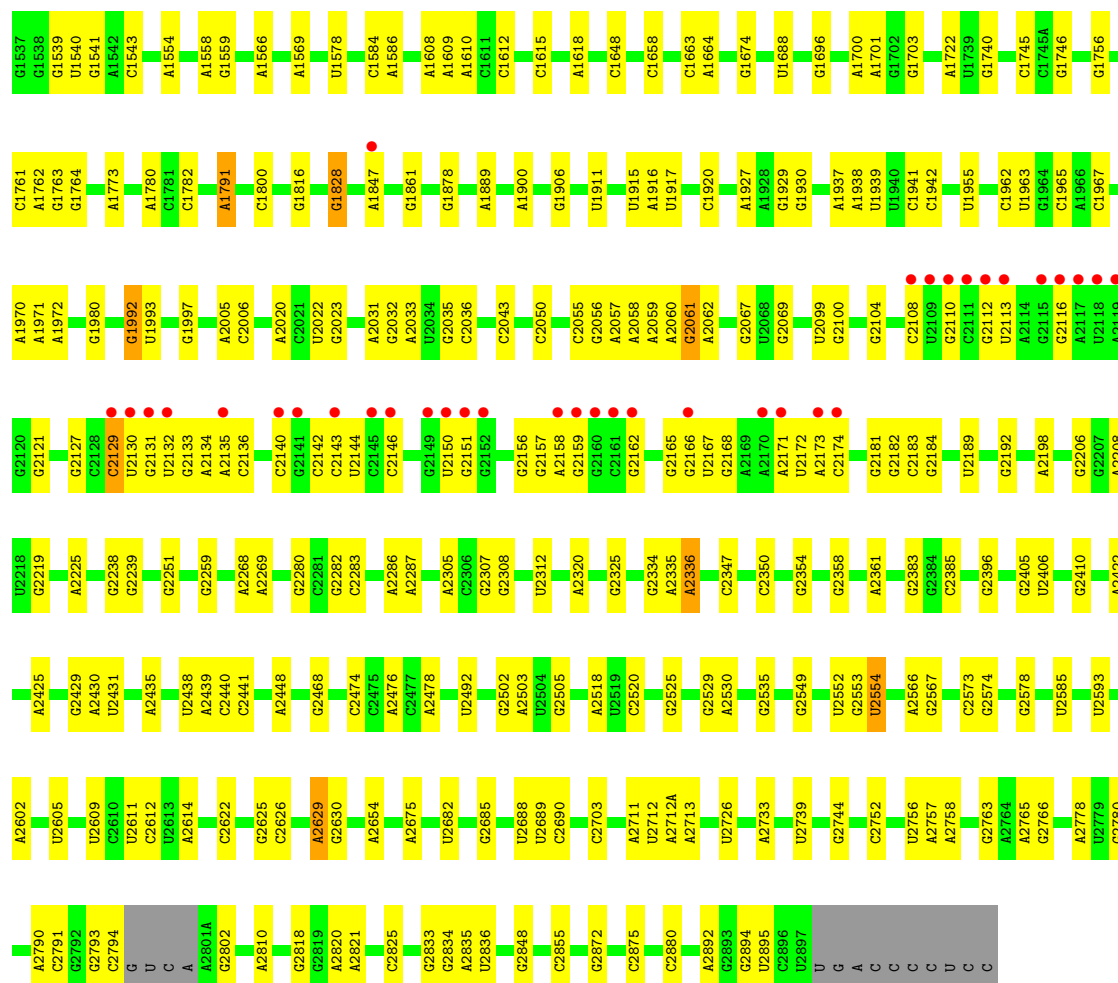
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2D	15	Total 15	O 15	0	0
62	2E	12	Total 12	O 12	0	0
62	2F	13	Total 13	O 13	0	0
62	2I	2	Total 2	O 2	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	10	Total 10	O 10	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	5	Total 5	O 5	0	0
62	2U	3	Total 3	O 3	0	0
62	2W	1	Total 1	O 1	0	0
62	2X	3	Total 3	O 3	0	0
62	2Y	1	Total 1	O 1	0	0
62	20	4	Total 4	O 4	0	0
62	21	8	Total 8	O 8	0	0
62	23	1	Total 1	O 1	0	0
62	25	1	Total 1	O 1	0	0
62	27	4	Total 4	O 4	0	0
62	28	2	Total 2	O 2	0	0
62	29	1	Total 1	O 1	0	0
62	2a	181	Total 181	O 181	0	0

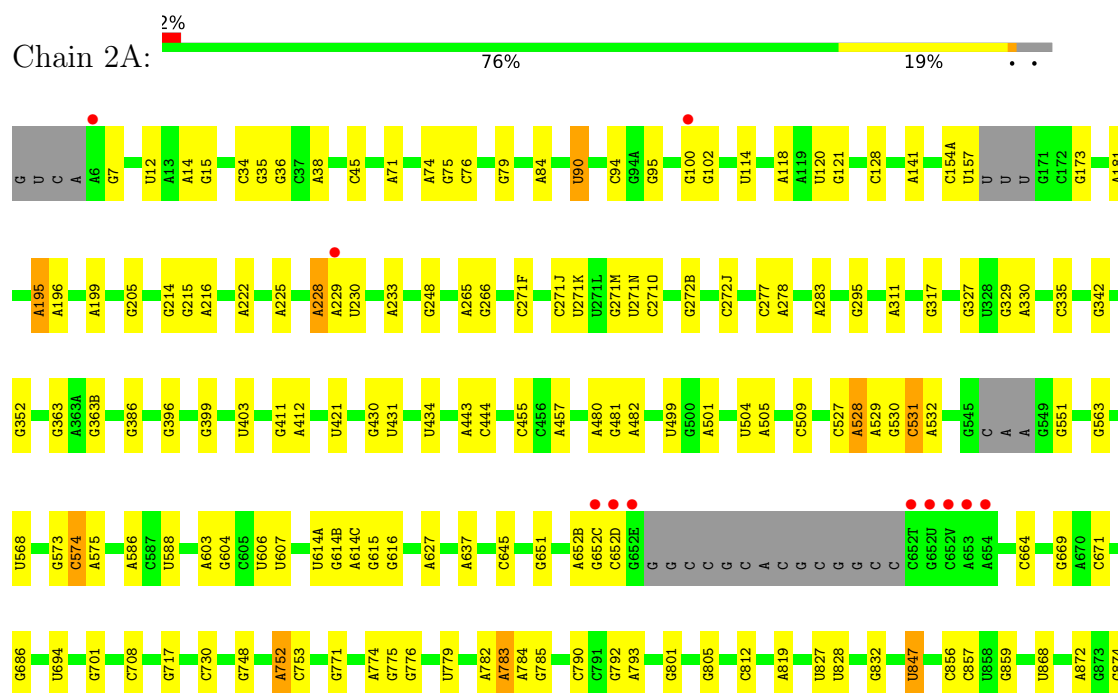
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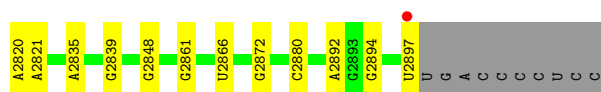
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2d	1	Total	O	0	0
			1	1		
62	2j	3	Total	O	0	0
			3	3		
62	2l	5	Total	O	0	0
			5	5		
62	2p	3	Total	O	0	0
			3	3		
62	2q	1	Total	O	0	0
			1	1		
62	2r	1	Total	O	0	0
			1	1		
62	2t	2	Total	O	0	0
			2	2		
62	2v	4	Total	O	0	0
			4	4		
62	2w	1	Total	O	0	0
			1	1		
62	2x	3	Total	O	0	0
			3	3		
62	2y	4	Total	O	0	0
			4	4		



• Molecule 1: 23S Ribosomal RNA



A2854	A2497	A2366	U2189	G2123	C1941	A1762	C1543	G1385	A	U	C1012	G875
A2662	G2502	G2370	G2192	G2125	C1942	G1763	C1547	C1386	U	U	C1013	A878
A2679	A2198	G2374	A2198	A2126	U1955	G1764	A1558	A1392	A	A	G1017	G880
G2886	G2504	C2375	G2206	C2128	C1962	A1780	A1566	A1412	G1195	A	A1021	G881
U2605	U2506	A2376	G2207	C2129	U1963	C1781	A1566	G1416	A	A	G1022	G882
C2507	A2208	A2376	A2208	C2130	A1966	C1782	A1569	C1417	A	G	G1023	C884
U2689	U2218	G2383	U2218	U2132	C1967	A1786	U1578	U1420	A	U	G1024	C885
A2518	G2384	G2384	G2225	G2133	A1970	A1786	U1578	U1420	A	C	G1025	C886
C2703	G2385	G2385	A2225	A2134	A1971	A1786	A1579	G1421	A	C	U1026	A887
A2712A	C2520	A2391	G2238	A2135	A1971	A1791	A1580	C1428	A	G	A1027	C889
G2525	G2525	C2137	G2237	C2136	A1972	C1800	A1583	C1428	A	U	U1033	
G2714	G2529	C2403	G2251	C2138	U1993	G1801	C1584	C1437	A	A	U1033	
G2718	G2532	U2406	A2267	C2140	G1997	A1812	C1588	C1437	A	U	G1036	C893
U2726	U2537	G2414	A2268	G2141	G1997	G1816	A1608	G1442	A	A	G1037	C894
A2733	U2552	A2422	A2274	C2143	A2020	A1829	A1609	A1445	A	G	G1038	U895
G2751	U2553	A2425	A2278	C2146	A2031	G1835	A1616	A1449	A	U	G1039	A896
C2752	U2554	A2426	A2287	G2147	A2032	A1847	C1648	G1461	A	C	A	C904
A2753	U2555	C2427	C2283	G2148	A2033	A1848	G1653	A1461	A	U	G1042	A897
U2562	U2562	G2428	A2286	C2149	A2036	G1858	A1654	C1462	A	C	C1043	C898
G2758	U2566	G2429	A2287	U2150	C2036	G1858	A1654	C1462	A	C	G	A900
A2759	G2567	A2430	A2287	G2152	C2036	G1858	A1654	C1462	A	C	G	A901
C2760	U2567	A2434	A2288	C2153	C2043	G1861	A1664	C1467	A	U	A	
G2761	C2573	A2435	A2305	G2154	C2043	G1861	A1664	C1467	A	U	A	
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A2765	G2578	A2439	G2308	G2156	A2057	G1878	G1674	A1471	A	U	A	
A2778	G2578	C2440	A2309	G2157	A2058	C1881	G1674	A1471	A	U	A	
U2779	G2582	C2441	A2310	A2158	A2059	C1881	C1675	G1479	A	U	A	
G2780	A2602	G2445	U2311	G2159	A2060	A1900	C1675	G1479	A	U	A	
C2789	A2602	G2446	U2312	C2160	G2061	A1900	C1675	G1479	A	U	A	
A	U2605	G2447	U2312	C2161	G2062	G1906	G1695	A1490	A	U	A	
C	U2605	A2448	G2318	C2162	C2063	G1906	G1695	A1490	A	U	A	
G2792	U2609	U2457	G2319	G2165	G2069	U1911	G1697	C1493	A	U	A	
G2793	C2610	G2458	A2320	U2167	G2069	A1912	G1697	C1493	A	U	A	
C2794	U2611	A2459	G2325	C2168	G2093	A1913	A1698	A1496	A	U	A	
G	C2612	A2459	G2325	A2169	G2093	C1914	A1700	U1497	A	U	A	
U	U	C2465	C2326	A2169	G2093	U1915	A1701	U1352	A	U	A	
U	U	C2465	A2327	A2170	U2109	A1916	G1707	A1508	A	U	A	
C	U2616	A2469	G2334	A2171	G2110	U1917	G1707	A1508	A	U	A	
A	A2629	A2469	G2334	U2172	G2111	C1920	G1707	A1508	A	U	A	
A2801A	G2629	A2476	A2335	A2173	U2112	C1920	G1721	A1509A	A	U	A	
G2802	G2630	C2477	A2336	C2174	G2113	C1920	A1722	C1530	A	U	A	
C2803	C2634	C2477	A2336	C2175	U1739	G1929	U1739	C1531	A	U	A	
C2804	C2635	C2477	A2346	G2176	G2114	G1930	G1740	C1532	A	U	A	
G2805	U2636	C2480	C2347	A2176	G2115	G1930	G1740	C1532	A	U	A	
G2807	U2636	G2481	C2347	C2177	G2116	U1931	G1368	G1533	A	U	A	
A2810	C2646	G2490	C2350	C2178	U2117	A1936	G1747	U	A	U	A	
U2847	U2647	U2491	C2350	G2182	U2118	A1937	G1750	A	A	U	A	
C2648	C2648	U2491	G2354	G2182	A2119	A1937	G1750	C1536	A	U	A	
G2818	C2648	C2464	G2358	C2185	G2120	U1939	G1756	G1541	A	U	A	
C2819	C2648	C2464	C2358	U2192	C2121	U1940	A1542	A1542	A	U	A	



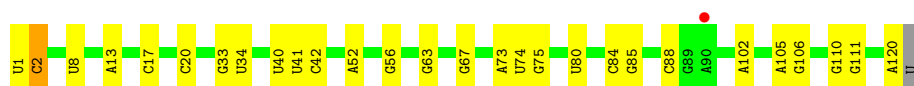
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 89% 10%



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 76% 22% 2%



- Molecule 3: 50S ribosomal protein L2

Chain 1D: 94% 5%



- Molecule 3: 50S ribosomal protein L2

Chain 2D: 94% 6%



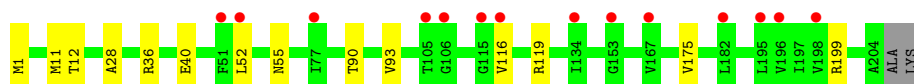
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 94% 5%




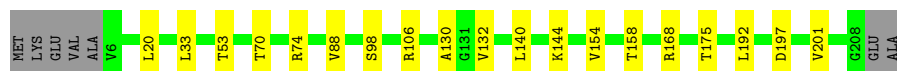
- Molecule 4: 50S ribosomal protein L3

Chain 2E: 92% 7% 7%

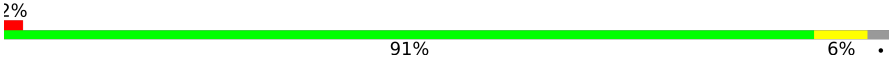


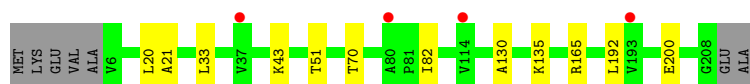
- Molecule 5: 50S ribosomal protein L4

Chain 1F:  88% 9% .

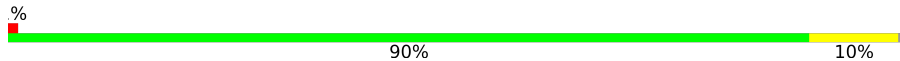


- Molecule 5: 50S ribosomal protein L4

Chain 2F:  91% 6% .




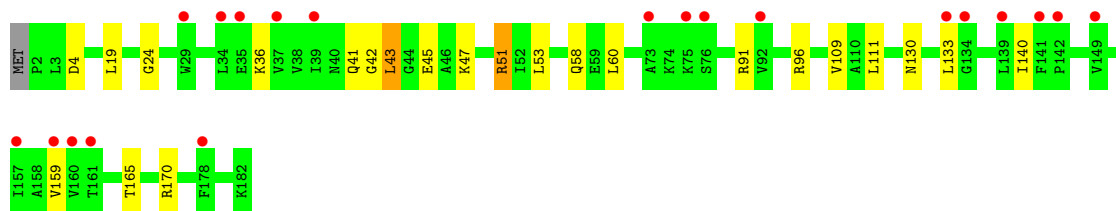
- Molecule 6: 50S ribosomal protein L5

Chain 1G:  90% 10% .




- Molecule 6: 50S ribosomal protein L5

Chain 2G:  87% 12% ..

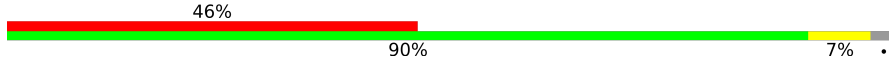


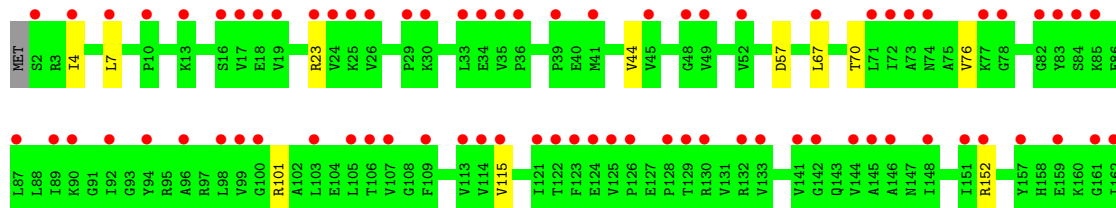
- Molecule 7: 50S ribosomal protein L6

Chain 1H:  89% 7% .



- Molecule 7: 50S ribosomal protein L6

Chain 2H:  90% 7% .





- Molecule 8: 50S ribosomal protein L9

Chain 1I: 89% 9% .



- Molecule 8: 50S ribosomal protein L9

Chain 2I: 3% 86% 13% .



- Molecule 9: 50S ribosomal protein L13

Chain 1N: 0% 91% 9% .



- Molecule 9: 50S ribosomal protein L13

Chain 2N: 7% 91% 9% .



- Molecule 10: 50S ribosomal protein L14

Chain 1O: 98% .

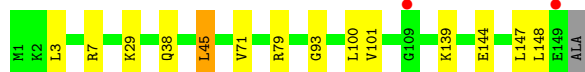
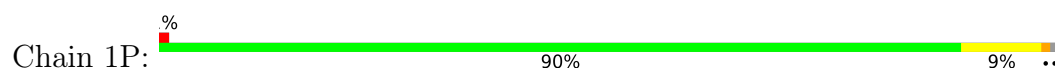


- Molecule 10: 50S ribosomal protein L14

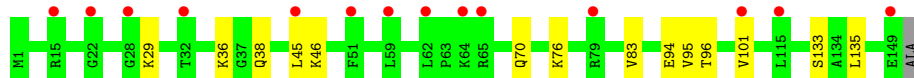
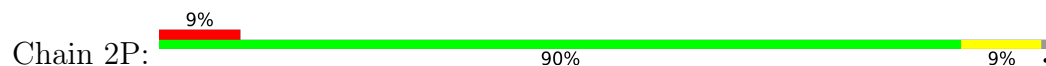
Chain 2O: 0% 92% 8% .



- Molecule 11: 50S ribosomal protein L15



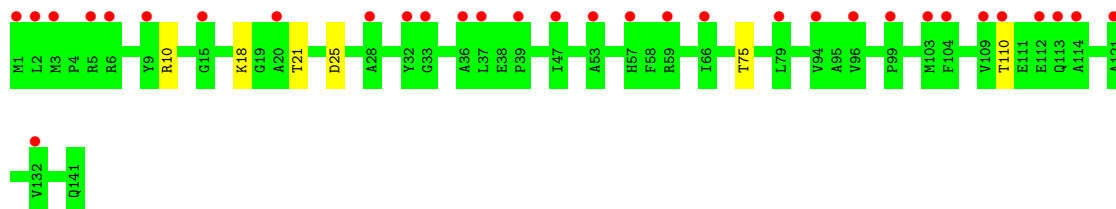
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



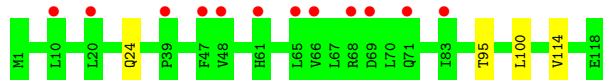
- Molecule 12: 50S ribosomal protein L16



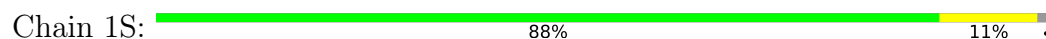
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

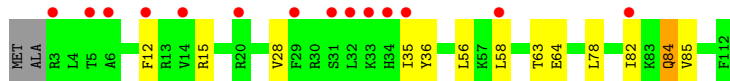
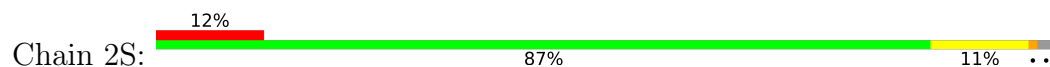


- Molecule 14: 50S ribosomal protein L18

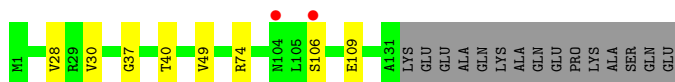
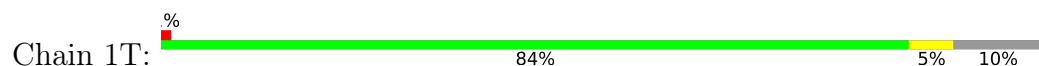




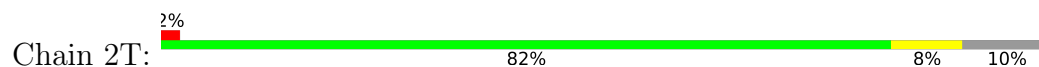
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



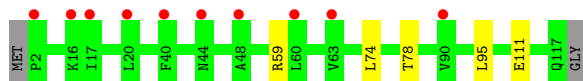
- Molecule 15: 50S ribosomal protein L19



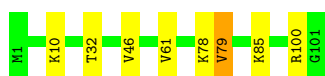
- Molecule 16: 50S ribosomal protein L20



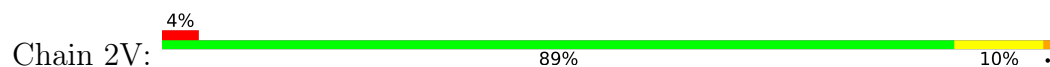
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21





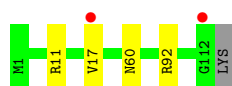
- Molecule 18: 50S ribosomal protein L22

Chain 1W: 93% 6% .



- Molecule 18: 50S ribosomal protein L22

Chain 2W: 2% 96% ..



- Molecule 19: 50S ribosomal protein L23

Chain 1X: 96% ..



- Molecule 19: 50S ribosomal protein L23

Chain 2X: 1% 96% ..



- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 1% 89% 8% .

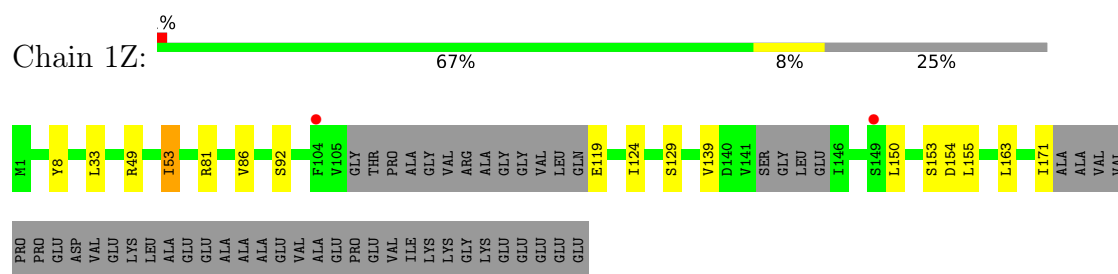


- Molecule 20: 50S ribosomal protein L24

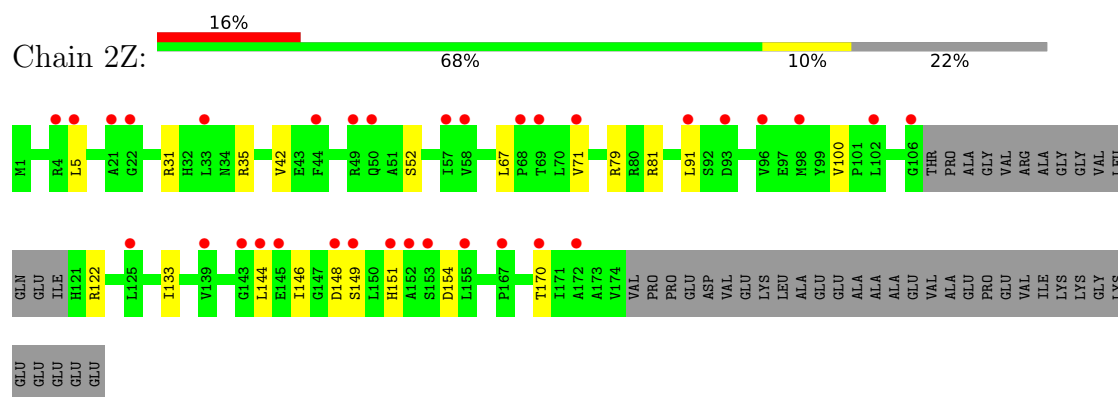
Chain 2Y: 1% 90% 7% .



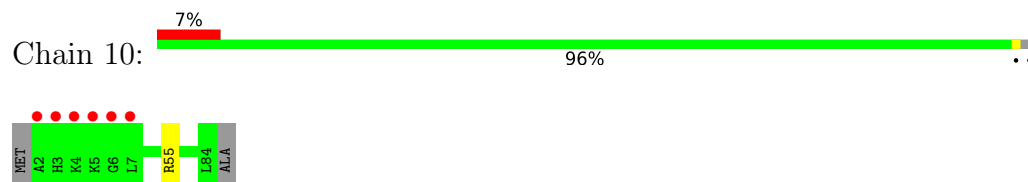
- Molecule 21: 50S ribosomal protein L25



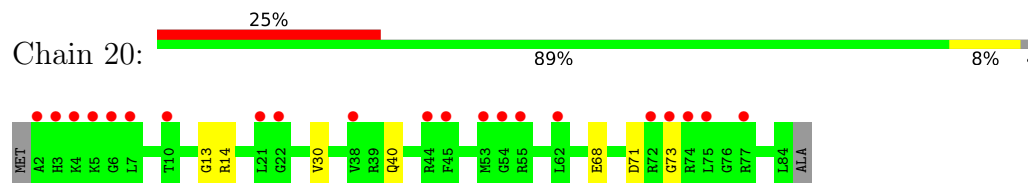
- Molecule 21: 50S ribosomal protein L25



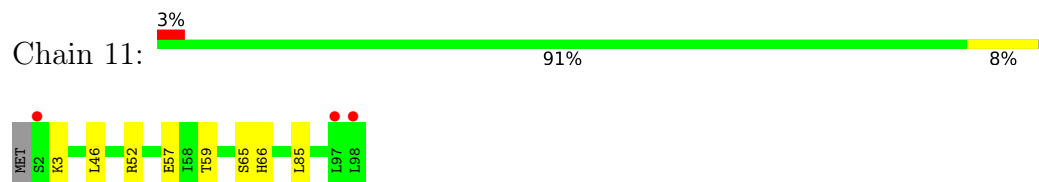
- Molecule 22: 50S ribosomal protein L27



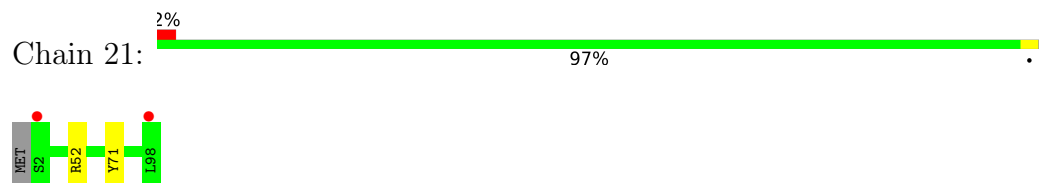
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

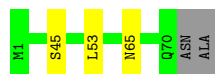


- Molecule 23: 50S ribosomal protein L28




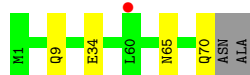
- Molecule 24: 50S ribosomal protein L29

Chain 12:  93% . .




- Molecule 24: 50S ribosomal protein L29

Chain 22:  92% 6% .



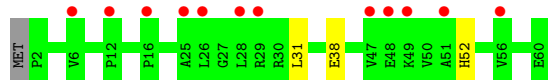
- Molecule 25: 50S ribosomal protein L30

Chain 13:  83% 15% .




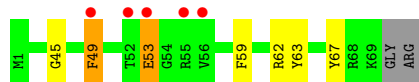
- Molecule 25: 50S ribosomal protein L30

Chain 23:  20% 93% 5% .




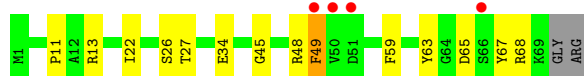
- Molecule 26: 50S ribosomal protein L31

Chain 14:  7% 87% 7% . .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  6% 77% 18% . .

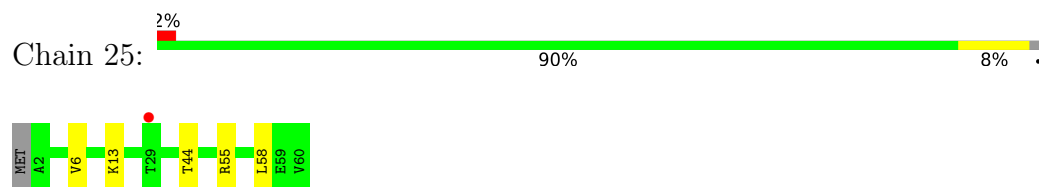


- Molecule 27: 50S ribosomal protein L32

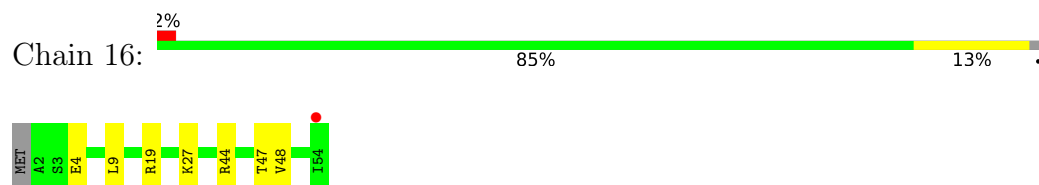
Chain 15:  92% 7% .



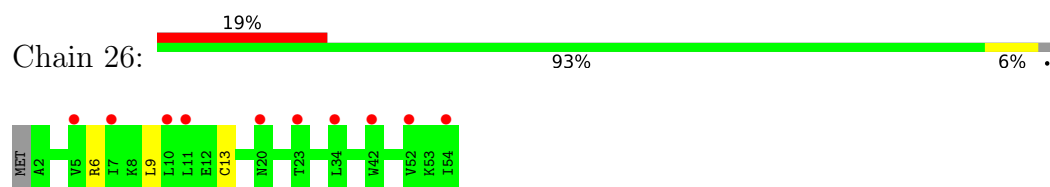
- Molecule 27: 50S ribosomal protein L32



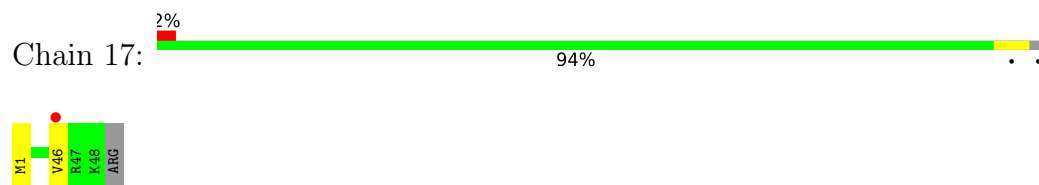
- Molecule 28: 50S ribosomal protein L33



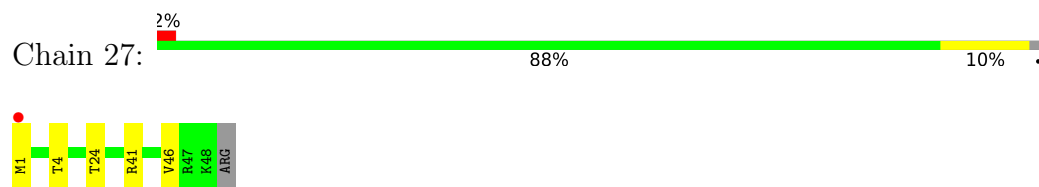
- Molecule 28: 50S ribosomal protein L33



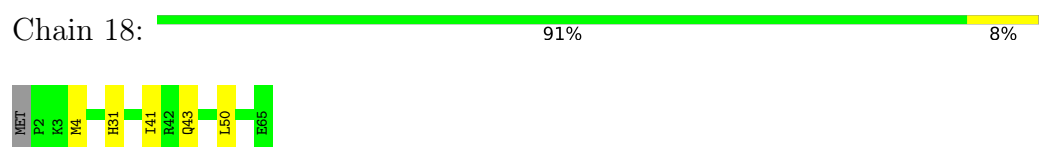
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

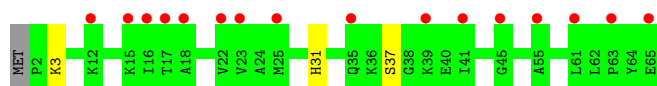


- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35





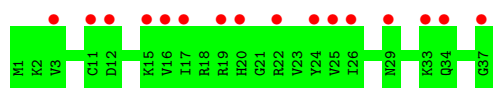
- Molecule 31: 50S ribosomal protein L36

Chain 19: 97%



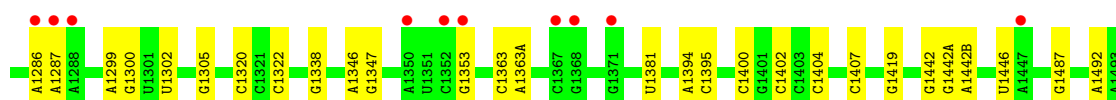
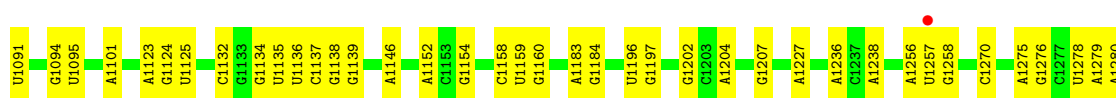
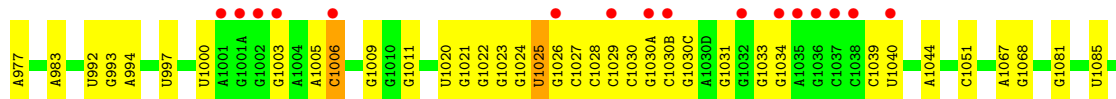
- Molecule 31: 50S ribosomal protein L36

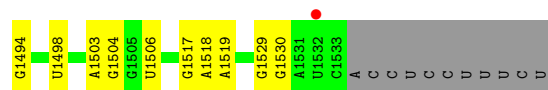
Chain 29: 43% 100%



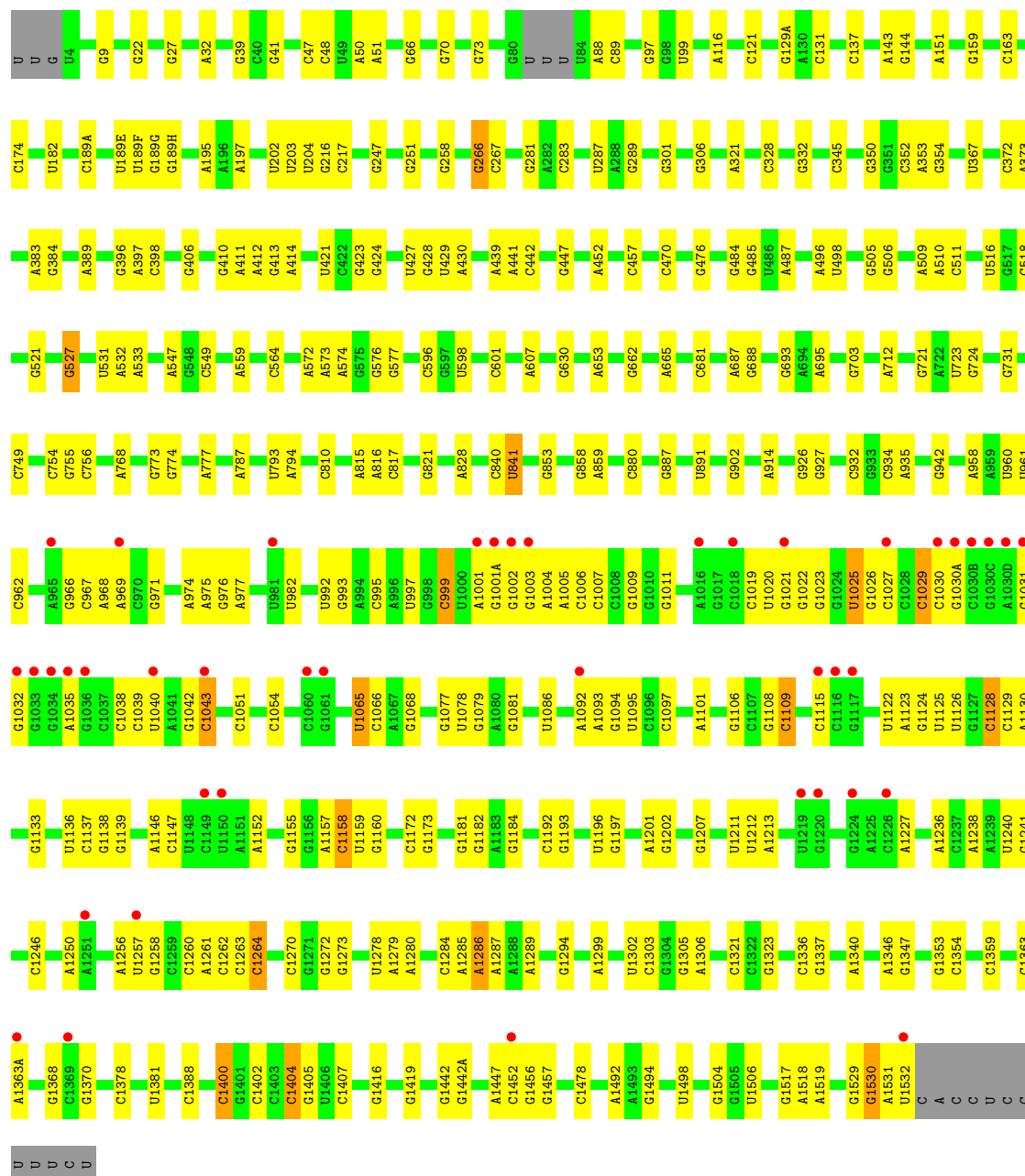
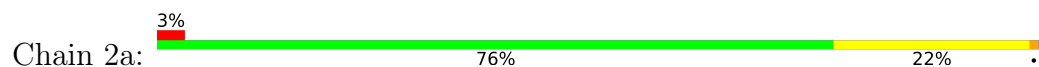
- Molecule 32: 16S Ribosomal RNA

Chain 1a: 2% 80% 18%

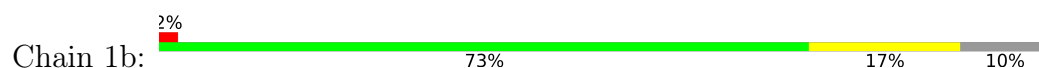


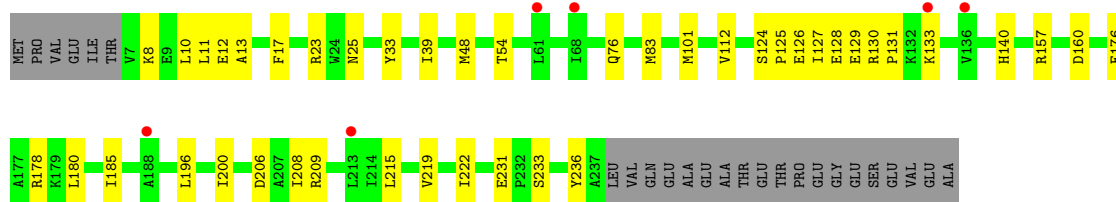


- Molecule 32: 16S Ribosomal RNA

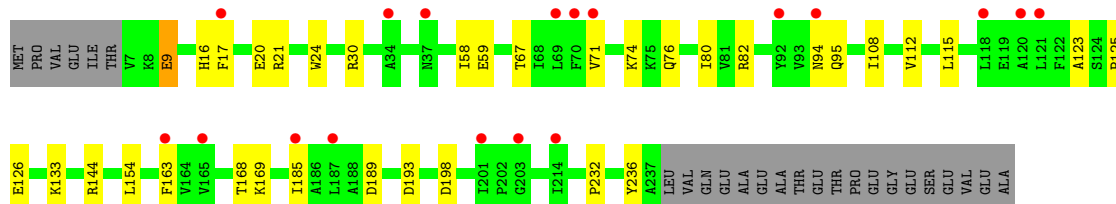
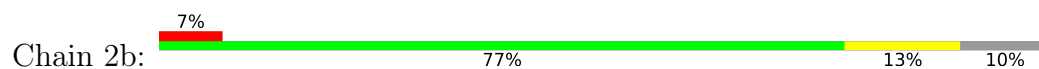


- Molecule 33: 30S ribosomal protein S2

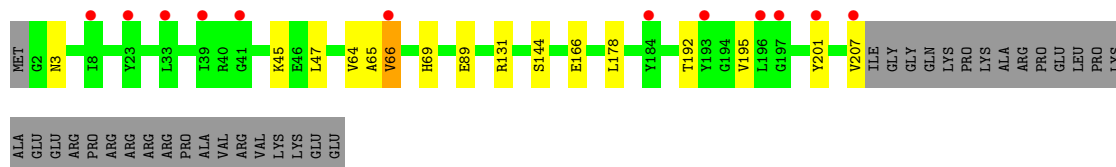
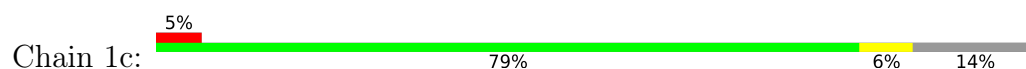




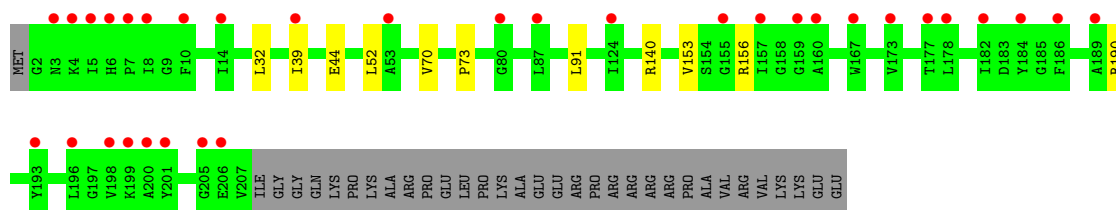
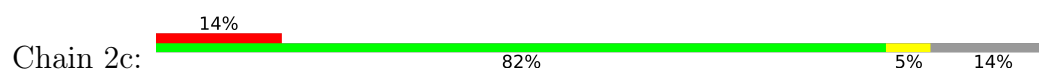
- Molecule 33: 30S ribosomal protein S2



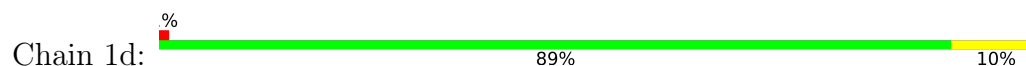
- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3

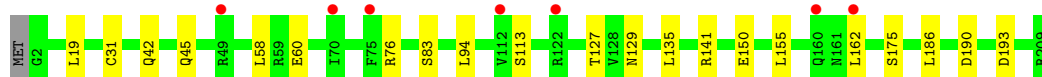


- Molecule 35: 30S ribosomal protein S4

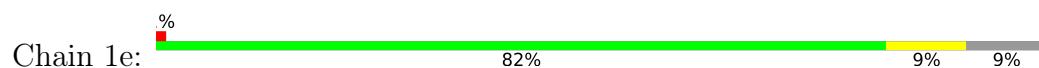


- Molecule 35: 30S ribosomal protein S4

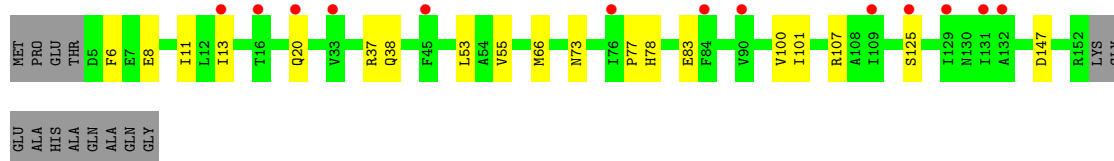
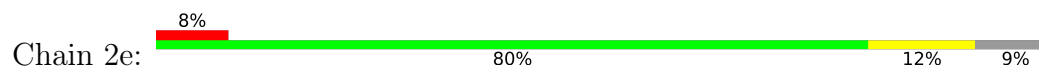




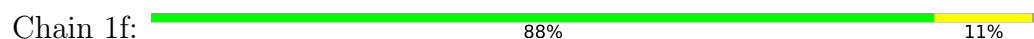
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



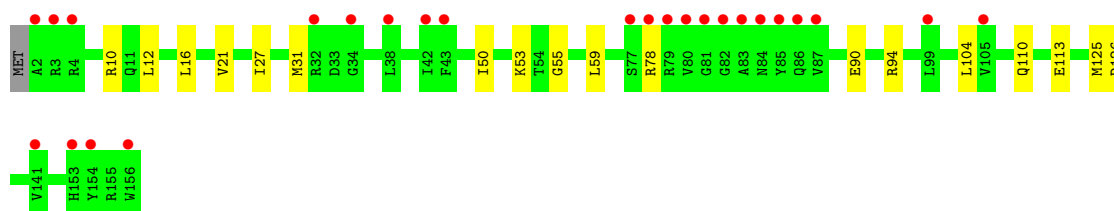
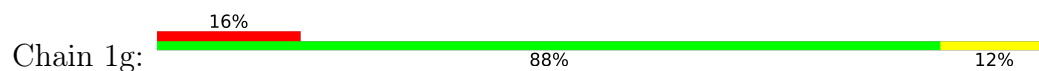
- Molecule 37: 30S ribosomal protein S6



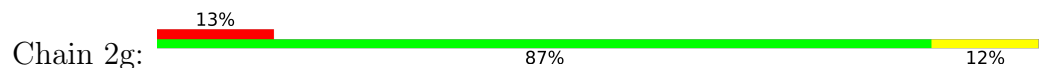
- Molecule 37: 30S ribosomal protein S6

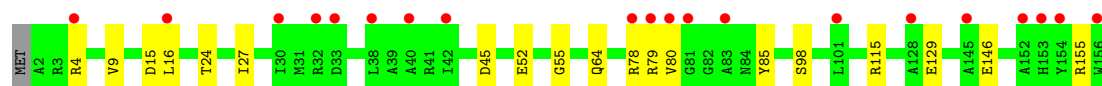


- Molecule 38: 30S ribosomal protein S7

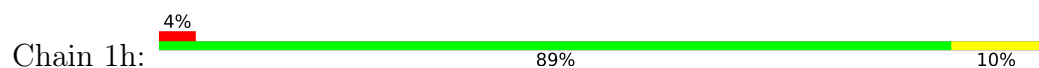


- Molecule 38: 30S ribosomal protein S7

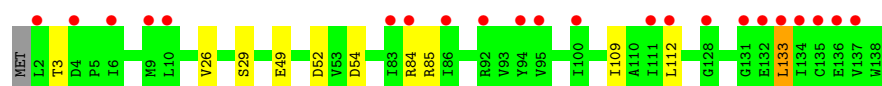
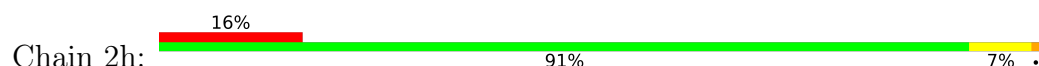




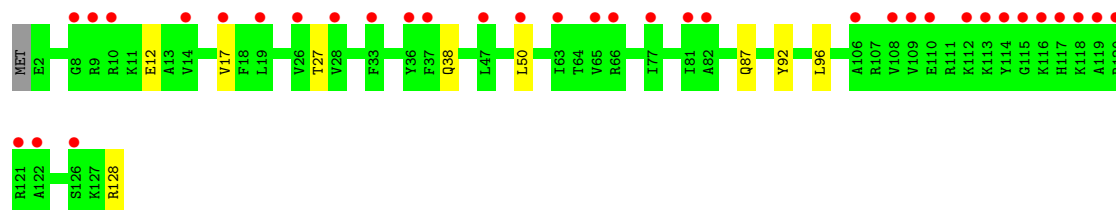
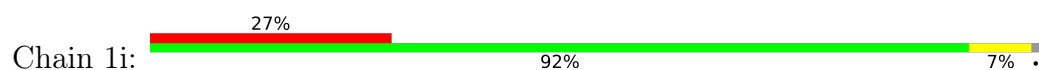
- Molecule 39: 30S ribosomal protein S8



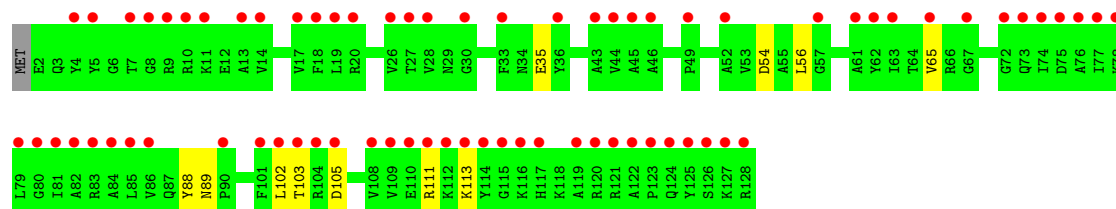
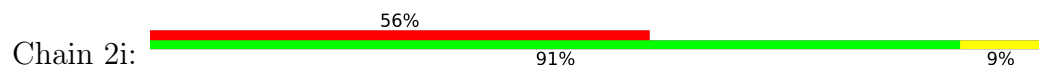
- Molecule 39: 30S ribosomal protein S8



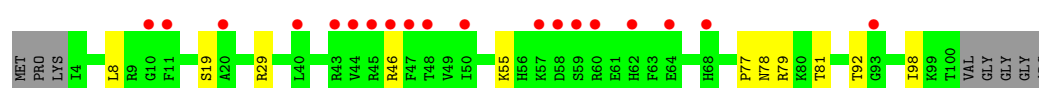
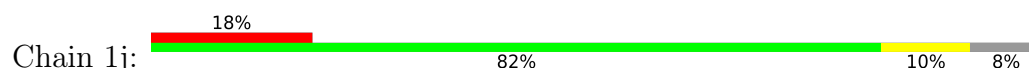
- Molecule 40: 30S ribosomal protein S9



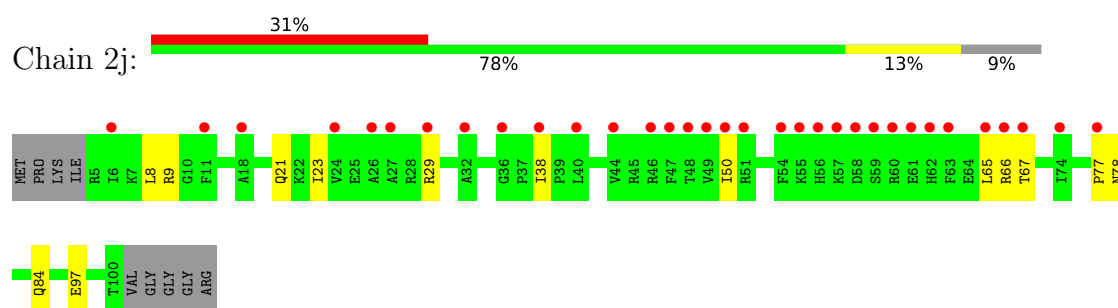
- Molecule 40: 30S ribosomal protein S9



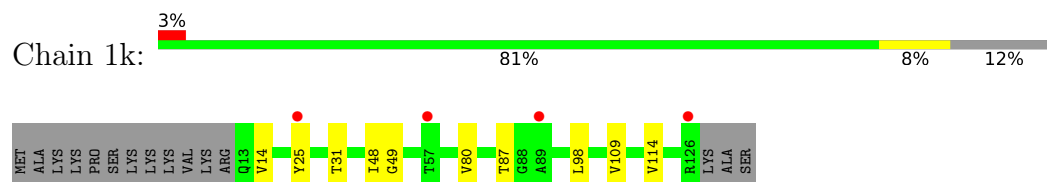
- Molecule 41: 30S ribosomal protein S10



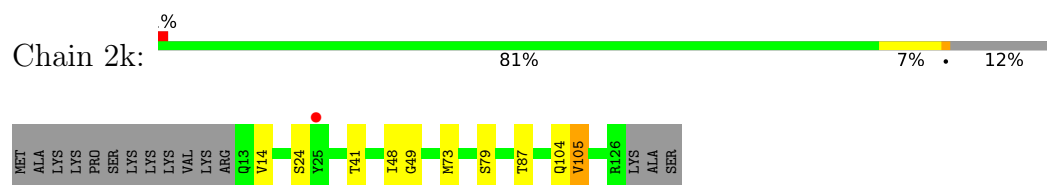
- Molecule 41: 30S ribosomal protein S10



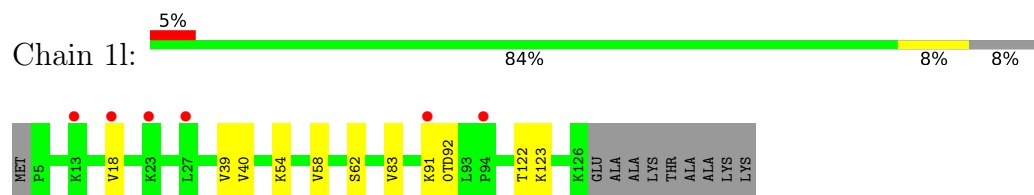
- Molecule 42: 30S ribosomal protein S11



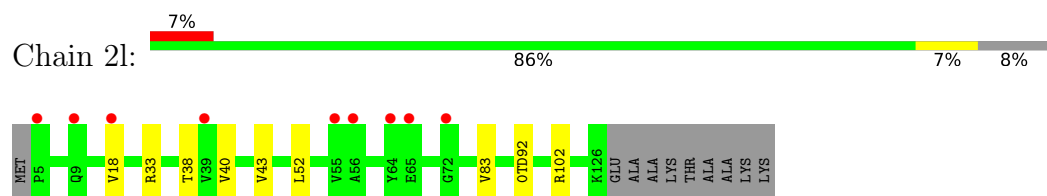
- Molecule 42: 30S ribosomal protein S11



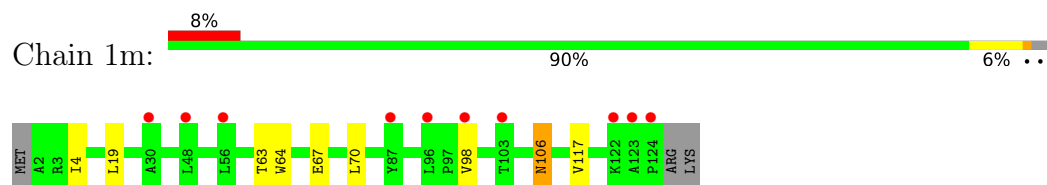
- Molecule 43: 30S ribosomal protein S12



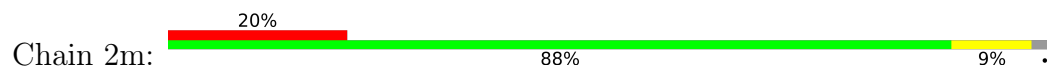
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13

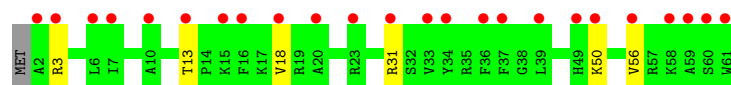
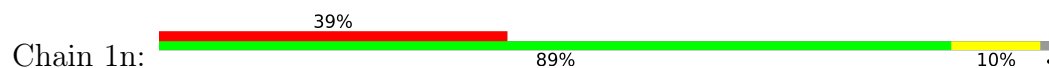


- Molecule 44: 30S ribosomal protein S13

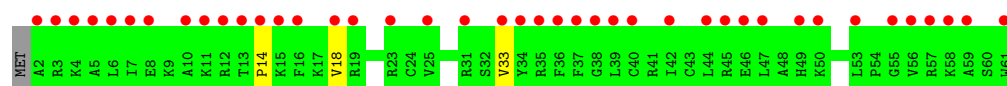




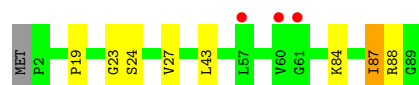
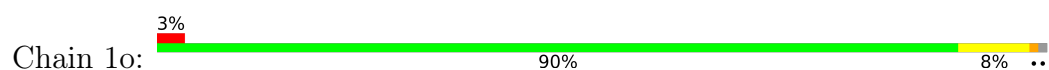
- Molecule 45: 30S ribosomal protein S14 type Z



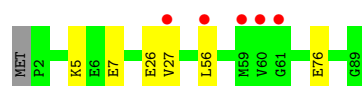
- Molecule 45: 30S ribosomal protein S14 type Z



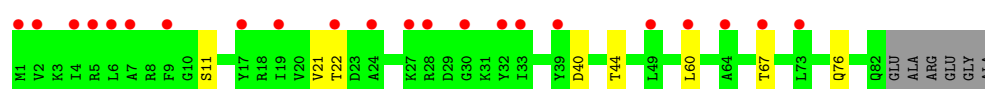
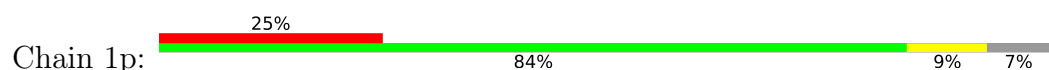
- Molecule 46: 30S ribosomal protein S15



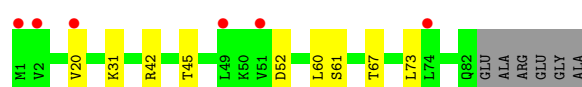
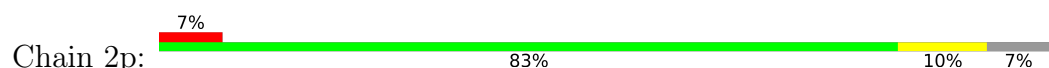
- Molecule 46: 30S ribosomal protein S15



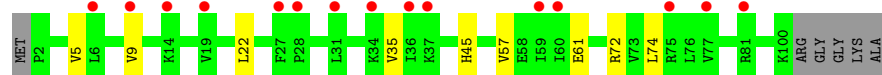
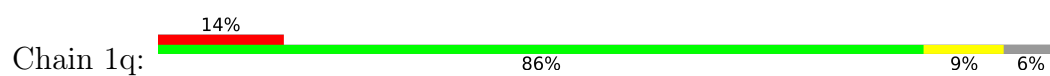
- Molecule 47: 30S ribosomal protein S16



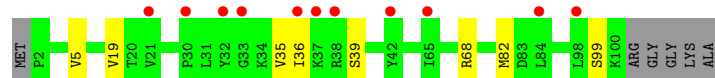
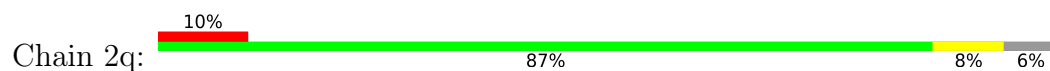
- Molecule 47: 30S ribosomal protein S16



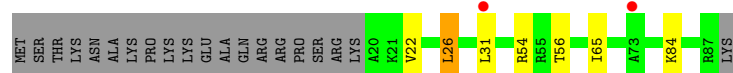
- Molecule 48: 30S ribosomal protein S17



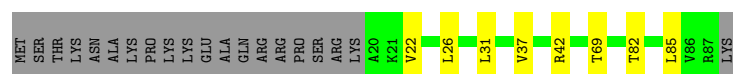
- Molecule 48: 30S ribosomal protein S17



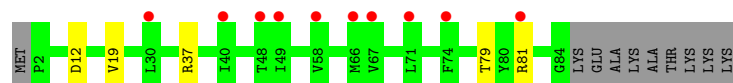
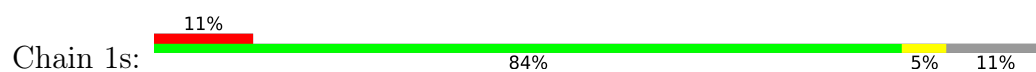
- Molecule 49: 30S ribosomal protein S18



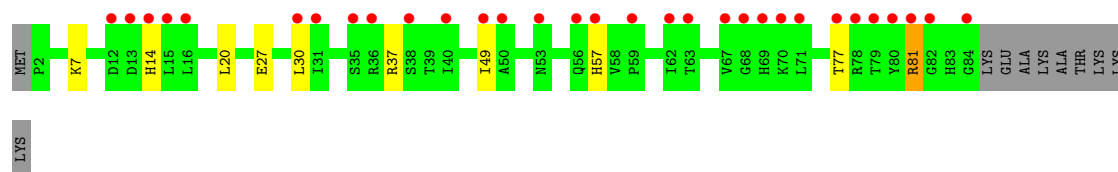
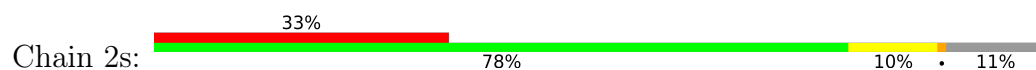
- Molecule 49: 30S ribosomal protein S18



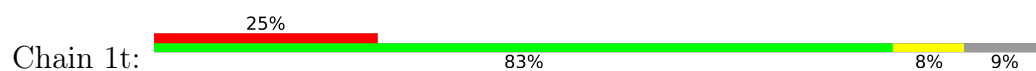
- Molecule 50: 30S ribosomal protein S19

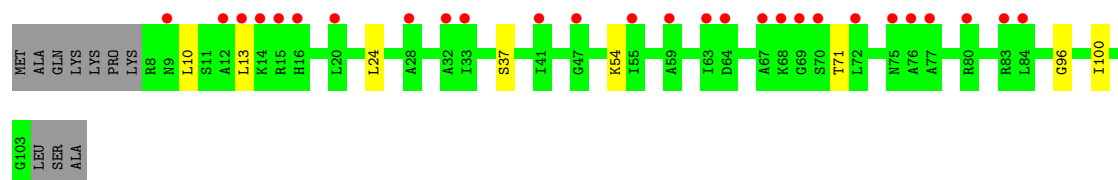


- Molecule 50: 30S ribosomal protein S19

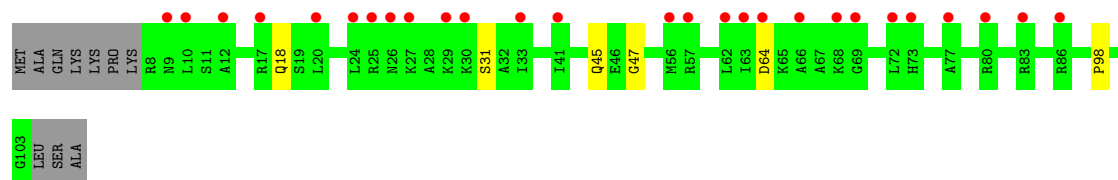
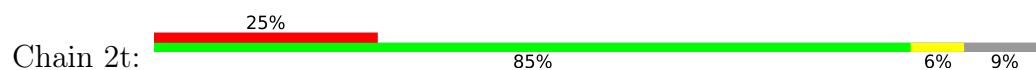


- Molecule 51: 30S ribosomal protein S20

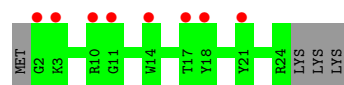
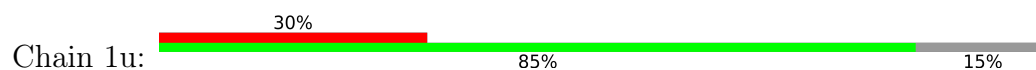




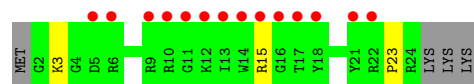
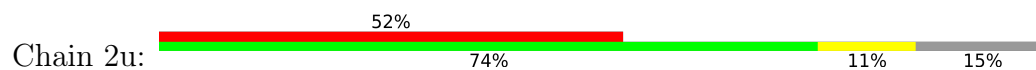
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA



- Molecule 54: A-site tRNA





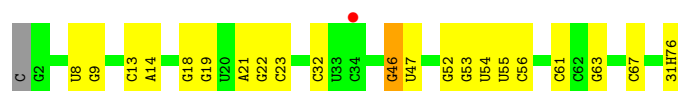
• Molecule 54: A-site tRNA



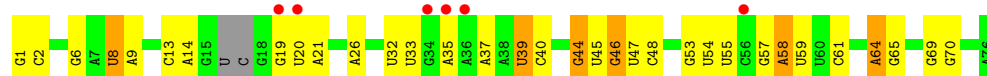
• Molecule 55: P-site tRNA



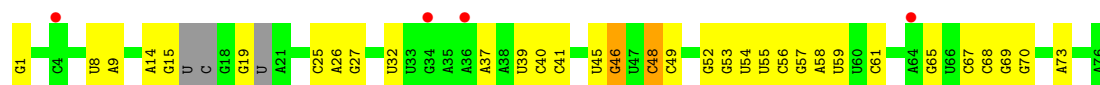
• Molecule 55: P-site tRNA



• Molecule 56: E-site tRNA



• Molecule 56: E-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.80Å 444.65Å 619.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.53 – 2.60 180.77 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (106.53-2.60) 98.0 (180.77-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.241 , 0.298 0.241 , 0.298	Depositor DCC
R_{free} test set	85661 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	299665	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 5MU, SF4, ZN, 2MG, 0TD, MG, 4OC, OMG, K, 4SU, M2G, MA6, MIA, 6IF, PSU, 7MG, 2MA, OMU, 31H, 5MC, UR3

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	0.55	1/68984 (0.0%)	1.03	90/107673 (0.1%)
1	2A	0.41	0/67268	0.91	36/104995 (0.0%)
2	1B	0.52	1/2882 (0.0%)	0.95	0/4494
2	2B	0.41	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.38	0/2186	0.58	0/2944
3	2D	0.32	0/2186	0.52	0/2944
4	1E	0.36	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.35	0/1619	0.55	0/2193
5	2F	0.32	0/1615	0.50	0/2188
6	1G	0.31	0/1448	0.51	0/1957
6	2G	0.30	0/1453	0.48	0/1963
7	1H	0.33	0/1356	0.50	0/1834
7	2H	0.29	0/1356	0.46	0/1834
8	1I	0.29	0/1112	0.50	0/1514
8	2I	0.29	0/1079	0.52	0/1475
9	1N	0.34	0/1144	0.52	0/1543
9	2N	0.29	0/1144	0.45	0/1543
10	1O	0.37	0/943	0.55	0/1269
10	2O	0.31	0/943	0.52	0/1269
11	1P	0.34	0/1152	0.60	0/1533
11	2P	0.32	0/1152	0.53	0/1533
12	1Q	0.37	0/1143	0.55	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.36	0/982	0.55	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.33	0/883	0.52	0/1176
14	2S	0.31	0/880	0.51	0/1172
15	1T	0.34	0/1105	0.54	0/1477
15	2T	0.30	0/1097	0.47	0/1468
16	1U	0.38	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.31	0/977	0.46	0/1301
17	1V	0.36	0/782	0.63	0/1049
17	2V	0.30	0/782	0.55	0/1049
18	1W	0.40	0/897	0.56	0/1205
18	2W	0.31	0/897	0.47	0/1205
19	1X	0.38	0/764	0.57	0/1025
19	2X	0.31	0/764	0.55	0/1025
20	1Y	0.34	0/819	0.53	0/1095
20	2Y	0.32	0/819	0.50	0/1095
21	1Z	0.33	0/1267	0.55	0/1717
21	2Z	0.29	0/1299	0.50	0/1763
22	10	0.38	0/662	0.55	0/881
22	20	0.32	0/662	0.51	0/881
23	11	0.38	0/762	0.52	0/1014
23	21	0.32	0/762	0.50	0/1014
24	12	0.34	0/590	0.48	0/781
24	22	0.29	0/590	0.43	0/781
25	13	0.35	0/474	0.55	0/635
25	23	0.29	0/469	0.46	0/630
26	14	0.33	0/565	0.54	0/761
26	24	0.32	0/545	0.51	0/737
27	15	0.34	0/469	0.54	0/635
27	25	0.31	0/469	0.50	0/635
28	16	0.38	0/460	0.54	0/613
28	26	0.31	0/456	0.52	0/608
29	17	0.35	0/426	0.56	0/561
29	27	0.31	0/426	0.51	0/561
30	18	0.34	0/525	0.57	0/691
30	28	0.28	0/525	0.49	0/691
31	19	0.35	0/310	0.52	0/407
31	29	0.30	0/310	0.50	0/407
32	1a	0.39	0/35795	0.92	27/55864 (0.0%)
32	2a	0.37	2/35886 (0.0%)	0.94	54/56005 (0.1%)
33	1b	0.29	0/1881	0.50	0/2542
33	2b	0.31	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.48	0/2126
34	2c	0.29	0/1566	0.52	1/2119 (0.0%)
35	1d	0.30	0/1685	0.46	0/2262
35	2d	0.30	0/1704	0.47	0/2284
36	1e	0.30	0/1145	0.53	0/1543
36	2e	0.29	0/1149	0.51	0/1548
37	1f	0.30	0/823	0.49	0/1115
37	2f	0.31	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.43	0/1679
38	2g	0.28	0/1254	0.44	0/1683
39	1h	0.31	0/1108	0.49	0/1494
39	2h	0.28	0/1108	0.45	0/1494
40	1i	0.30	0/1002	0.51	0/1346
40	2i	0.29	0/997	0.51	0/1343
41	1j	0.30	0/722	0.53	0/982
41	2j	0.30	0/727	0.53	0/988
42	1k	0.28	0/844	0.48	0/1145
42	2k	0.29	0/848	0.48	0/1149
43	1l	0.31	0/937	0.54	0/1260
43	2l	0.30	0/937	0.52	0/1260
44	1m	0.29	0/969	0.50	0/1302
44	2m	0.30	0/961	0.49	0/1291
45	1n	0.33	0/501	0.47	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.29	0/739	0.46	0/985
46	2o	0.26	0/739	0.45	0/985
47	1p	0.31	0/697	0.53	0/939
47	2p	0.28	0/693	0.51	0/935
48	1q	0.31	0/836	0.48	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.29	0/560	0.48	0/746
49	2r	0.28	0/560	0.42	0/746
50	1s	0.30	0/667	0.55	0/900
50	2s	0.29	0/661	0.54	0/893
51	1t	0.28	0/730	0.44	0/965
51	2t	0.28	0/729	0.42	0/965
52	1u	0.26	0/203	0.46	0/266
52	2u	0.33	0/203	0.54	0/266
53	1v	0.45	0/310	0.91	0/480
53	2v	0.38	0/310	0.91	0/480
54	1w	0.54	1/1559 (0.1%)	1.21	10/2424 (0.4%)
54	2w	0.47	0/1509	1.15	3/2345 (0.1%)
55	1x	0.62	6/1700 (0.4%)	1.23	23/2650 (0.9%)
55	2x	0.49	1/1700 (0.1%)	1.09	18/2650 (0.7%)
56	1y	0.48	1/1606 (0.1%)	1.08	5/2497 (0.2%)
56	2y	0.48	1/1583 (0.1%)	1.00	1/2459 (0.0%)
All	All	0.42	15/316492 (0.0%)	0.87	270/473811 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	1	G	OP3-P	-10.69	1.48	1.61
2	2B	1	U	OP3-P	-10.43	1.48	1.61
54	1w	1	G	OP3-P	-10.23	1.48	1.61
2	1B	1	U	OP3-P	-10.22	1.48	1.61
56	1y	1	G	OP3-P	-10.15	1.49	1.61
32	2a	1272	G	N1-C2	-7.73	1.31	1.37
55	1x	22	G	N7-C5	6.78	1.43	1.39
32	2a	1272	G	C6-N1	-6.50	1.35	1.39
55	1x	46	G	C6-N1	6.27	1.44	1.39
55	1x	22	G	C8-N7	5.51	1.34	1.30
55	2x	22	G	N7-C5	5.26	1.42	1.39
1	1A	2059	A	N9-C4	-5.24	1.34	1.37
55	1x	14	A	C8-N7	-5.16	1.27	1.31
55	1x	14	A	N7-C5	-5.07	1.36	1.39
55	1x	22	G	N9-C4	-5.04	1.33	1.38

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.79	132.57	118.90
32	2a	1272	G	N3-C2-N2	19.44	133.51	119.90
32	2a	1272	G	N1-C2-N2	-15.43	102.31	116.20
32	2a	1272	G	C5-C6-O6	15.06	137.63	128.60
32	2a	1263	C	C2-N3-C4	13.83	126.82	119.90
1	1A	975	C	N1-C2-O2	-13.73	110.66	118.90
32	2a	1263	C	C5-C6-N1	12.18	127.09	121.00
32	2a	1272	G	C6-N1-C2	12.03	132.32	125.10
32	2a	1263	C	N3-C2-O2	-11.82	113.63	121.90
55	1x	46	G	C6-N1-C2	-11.26	118.34	125.10
55	2x	46	G	C6-N1-C2	-10.74	118.65	125.10
1	1A	1075	C	N1-C2-O2	10.74	125.34	118.90
2	2B	80	U	O4'-C1'-N1	10.41	116.53	108.20
32	2a	1272	G	C5-C6-N1	-10.23	106.39	111.50
55	1x	22	G	C5-N7-C8	-9.77	99.41	104.30
1	1A	1063	G	C5-C6-O6	9.47	134.28	128.60
55	2x	14	A	C4-C5-C6	9.28	121.64	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C4-C5-C6	9.15	121.57	117.00
55	1x	22	G	C4-C5-C6	-9.13	113.32	118.80
55	1x	22	G	N3-C4-N9	-9.12	120.53	126.00
32	2a	754	C	C2-N1-C1'	9.01	128.71	118.80
55	1x	46	G	N3-C2-N2	-8.96	113.63	119.90
32	2a	1263	C	C4-C5-C6	-8.91	112.94	117.40
1	1A	975	C	C2-N1-C1'	-8.90	109.01	118.80
32	2a	1263	C	C2-N1-C1'	8.80	128.48	118.80
32	2a	754	C	N1-C2-O2	8.66	124.09	118.90
55	1x	14	A	C5-N7-C8	8.48	108.14	103.90
54	1w	47	U	C2-N1-C1'	8.47	127.87	117.70
55	2x	14	A	C5-N7-C8	8.47	108.13	103.90
32	2a	1272	G	C4-N9-C1'	8.32	137.31	126.50
32	2a	1272	G	C8-N9-C1'	-8.20	116.33	127.00
32	2a	1029	C	N1-C2-O2	8.06	123.73	118.90
32	1a	1030(B)	C	C2-N1-C1'	8.03	127.64	118.80
55	1x	22	G	N3-C4-C5	8.01	132.60	128.60
1	1A	1063	G	C6-N1-C2	8.01	129.90	125.10
1	1A	1075	C	C2-N3-C4	7.92	123.86	119.90
1	1A	2006	C	O5'-P-OP1	-7.91	98.58	105.70
32	1a	841	U	C5-C6-N1	7.86	126.63	122.70
32	1a	1030(B)	C	N1-C2-O2	7.85	123.61	118.90
1	2A	801	G	O5'-P-OP2	-7.79	98.69	105.70
32	2a	1263	C	N1-C2-N3	-7.74	113.78	119.20
1	1A	2067	G	C8-N9-C4	-7.71	103.31	106.40
55	1x	22	G	C8-N9-C1'	7.65	136.95	127.00
32	2a	1263	C	C6-N1-C2	-7.62	117.25	120.30
1	1A	975	C	C2-N3-C4	-7.55	116.13	119.90
55	2x	14	A	C5-C6-N1	-7.54	113.93	117.70
1	1A	2682	U	O5'-P-OP2	-7.46	98.98	105.70
1	1A	2167	U	C2-N1-C1'	7.37	126.54	117.70
54	1w	47	U	N1-C2-O2	7.33	127.93	122.80
1	2A	2129	C	N1-C2-O2	7.30	123.28	118.90
1	1A	1086	A	N1-C6-N6	-7.24	114.26	118.60
55	2x	22	G	C4-C5-C6	-7.23	114.46	118.80
32	1a	299	G	C5-C6-O6	-7.18	124.29	128.60
1	1A	1063	G	N3-C2-N2	7.10	124.87	119.90
55	2x	22	G	C5-N7-C8	-6.99	100.80	104.30
32	2a	1054	C	C2-N1-C1'	6.99	126.49	118.80
1	1A	975	C	C6-N1-C1'	6.95	129.14	120.80
55	1x	22	G	C4-N9-C1'	-6.91	117.52	126.50
55	2x	22	G	N1-C6-O6	-6.88	115.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1337	G	N3-C4-N9	-6.88	121.87	126.00
32	2a	754	C	C6-N1-C1'	-6.81	112.63	120.80
55	1x	46	G	C5-C6-O6	-6.80	124.52	128.60
1	1A	975	C	N3-C2-O2	6.76	126.63	121.90
1	1A	203	C	N1-C2-O2	-6.71	114.87	118.90
54	2w	66	U	C5-C4-O4	-6.69	121.88	125.90
32	2a	1264	C	N1-C2-O2	6.69	122.92	118.90
55	2x	46	G	C5-C6-N1	6.67	114.83	111.50
56	1y	33	U	C2-N1-C1'	6.60	125.62	117.70
32	2a	1272	G	N1-C6-O6	-6.59	115.95	119.90
55	1x	22	G	N1-C6-O6	-6.57	115.96	119.90
1	1A	1992	G	P-O3'-C3'	6.56	127.57	119.70
1	1A	2129	C	C2-N1-C1'	6.54	126.00	118.80
1	1A	2593	U	N3-C4-O4	-6.54	114.82	119.40
32	1a	1158	C	C2-N1-C1'	6.52	125.97	118.80
1	1A	2614	A	C8-N9-C4	6.51	108.40	105.80
54	1w	47	U	N3-C2-O2	-6.47	117.67	122.20
32	1a	266	G	P-O3'-C3'	6.43	127.41	119.70
32	2a	1043	C	N1-C2-O2	6.42	122.75	118.90
1	1A	1075	C	N3-C2-O2	-6.41	117.41	121.90
1	1A	2061	G	O5'-P-OP2	-6.40	99.94	105.70
32	1a	1025	U	N1-C2-O2	6.39	127.28	122.80
32	2a	1065	U	P-O3'-C3'	6.36	127.34	119.70
1	2A	2155	G	C6-N1-C2	6.33	128.90	125.10
1	1A	748	G	O4'-C1'-N9	6.31	113.25	108.20
1	2A	2136	C	N1-C2-O2	6.29	122.67	118.90
54	1w	9	A	N1-C6-N6	-6.28	114.83	118.60
1	1A	975	C	C5-C6-N1	-6.27	117.87	121.00
55	1x	22	G	C6-C5-N7	6.26	134.16	130.40
1	1A	2129	C	N1-C2-O2	6.24	122.64	118.90
1	2A	1313	U	C2-N1-C1'	6.20	125.14	117.70
32	1a	841	U	C2-N1-C1'	6.20	125.14	117.70
32	1a	841	U	C6-N1-C2	-6.18	117.29	121.00
56	1y	58	A	OP1-P-O3'	6.17	118.78	105.20
1	2A	2155	G	C5-C6-O6	6.15	132.29	128.60
32	1a	1030(B)	C	C6-N1-C2	-6.15	117.84	120.30
55	1x	46	G	N9-C4-C5	6.12	107.85	105.40
1	1A	2036	C	O5'-P-OP1	-6.05	100.26	105.70
1	2A	2318	G	O4'-C1'-N9	6.04	113.03	108.20
1	2A	1698	A	O4'-C1'-N9	6.03	113.02	108.20
1	1A	1618	A	O5'-P-OP1	-6.02	100.29	105.70
32	1a	1030(B)	C	N3-C2-O2	-6.01	117.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	46	G	N1-C2-N3	6.00	127.50	123.90
32	1a	1006	C	N1-C2-O2	6.00	122.50	118.90
32	2a	841	U	C5-C6-N1	5.99	125.70	122.70
1	1A	226	G	O4'-C1'-N9	5.99	112.99	108.20
55	1x	14	A	C5-C6-N1	-5.99	114.71	117.70
1	1A	1253	A	C8-N9-C4	5.98	108.19	105.80
1	1A	2554	U	O5'-P-OP1	-5.95	100.34	105.70
55	2x	22	G	N3-C4-N9	-5.94	122.43	126.00
1	1A	624	C	O5'-P-OP1	-5.91	100.38	105.70
32	2a	1065	U	OP2-P-O3'	5.91	118.21	105.20
32	2a	754	C	N3-C2-O2	-5.90	117.77	121.90
56	1y	44	G	C5-C6-O6	-5.89	125.06	128.60
32	2a	1272	G	C2-N3-C4	-5.87	108.96	111.90
32	2a	1530	G	O5'-P-OP1	5.83	117.70	110.70
32	2a	266	G	P-O3'-C3'	5.83	126.69	119.70
1	1A	1313	U	O4'-C1'-N1	5.82	112.86	108.20
55	2x	46	G	N1-C2-N3	5.82	127.39	123.90
1	1A	2167	U	N3-C2-O2	-5.80	118.14	122.20
1	1A	2712	U	N3-C2-O2	-5.79	118.15	122.20
55	2x	22	G	C8-N9-C1'	5.78	134.51	127.00
1	1A	847	U	N1-C2-O2	5.78	126.84	122.80
1	1A	512	G	O4'-C1'-N9	5.75	112.80	108.20
32	2a	70	G	C5-C6-O6	5.74	132.04	128.60
32	2a	1054	C	N1-C2-O2	5.73	122.34	118.90
1	2A	228	A	P-O3'-C3'	5.72	126.56	119.70
1	1A	1247	A	C8-N9-C4	5.70	108.08	105.80
55	2x	22	G	C5-C6-N1	5.68	114.34	111.50
1	1A	12	U	C2-N1-C1'	5.67	124.51	117.70
54	2w	66	U	C2-N1-C1'	5.67	124.51	117.70
1	1A	591	C	N1-C2-O2	-5.66	115.50	118.90
32	2a	1158	C	C2-N1-C1'	5.66	125.03	118.80
1	2A	879	G	C4-N9-C1'	5.66	133.85	126.50
1	2A	228	A	OP1-P-O3'	5.65	117.64	105.20
1	2A	748	G	O4'-C1'-N9	5.65	112.72	108.20
1	1A	847	U	C2-N1-C1'	5.64	124.47	117.70
1	1A	2685	G	C8-N9-C1'	5.63	134.32	127.00
32	2a	1272	G	N3-C4-N9	5.63	129.38	126.00
55	1x	46	G	C4-C5-N7	-5.63	108.55	110.80
55	1x	22	G	C5-C6-N1	5.62	114.31	111.50
1	2A	2447	G	C4-N9-C1'	-5.62	119.19	126.50
32	1a	90	U	C2-N1-C1'	5.62	124.45	117.70
1	1A	2848	G	O4'-C1'-N9	5.62	112.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1034	G	C6-N1-C2	5.61	128.47	125.10
1	2A	2689	U	P-O3'-C3'	5.61	126.43	119.70
32	2a	99	U	N1-C2-O2	-5.61	118.88	122.80
1	1A	1430	C	C6-N1-C2	-5.60	118.06	120.30
56	1y	33	U	N1-C2-O2	5.60	126.72	122.80
1	2A	528	A	OP1-P-O3'	5.59	117.51	105.20
1	1A	2050	C	N1-C2-O2	-5.59	115.55	118.90
2	2B	2	C	C6-N1-C2	-5.58	118.07	120.30
32	2a	1284	C	C2-N3-C4	5.58	122.69	119.90
1	2A	531	C	C6-N1-C2	5.57	122.53	120.30
1	1A	955	C	N1-C2-O2	-5.57	115.56	118.90
32	1a	928	G	N3-C4-N9	-5.56	122.67	126.00
1	1A	2167	U	N1-C2-O2	5.56	126.69	122.80
55	1x	46	G	C5-C6-N1	5.55	114.28	111.50
32	2a	1263	C	N3-C4-N4	-5.55	114.11	118.00
32	2a	1286	A	N7-C8-N9	5.55	116.58	113.80
54	1w	4	C	C2-N3-C4	5.54	122.67	119.90
1	2A	898	C	C6-N1-C2	-5.54	118.08	120.30
1	1A	1828	G	N1-C6-O6	5.54	123.22	119.90
1	1A	139(A)	G	N1-C6-O6	5.53	123.22	119.90
32	2a	1043	C	C2-N3-C4	5.52	122.66	119.90
32	2a	1263	C	C6-N1-C1'	-5.51	114.19	120.80
32	2a	1337	G	C8-N9-C1'	5.51	134.16	127.00
1	1A	944	G	C4-N9-C1'	5.50	133.65	126.50
32	2a	1337	G	C4-N9-C1'	-5.50	119.35	126.50
55	2x	46	G	N3-C2-N2	-5.50	116.05	119.90
32	2a	999	C	N1-C2-O2	5.48	122.19	118.90
32	2a	70	G	C6-N1-C2	5.48	128.39	125.10
1	1A	2614	A	N9-C4-C5	-5.46	103.62	105.80
1	1A	1791	A	O5'-P-OP1	-5.46	100.79	105.70
1	1A	1187	G	N1-C6-O6	-5.45	116.63	119.90
1	2A	2129	C	C2-N3-C4	5.43	122.62	119.90
1	1A	2005	A	OP1-P-O3'	5.43	117.14	105.20
1	1A	774	A	C8-N9-C4	-5.42	103.63	105.80
1	1A	1063	G	N1-C6-O6	-5.41	116.65	119.90
55	1x	56	C	N1-C2-O2	5.40	122.14	118.90
54	1w	47	U	C5-C6-N1	5.39	125.40	122.70
54	1w	47	U	C6-N1-C1'	-5.38	113.67	121.20
55	2x	22	G	C6-C5-N7	5.37	133.62	130.40
1	2A	90	U	C2-N1-C1'	5.36	124.14	117.70
1	1A	139(A)	G	C5-C6-O6	-5.34	125.40	128.60
32	1a	1067	A	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	4	C	C5-C4-N4	5.34	123.94	120.20
32	2a	1263	C	C5-C4-N4	5.34	123.94	120.20
1	1A	2622	C	N1-C2-O2	-5.33	115.70	118.90
1	2A	1616	A	N1-C6-N6	5.31	121.79	118.60
1	1A	577	G	C5-C6-O6	-5.31	125.41	128.60
1	1A	2629	A	P-O3'-C3'	5.31	126.07	119.70
55	2x	14	A	C4-C5-N7	-5.31	108.05	110.70
1	2A	752	A	P-O3'-C3'	5.30	126.06	119.70
55	2x	46	G	C4-C5-N7	-5.30	108.68	110.80
32	1a	1030(B)	C	C6-N1-C1'	-5.29	114.45	120.80
1	2A	783	A	C2-N3-C4	5.29	113.24	110.60
34	2c	91	LEU	CA-CB-CG	5.28	127.45	115.30
1	2A	2866	U	C2-N1-C1'	5.28	124.03	117.70
32	2a	1029	C	N3-C2-O2	-5.26	118.22	121.90
32	2a	841	U	C6-N1-C2	-5.26	117.84	121.00
1	2A	2059	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	2167	U	C5-C6-N1	5.25	125.33	122.70
1	1A	2022	U	N1-C2-O2	-5.25	119.12	122.80
1	1A	2335	A	O4'-C1'-N9	5.25	112.40	108.20
1	1A	1174	A	P-O3'-C3'	5.25	126.00	119.70
56	1y	64	A	C5-C6-N6	5.25	127.90	123.70
54	2w	67	C	C5-C4-N4	5.23	123.86	120.20
1	2A	574	C	O5'-P-OP1	-5.23	100.99	105.70
1	2A	114	U	C2-N1-C1'	5.23	123.97	117.70
1	2A	528	A	P-O3'-C3'	5.21	125.96	119.70
1	1A	195	A	P-O3'-C3'	5.21	125.95	119.70
1	1A	2688	U	N3-C2-O2	5.21	125.85	122.20
32	1a	1395	C	C2-N3-C4	5.21	122.51	119.90
32	1a	1034	G	C5-C6-O6	5.20	131.72	128.60
1	1A	746	A	O4'-C1'-N9	5.20	112.36	108.20
32	2a	754	C	C5-C6-N1	5.20	123.60	121.00
1	1A	2492	U	O5'-P-OP1	-5.19	101.03	105.70
32	1a	560	U	C3'-C2'-C1'	5.19	105.66	101.50
1	1A	2626	C	N1-C2-O2	-5.19	115.78	118.90
32	1a	204	U	C2-N1-C1'	5.19	123.93	117.70
1	2A	1992	G	P-O3'-C3'	5.19	125.92	119.70
1	2A	847	U	C2-N1-C1'	5.18	123.92	117.70
1	1A	1236	G	N3-C4-C5	5.17	131.19	128.60
1	2A	2848	G	O4'-C1'-N9	5.17	112.33	108.20
1	1A	372	G	O4'-C1'-N9	5.15	112.32	108.20
54	1w	66	U	C5-C4-O4	-5.14	122.82	125.90
1	1A	1174	A	OP1-P-O3'	5.14	116.50	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2625	G	N3-C2-N2	-5.13	116.31	119.90
55	1x	22	G	N7-C8-N9	5.13	115.67	113.10
1	1A	1313	U	C2-N1-C1'	5.13	123.86	117.70
1	1A	2282	G	C8-N9-C4	5.13	108.45	106.40
55	2x	46	G	N9-C4-C5	5.12	107.45	105.40
32	1a	748	C	P-O3'-C3'	5.12	125.84	119.70
55	1x	14	A	C4-N9-C1'	5.11	135.50	126.30
1	1A	568	U	C5-C4-O4	-5.11	122.83	125.90
1	1A	748	G	N1-C6-O6	-5.11	116.83	119.90
32	2a	1109	C	C6-N1-C2	-5.11	118.26	120.30
1	1A	1828	G	C5-C6-O6	-5.11	125.53	128.60
1	2A	2318	G	C4-N9-C1'	5.11	133.14	126.50
1	1A	697	C	N3-C2-O2	-5.11	118.33	121.90
1	1A	960	A	C8-N9-C4	-5.10	103.76	105.80
32	2a	1128	C	P-O3'-C3'	5.09	125.81	119.70
1	1A	1265	A	O5'-P-OP2	-5.09	101.12	105.70
55	2x	14	A	C4-N9-C1'	5.09	135.47	126.30
1	1A	884	C	C2-N1-C1'	5.09	124.40	118.80
1	1A	1688	U	N1-C2-O2	-5.09	119.24	122.80
1	1A	2057	A	O5'-P-OP2	-5.09	101.12	105.70
32	1a	1395	C	N1-C2-O2	5.09	121.95	118.90
1	2A	128	C	C6-N1-C2	-5.08	118.27	120.30
54	1w	4	C	N1-C2-O2	5.08	121.95	118.90
1	1A	789	A	C8-N9-C4	5.07	107.83	105.80
32	1a	1030(B)	C	C5-C6-N1	5.07	123.53	121.00
32	2a	1025	U	N1-C2-O2	5.05	126.34	122.80
1	1A	944	G	C8-N9-C1'	-5.05	120.44	127.00
32	1a	299	G	N1-C6-O6	5.04	122.92	119.90
32	2a	1337	G	N3-C2-N2	-5.04	116.37	119.90
32	1a	115	G	P-O3'-C3'	5.04	125.74	119.70
1	2A	195	A	P-O3'-C3'	5.03	125.73	119.70
1	1A	1075	C	C2-N1-C1'	5.03	124.33	118.80
1	1A	2336	A	O4'-C1'-N9	-5.03	104.18	108.20
1	2A	1021	A	C8-N9-C4	-5.02	103.79	105.80
32	2a	1158	C	N1-C2-O2	5.02	121.91	118.90
1	2A	694	U	C5-C4-O4	-5.02	122.89	125.90
1	1A	2553	G	N3-C4-N9	5.01	129.01	126.00
56	2y	48	C	N1-C2-O2	-5.01	115.89	118.90
1	1A	944	G	C6-C5-N7	-5.01	127.39	130.40
1	1A	2685	G	O4'-C1'-N9	5.01	112.20	108.20
1	2A	1022	G	N3-C4-N9	-5.01	123.00	126.00
55	1x	14	A	C8-N9-C1'	-5.00	118.69	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	299	G	N9-C4-C5	-5.00	103.40	105.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide
33	1b	130	ARG	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%)	251 (92%)	19 (7%)	3 (1%)	14	30
3	2D	273/276 (99%)	250 (92%)	22 (8%)	1 (0%)	34	57
4	1E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	32
4	2E	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	15	32
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	52
5	2F	201/210 (96%)	184 (92%)	15 (8%)	2 (1%)	15	32
6	1G	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	9	18
6	2G	179/182 (98%)	149 (83%)	24 (13%)	6 (3%)	3	5
7	1H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	25	47
7	2H	172/180 (96%)	153 (89%)	19 (11%)	0	100	100
8	1I	144/148 (97%)	128 (89%)	16 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	2I	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	22	43
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	39
11	1P	147/150 (98%)	128 (87%)	14 (10%)	5 (3%)	3	5
11	2P	147/150 (98%)	129 (88%)	14 (10%)	4 (3%)	5	8
12	1Q	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
12	2Q	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	35
13	2R	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	35
15	1T	129/146 (88%)	115 (89%)	13 (10%)	1 (1%)	19	39
15	2T	129/146 (88%)	114 (88%)	14 (11%)	1 (1%)	19	39
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	32
17	2V	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	7	14
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	102 (93%)	7 (6%)	1 (1%)	17	35
19	1X	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	14	30
19	2X	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	14	30
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	127 (86%)	19 (13%)	2 (1%)	11	22
21	2Z	156/206 (76%)	130 (83%)	24 (15%)	2 (1%)	12	24
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	2 (2%)	2 (2%)	5	9
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	30
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	12	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	16
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
26	24	67/71 (94%)	46 (69%)	16 (24%)	5 (8%)	1	1
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	184 (80%)	37 (16%)	8 (4%)	3	5
33	2b	229/256 (90%)	185 (81%)	36 (16%)	8 (4%)	3	5
34	1c	204/239 (85%)	177 (87%)	25 (12%)	2 (1%)	15	32
34	2c	204/239 (85%)	168 (82%)	34 (17%)	2 (1%)	15	32
35	1d	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	15	32
35	2d	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	29	52
36	1e	146/162 (90%)	132 (90%)	12 (8%)	2 (1%)	11	22
36	2e	146/162 (90%)	119 (82%)	22 (15%)	5 (3%)	3	5
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	22	43
38	2g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	12	24
39	1h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	22	43
40	1i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	6 (6%)	5 (5%)	2	2
41	2j	94/105 (90%)	77 (82%)	14 (15%)	3 (3%)	4	6
42	1k	112/129 (87%)	95 (85%)	16 (14%)	1 (1%)	17	35
42	2k	112/129 (87%)	91 (81%)	18 (16%)	3 (3%)	5	8
43	1l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	121/126 (96%)	109 (90%)	10 (8%)	2 (2%)	9	18
44	2m	120/126 (95%)	99 (82%)	21 (18%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	18
46	1o	86/89 (97%)	76 (88%)	6 (7%)	4 (5%)	2	2
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12	24
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	12	24
48	1q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	32
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	32
49	1r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	21
49	2r	66/88 (75%)	57 (86%)	9 (14%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	13	27
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	13	27
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	13
51	2t	94/106 (89%)	82 (87%)	10 (11%)	2 (2%)	7	13
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	0	2 (10%)	0	0
All	All	11370/12128 (94%)	10197 (90%)	1047 (9%)	126 (1%)	14	30

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	29	LYS
11	1P	45	LEU

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Mol	Chain	Res	Type
21	1Z	53	ILE
23	11	3	LYS
26	14	62	ARG
41	1j	79	ARG
44	1m	67	GLU
44	1m	106	ASN
6	2G	43	LEU
6	2G	51	ARG
8	2I	10	GLU
11	2P	29	LYS
17	2V	79	VAL
26	24	48	ARG
33	2b	9	GLU
33	2b	17	PHE
33	2b	74	LYS
42	2k	104	GLN
48	2q	68	ARG
4	1E	28	ALA
6	1G	181	ARG
15	1T	37	GLY
21	1Z	163	LEU
26	14	45	GLY
33	1b	17	PHE
33	1b	126	GLU
33	1b	129	GLU
34	1c	66	VAL
35	1d	195	ALA
38	1g	55	GLY
41	1j	29	ARG
42	1k	49	GLY
47	1p	44	THR
50	1s	81	ARG
51	1t	100	ILE
5	2F	130	ALA
6	2G	42	GLY
6	2G	47	LYS
6	2G	96	ARG
22	20	73	GLY
33	2b	123	ALA
33	2b	126	GLU
34	2c	156	ARG
36	2e	77	PRO

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Mol	Chain	Res	Type
38	2g	55	GLY
38	2g	80	VAL
39	2h	133	LEU
42	2k	49	GLY
42	2k	105	VAL
3	1D	257	LEU
11	1P	139	LYS
17	1V	79	VAL
26	14	49	PHE
33	1b	13	ALA
33	1b	124	SER
49	1r	26	LEU
4	2E	28	ALA
5	2F	21	ALA
11	2P	45	LEU
14	2S	84	GLN
17	2V	53	GLU
25	23	38	GLU
26	24	49	PHE
33	2b	20	GLU
33	2b	21	ARG
36	2e	66	MET
36	2e	107	ARG
41	2j	78	ASN
50	2s	81	ARG
52	2u	3	LYS
4	1E	52	LEU
11	1P	38	GLN
11	1P	93	GLY
13	1R	107	ASP
33	1b	8	LYS
34	1c	65	ALA
40	1i	12	GLU
41	1j	55	LYS
41	1j	78	ASN
46	1o	19	PRO
48	1q	61	GLU
4	2E	52	LEU
11	2P	36	LYS
11	2P	38	GLN
21	2Z	52	SER
36	2e	37	ARG

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Mol	Chain	Res	Type
41	2j	29	ARG
26	14	53	GLU
33	1b	231	GLU
36	1e	70	PRO
36	1e	85	GLY
18	2W	60	ASN
21	2Z	146	ILE
33	2b	125	PRO
35	2d	186	LEU
45	2n	14	PRO
47	2p	52	ASP
3	1D	49	ILE
6	1G	24	GLY
7	1H	55	PRO
46	1o	88	ARG
22	20	13	GLY
26	24	65	ASP
34	2c	73	PRO
36	2e	11	ILE
41	2j	77	PRO
33	1b	131	PRO
3	2D	271	ILE
26	24	11	PRO
26	24	45	GLY
51	2t	98	PRO
52	2u	23	PRO
19	1X	94	GLY
41	1j	77	PRO
46	1o	23	GLY
10	2O	43	VAL
3	1D	244	ARG
35	1d	178	VAL
46	1o	87	ILE
51	1t	96	GLY
6	2G	24	GLY
19	2X	94	GLY
51	2t	47	GLY
6	1G	44	GLY
15	2T	37	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	203 (94%)	12 (6%)	21	42
3	2D	215/218 (99%)	200 (93%)	15 (7%)	15	30
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	48
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	28
5	1F	160/166 (96%)	142 (89%)	18 (11%)	6	10
5	2F	159/166 (96%)	149 (94%)	10 (6%)	18	36
6	1G	143/156 (92%)	128 (90%)	15 (10%)	7	13
6	2G	143/156 (92%)	124 (87%)	19 (13%)	4	7
7	1H	144/148 (97%)	132 (92%)	12 (8%)	11	22
7	2H	144/148 (97%)	132 (92%)	12 (8%)	11	22
8	1I	113/124 (91%)	99 (88%)	14 (12%)	4	8
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2	3
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7	14
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	11
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	67
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9	18
11	1P	115/116 (99%)	105 (91%)	10 (9%)	10	20
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	20
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	52
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22	44
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	39
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31	57
14	1S	86/88 (98%)	74 (86%)	12 (14%)	3	6
14	2S	85/88 (97%)	72 (85%)	13 (15%)	2	4
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18	38
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	44
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	44
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7	14
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	8
18	1W	90/92 (98%)	83 (92%)	7 (8%)	12	25
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38	64
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	72
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	12
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	17
21	1Z	135/179 (75%)	119 (88%)	16 (12%)	5	9
21	2Z	137/179 (76%)	119 (87%)	18 (13%)	4	7
22	10	65/67 (97%)	64 (98%)	1 (2%)	65	83
22	20	65/67 (97%)	60 (92%)	5 (8%)	13	25
23	11	80/83 (96%)	73 (91%)	7 (9%)	10	19
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	73
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	51
24	22	65/67 (97%)	61 (94%)	4 (6%)	18	37
25	13	51/52 (98%)	42 (82%)	9 (18%)	2	3
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	21
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	2
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	24
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	14
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	6
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	39
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	48
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	9
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	17
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	42
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	159 (83%)	33 (17%)	2	3
33	2b	187/220 (85%)	159 (85%)	28 (15%)	3	5
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	12
34	2c	140/188 (74%)	132 (94%)	8 (6%)	20	41
35	1d	169/181 (93%)	148 (88%)	21 (12%)	4	8
35	2d	173/181 (96%)	153 (88%)	20 (12%)	5	10
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5	10
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	9
37	1f	84/90 (93%)	73 (87%)	11 (13%)	4	7
37	2f	85/90 (94%)	79 (93%)	6 (7%)	14	29
38	1g	119/127 (94%)	102 (86%)	17 (14%)	3	5
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	5
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4	9
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	16
40	1i	90/99 (91%)	82 (91%)	8 (9%)	9	19
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	8
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9	18
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2	4
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	11
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	16
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	13
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	22
44	1m	93/101 (92%)	85 (91%)	8 (9%)	10	20
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	9
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	9
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	56
46	1o	78/80 (98%)	73 (94%)	5 (6%)	17	35
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	25
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	14
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	21
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	28
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	9
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	6
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	40
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	5
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	20
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	41
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	42
All	All	9303/10064 (92%)	8434 (91%)	869 (9%)	9	17

All (869) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	32	SER
3	1D	37	LEU
3	1D	88	ARG
3	1D	99	ASP
3	1D	173	VAL
3	1D	181	GLU
3	1D	229	VAL
3	1D	242	ARG
3	1D	254	THR
3	1D	259	THR
3	1D	261	LYS
4	1E	7	VAL
4	1E	47	VAL
4	1E	49	LEU
4	1E	75	VAL
4	1E	83	ASP
4	1E	89	ASP
4	1E	97	LYS
4	1E	145	LYS
5	1F	20	LEU
5	1F	33	LEU
5	1F	53	THR

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Mol	Chain	Res	Type
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	98	SER
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	154	VAL
5	1F	158	THR
5	1F	168	ARG
5	1F	175	THR
5	1F	192	LEU
5	1F	197	ASP
5	1F	201	VAL
6	1G	3	LEU
6	1G	21	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	49	ASP
6	1G	62	LEU
6	1G	82	LEU
6	1G	91	ARG
6	1G	108	ASN
6	1G	114	ILE
6	1G	126	ASP
6	1G	132	ASN
6	1G	133	LEU
6	1G	139	LEU
7	1H	16	SER
7	1H	17	VAL
7	1H	24	VAL
7	1H	40	GLU
7	1H	56	SER
7	1H	77	LYS
7	1H	88	LEU
7	1H	99	VAL
7	1H	113	VAL
7	1H	119	GLU
7	1H	129	THR
7	1H	132	ARG

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Mol	Chain	Res	Type
8	1I	2	LYS
8	1I	37	VAL
8	1I	45	LYS
8	1I	47	LEU
8	1I	50	ARG
8	1I	75	LEU
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	91	SER
8	1I	101	LEU
8	1I	133	HIS
8	1I	140	LEU
8	1I	141	LYS
9	1N	1	MET
9	1N	28	THR
9	1N	32	THR
9	1N	38	HIS
9	1N	58	ASP
9	1N	61	ARG
9	1N	67	LEU
9	1N	68	GLU
9	1N	96	GLU
9	1N	131	GLN
9	1N	137	LYS
9	1N	138	LEU
10	1O	77	ILE
10	1O	89	ASN
10	1O	112	MET
11	1P	3	LEU
11	1P	7	ARG
11	1P	45	LEU
11	1P	71	VAL
11	1P	79	ARG
11	1P	100	LEU
11	1P	101	VAL
11	1P	144	GLU
11	1P	147	LEU
11	1P	148	LEU
12	1Q	10	ARG
12	1Q	43	THR
12	1Q	75	THR

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Mol	Chain	Res	Type
12	1Q	85	LYS
12	1Q	109	VAL
13	1R	15	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	73	VAL
13	1R	100	LEU
13	1R	111	LEU
14	1S	3	ARG
14	1S	8	GLU
14	1S	13	ARG
14	1S	15	ARG
14	1S	25	ARG
14	1S	49	VAL
14	1S	50	SER
14	1S	68	GLN
14	1S	69	VAL
14	1S	73	LEU
14	1S	88	ASP
14	1S	110	LEU
15	1T	28	VAL
15	1T	30	VAL
15	1T	40	THR
15	1T	49	VAL
15	1T	74	ARG
15	1T	106	SER
15	1T	109	GLU
16	1U	59	ARG
16	1U	74	LEU
16	1U	78	THR
16	1U	95	LEU
16	1U	117	GLN
17	1V	10	LYS
17	1V	32	THR
17	1V	46	VAL
17	1V	61	VAL
17	1V	78	LYS
17	1V	79	VAL
17	1V	85	LYS
17	1V	100	ARG
18	1W	4	LYS
18	1W	11	ARG

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Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	30	GLU
18	1W	63	ASP
18	1W	67	ASP
18	1W	96	ILE
19	1X	75	ASP
19	1X	90	GLU
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	14	LEU
20	1Y	21	LYS
20	1Y	26	LYS
20	1Y	55	TYR
20	1Y	67	LEU
20	1Y	85	VAL
20	1Y	99	CYS
21	1Z	8	TYR
21	1Z	33	LEU
21	1Z	49	ARG
21	1Z	53	ILE
21	1Z	81	ARG
21	1Z	86	VAL
21	1Z	92	SER
21	1Z	119	GLU
21	1Z	124	ILE
21	1Z	129	SER
21	1Z	139	VAL
21	1Z	150	LEU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	171	ILE
22	10	55	ARG
23	11	46	LEU
23	11	52	ARG
23	11	57	GLU
23	11	59	THR
23	11	65	SER
23	11	66	HIS
23	11	85	LEU
24	12	45	SER
24	12	53	LEU

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Mol	Chain	Res	Type
24	12	65	ASN
25	13	18	ASP
25	13	23	LEU
25	13	24	LYS
25	13	29	ARG
25	13	34	GLU
25	13	40	THR
25	13	54	VAL
25	13	56	VAL
25	13	60	GLU
26	14	49	PHE
26	14	53	GLU
26	14	59	PHE
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	15	ARG
27	15	40	LYS
27	15	58	LEU
28	16	4	GLU
28	16	9	LEU
28	16	19	ARG
28	16	27	LYS
28	16	44	ARG
28	16	47	THR
28	16	48	VAL
29	17	1	MET
29	17	46	VAL
30	18	4	MET
30	18	31	HIS
30	18	41	ILE
30	18	43	GLN
30	18	50	LEU
31	19	6	SER
33	1b	10	LEU
33	1b	11	LEU
33	1b	12	GLU
33	1b	23	ARG
33	1b	25	ASN
33	1b	33	TYR
33	1b	39	ILE
33	1b	48	MET

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Mol	Chain	Res	Type
33	1b	54	THR
33	1b	76	GLN
33	1b	83	MET
33	1b	101	MET
33	1b	112	VAL
33	1b	127	ILE
33	1b	128	GLU
33	1b	133	LYS
33	1b	140	HIS
33	1b	157	ARG
33	1b	160	ASP
33	1b	176	GLU
33	1b	178	ARG
33	1b	180	LEU
33	1b	185	ILE
33	1b	196	LEU
33	1b	200	ILE
33	1b	206	ASP
33	1b	208	ILE
33	1b	209	ARG
33	1b	215	LEU
33	1b	219	VAL
33	1b	222	ILE
33	1b	233	SER
33	1b	236	TYR
34	1c	3	ASN
34	1c	45	LYS
34	1c	47	LEU
34	1c	64	VAL
34	1c	66	VAL
34	1c	69	HIS
34	1c	89	GLU
34	1c	131	ARG
34	1c	144	SER
34	1c	166	GLU
34	1c	178	LEU
34	1c	192	THR
34	1c	195	VAL
34	1c	201	TYR
34	1c	207	VAL
35	1d	15	GLU
35	1d	19	LEU

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Mol	Chain	Res	Type
35	1d	24	GLU
35	1d	28	SER
35	1d	49	ARG
35	1d	52	SER
35	1d	76	ARG
35	1d	83	SER
35	1d	86	LYS
35	1d	112	VAL
35	1d	115	ARG
35	1d	135	LEU
35	1d	141	ARG
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	176	LEU
35	1d	178	VAL
35	1d	188	LEU
35	1d	193	ASP
35	1d	194	LEU
36	1e	8	GLU
36	1e	12	LEU
36	1e	15	ARG
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	53	LEU
36	1e	63	ARG
36	1e	67	VAL
36	1e	75	THR
36	1e	82	VAL
36	1e	91	LEU
36	1e	135	THR
37	1f	1	MET
37	1f	19	LEU
37	1f	21	LEU
37	1f	24	GLU
37	1f	36	ARG
37	1f	55	ASP
37	1f	70	ASP
37	1f	72	VAL
37	1f	77	ARG
37	1f	78	GLU

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Mol	Chain	Res	Type
37	1f	87	ARG
38	1g	10	ARG
38	1g	12	LEU
38	1g	16	LEU
38	1g	21	VAL
38	1g	27	ILE
38	1g	31	MET
38	1g	50	ILE
38	1g	53	LYS
38	1g	59	LEU
38	1g	78	ARG
38	1g	90	GLU
38	1g	94	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	125	MET
38	1g	126	ASP
39	1h	24	THR
39	1h	25	ASP
39	1h	29	SER
39	1h	41	ARG
39	1h	45	ILE
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	68	ARG
39	1h	82	HIS
39	1h	83	ILE
39	1h	112	LEU
39	1h	118	VAL
39	1h	133	LEU
40	1i	17	VAL
40	1i	27	THR
40	1i	38	GLN
40	1i	50	LEU
40	1i	87	GLN
40	1i	92	TYR
40	1i	96	LEU
40	1i	128	ARG
41	1j	8	LEU
41	1j	19	SER

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Mol	Chain	Res	Type
41	1j	46	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
42	1k	14	VAL
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	80	VAL
42	1k	87	THR
42	1k	98	LEU
42	1k	109	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	39	VAL
43	1l	40	VAL
43	1l	54	LYS
43	1l	58	VAL
43	1l	62	SER
43	1l	83	VAL
43	1l	91	LYS
43	1l	122	THR
43	1l	123	LYS
44	1m	4	ILE
44	1m	19	LEU
44	1m	63	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	98	VAL
44	1m	106	ASN
44	1m	117	VAL
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	31	ARG
45	1n	50	LYS
45	1n	56	VAL
46	1o	24	SER
46	1o	27	VAL
46	1o	43	LEU
46	1o	84	LYS
46	1o	87	ILE

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Mol	Chain	Res	Type
47	1p	11	SER
47	1p	21	VAL
47	1p	22	THR
47	1p	40	ASP
47	1p	60	LEU
47	1p	67	THR
47	1p	76	GLN
48	1q	5	VAL
48	1q	9	VAL
48	1q	22	LEU
48	1q	35	VAL
48	1q	45	HIS
48	1q	57	VAL
48	1q	72	ARG
48	1q	74	LEU
49	1r	22	VAL
49	1r	26	LEU
49	1r	31	LEU
49	1r	54	ARG
49	1r	56	THR
49	1r	65	ILE
49	1r	84	LYS
50	1s	12	ASP
50	1s	19	VAL
50	1s	37	ARG
50	1s	79	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	54	LYS
51	1t	71	THR
3	2D	3	VAL
3	2D	14	ARG
3	2D	16	MET
3	2D	37	LEU
3	2D	71	ASP
3	2D	73	VAL
3	2D	88	ARG
3	2D	113	VAL
3	2D	141	VAL
3	2D	204	ILE

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Mol	Chain	Res	Type
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	273	ARG
4	2E	1	MET
4	2E	11	MET
4	2E	12	THR
4	2E	36	ARG
4	2E	40	GLU
4	2E	55	ASN
4	2E	90	THR
4	2E	93	VAL
4	2E	116	VAL
4	2E	119	ARG
4	2E	175	VAL
4	2E	199	ARG
5	2F	20	LEU
5	2F	33	LEU
5	2F	43	LYS
5	2F	51	THR
5	2F	70	THR
5	2F	82	ILE
5	2F	135	LYS
5	2F	165	ARG
5	2F	192	LEU
5	2F	200	GLU
6	2G	4	ASP
6	2G	19	LEU
6	2G	36	LYS
6	2G	41	GLN
6	2G	43	LEU
6	2G	45	GLU
6	2G	51	ARG
6	2G	53	LEU
6	2G	58	GLN
6	2G	60	LEU
6	2G	91	ARG
6	2G	109	VAL
6	2G	111	LEU
6	2G	130	ASN
6	2G	133	LEU

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Mol	Chain	Res	Type
6	2G	140	ILE
6	2G	159	VAL
6	2G	165	THR
6	2G	170	ARG
7	2H	4	ILE
7	2H	7	LEU
7	2H	23	ARG
7	2H	44	VAL
7	2H	57	ASP
7	2H	67	LEU
7	2H	70	THR
7	2H	76	VAL
7	2H	101	ARG
7	2H	115	VAL
7	2H	152	ARG
7	2H	172	LYS
8	2I	12	LEU
8	2I	19	VAL
8	2I	38	LEU
8	2I	43	ASN
8	2I	47	LEU
8	2I	52	ARG
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	77	LEU
8	2I	82	ARG
8	2I	86	THR
8	2I	87	LYS
8	2I	108	THR
8	2I	116	LEU
8	2I	117	GLU
8	2I	127	VAL
8	2I	144	VAL
9	2N	15	LEU
9	2N	29	LYS
9	2N	38	HIS
9	2N	43	THR
9	2N	48	MET
9	2N	55	VAL
9	2N	61	ARG
9	2N	62	VAL

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Mol	Chain	Res	Type
9	2N	63	THR
9	2N	85	ILE
9	2N	90	MET
9	2N	131	GLN
9	2N	137	LYS
10	2O	14	THR
10	2O	21	CYS
10	2O	35	VAL
10	2O	52	VAL
10	2O	53	LYS
10	2O	65	THR
10	2O	89	ASN
10	2O	96	THR
10	2O	113	LYS
11	2P	46	LYS
11	2P	70	GLN
11	2P	76	LYS
11	2P	83	VAL
11	2P	94	GLU
11	2P	95	VAL
11	2P	96	THR
11	2P	101	VAL
11	2P	133	SER
11	2P	135	LEU
12	2Q	10	ARG
12	2Q	18	LYS
12	2Q	21	THR
12	2Q	25	ASP
12	2Q	75	THR
12	2Q	110	THR
13	2R	24	GLN
13	2R	95	THR
13	2R	100	LEU
13	2R	114	VAL
14	2S	12	PHE
14	2S	15	ARG
14	2S	28	VAL
14	2S	35	ILE
14	2S	36	TYR
14	2S	56	LEU
14	2S	58	LEU
14	2S	63	THR

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Mol	Chain	Res	Type
14	2S	64	GLU
14	2S	78	LEU
14	2S	82	ILE
14	2S	84	GLN
14	2S	85	VAL
15	2T	9	LEU
15	2T	28	VAL
15	2T	31	SER
15	2T	40	THR
15	2T	46	GLU
15	2T	89	VAL
15	2T	96	ARG
15	2T	104	ASN
15	2T	107	ASP
15	2T	115	ARG
15	2T	124	ASP
16	2U	59	ARG
16	2U	74	LEU
16	2U	78	THR
16	2U	95	LEU
16	2U	111	GLU
17	2V	12	TYR
17	2V	32	THR
17	2V	38	LEU
17	2V	45	THR
17	2V	46	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	79	VAL
17	2V	84	LYS
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
18	2W	92	ARG
19	2X	80	ILE
19	2X	81	VAL
20	2Y	1	MET
20	2Y	11	ASP
20	2Y	14	LEU
20	2Y	37	VAL
20	2Y	49	VAL
20	2Y	72	VAL

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Mol	Chain	Res	Type
20	2Y	99	CYS
20	2Y	101	LYS
21	2Z	5	LEU
21	2Z	31	ARG
21	2Z	35	ARG
21	2Z	42	VAL
21	2Z	67	LEU
21	2Z	71	VAL
21	2Z	79	ARG
21	2Z	81	ARG
21	2Z	91	LEU
21	2Z	100	VAL
21	2Z	122	ARG
21	2Z	133	ILE
21	2Z	144	LEU
21	2Z	148	ASP
21	2Z	149	SER
21	2Z	151	HIS
21	2Z	154	ASP
21	2Z	170	THR
22	20	14	ARG
22	20	30	VAL
22	20	40	GLN
22	20	68	GLU
22	20	71	ASP
23	21	52	ARG
23	21	71	TYR
24	22	9	GLN
24	22	34	GLU
24	22	65	ASN
24	22	70	GLN
25	23	31	LEU
25	23	52	HIS
26	24	13	ARG
26	24	22	ILE
26	24	26	SER
26	24	27	THR
26	24	34	GLU
26	24	49	PHE
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR

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Mol	Chain	Res	Type
26	24	68	ARG
27	25	6	VAL
27	25	13	LYS
27	25	44	THR
27	25	55	ARG
27	25	58	LEU
28	26	6	ARG
28	26	9	LEU
28	26	13	CYS
29	27	1	MET
29	27	4	THR
29	27	24	THR
29	27	41	ARG
29	27	46	VAL
30	28	3	LYS
30	28	31	HIS
30	28	37	SER
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	30	ARG
33	2b	58	ILE
33	2b	59	GLU
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	80	ILE
33	2b	82	ARG
33	2b	94	ASN
33	2b	95	GLN
33	2b	108	ILE
33	2b	112	VAL
33	2b	115	LEU
33	2b	133	LYS
33	2b	144	ARG
33	2b	154	LEU
33	2b	163	PHE
33	2b	168	THR
33	2b	169	LYS
33	2b	185	ILE
33	2b	189	ASP
33	2b	193	ASP

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Mol	Chain	Res	Type
33	2b	198	ASP
33	2b	232	PRO
33	2b	236	TYR
34	2c	32	LEU
34	2c	39	ILE
34	2c	44	GLU
34	2c	52	LEU
34	2c	70	VAL
34	2c	140	ARG
34	2c	153	VAL
34	2c	190	ARG
35	2d	19	LEU
35	2d	31	CYS
35	2d	42	GLN
35	2d	45	GLN
35	2d	58	LEU
35	2d	60	GLU
35	2d	76	ARG
35	2d	83	SER
35	2d	94	LEU
35	2d	113	SER
35	2d	127	THR
35	2d	129	ASN
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	155	LEU
35	2d	162	LEU
35	2d	175	SER
35	2d	190	ASP
35	2d	193	ASP
36	2e	6	PHE
36	2e	8	GLU
36	2e	13	ILE
36	2e	20	GLN
36	2e	38	GLN
36	2e	53	LEU
36	2e	55	VAL
36	2e	73	ASN
36	2e	78	HIS
36	2e	83	GLU
36	2e	100	VAL

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Mol	Chain	Res	Type
36	2e	101	ILE
36	2e	125	SER
36	2e	147	ASP
37	2f	9	VAL
37	2f	15	ASP
37	2f	19	LEU
37	2f	63	TYR
37	2f	66	GLU
37	2f	75	LEU
38	2g	4	ARG
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	24	THR
38	2g	27	ILE
38	2g	45	ASP
38	2g	52	GLU
38	2g	64	GLN
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	98	SER
38	2g	115	ARG
38	2g	129	GLU
38	2g	146	GLU
38	2g	155	ARG
39	2h	3	THR
39	2h	26	VAL
39	2h	29	SER
39	2h	49	GLU
39	2h	52	ASP
39	2h	54	ASP
39	2h	84	ARG
39	2h	85	ARG
39	2h	109	ILE
39	2h	112	LEU
39	2h	133	LEU
40	2i	35	GLU
40	2i	54	ASP
40	2i	56	LEU
40	2i	65	VAL
40	2i	88	TYR

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Mol	Chain	Res	Type
40	2i	89	ASN
40	2i	102	LEU
40	2i	103	THR
40	2i	105	ASP
40	2i	111	ARG
40	2i	113	LYS
41	2j	8	LEU
41	2j	9	ARG
41	2j	21	GLN
41	2j	23	ILE
41	2j	38	ILE
41	2j	50	ILE
41	2j	65	LEU
41	2j	66	ARG
41	2j	67	THR
41	2j	84	GLN
41	2j	97	GLU
42	2k	14	VAL
42	2k	24	SER
42	2k	41	THR
42	2k	48	ILE
42	2k	73	MET
42	2k	79	SER
42	2k	87	THR
42	2k	105	VAL
43	2l	18	VAL
43	2l	33	ARG
43	2l	38	THR
43	2l	40	VAL
43	2l	43	VAL
43	2l	52	LEU
43	2l	83	VAL
43	2l	102	ARG
44	2m	14	ARG
44	2m	22	ILE
44	2m	32	GLU
44	2m	37	THR
44	2m	47	ASP
44	2m	62	ASN
44	2m	67	GLU
44	2m	73	GLU
44	2m	86	CYS

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Mol	Chain	Res	Type
44	2m	103	THR
44	2m	106	ASN
45	2n	18	VAL
45	2n	33	VAL
46	2o	5	LYS
46	2o	7	GLU
46	2o	26	GLU
46	2o	27	VAL
46	2o	56	LEU
46	2o	76	GLU
47	2p	20	VAL
47	2p	31	LYS
47	2p	42	ARG
47	2p	45	THR
47	2p	60	LEU
47	2p	61	SER
47	2p	67	THR
47	2p	73	LEU
48	2q	5	VAL
48	2q	19	VAL
48	2q	35	VAL
48	2q	36	ILE
48	2q	39	SER
48	2q	82	MET
48	2q	99	SER
49	2r	22	VAL
49	2r	26	LEU
49	2r	31	LEU
49	2r	37	VAL
49	2r	42	ARG
49	2r	69	THR
49	2r	82	THR
49	2r	85	LEU
50	2s	7	LYS
50	2s	14	HIS
50	2s	20	LEU
50	2s	27	GLU
50	2s	30	LEU
50	2s	37	ARG
50	2s	49	ILE
50	2s	57	HIS
50	2s	77	THR

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Mol	Chain	Res	Type
50	2s	81	ARG
51	2t	18	GLN
51	2t	31	SER
51	2t	45	GLN
51	2t	64	ASP
52	2u	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
4	1E	48	GLN
4	1E	54	GLN
5	1F	69	HIS
6	1G	26	GLN
6	1G	123	ASN
6	1G	132	ASN
9	1N	131	GLN
10	1O	3	GLN
10	1O	5	GLN
12	1Q	57	HIS
12	1Q	89	ASN
15	1T	43	GLN
15	1T	58	ASN
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	55	HIS
21	1Z	65	GLN
21	1Z	73	GLN
23	11	56	GLN
24	12	9	GLN
25	13	32	GLN
29	17	36	GLN
33	1b	16	HIS
33	1b	40	HIS
33	1b	113	HIS
33	1b	224	GLN
34	1c	6	HIS
34	1c	162	GLN
35	1d	123	HIS
36	1e	78	HIS
37	1f	13	ASN

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Mol	Chain	Res	Type
37	1f	57	GLN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	68	ASN
39	1h	82	HIS
40	1i	3	GLN
40	1i	38	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
41	1j	62	HIS
43	1l	99	HIS
44	1m	12	ASN
45	1n	49	HIS
46	1o	46	HIS
46	1o	50	HIS
46	1o	62	GLN
47	1p	14	ASN
47	1p	76	GLN
50	1s	47	HIS
50	1s	57	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	116	GLN
4	2E	48	GLN
5	2F	40	GLN
5	2F	69	HIS
6	2G	132	ASN
8	2I	105	HIS
8	2I	133	HIS
8	2I	139	GLN
10	2O	5	GLN
10	2O	90	GLN
11	2P	70	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	57	HIS
14	2S	38	GLN
15	2T	55	ASN
15	2T	58	ASN
16	2U	94	ASN

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Mol	Chain	Res	Type
19	2X	82	GLN
23	21	56	GLN
24	22	70	GLN
25	23	32	GLN
26	24	40	HIS
26	24	46	GLN
27	25	23	HIS
30	28	35	GLN
33	2b	76	GLN
33	2b	95	GLN
33	2b	135	GLN
34	2c	102	ASN
34	2c	104	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	56	GLN
37	2f	13	ASN
37	2f	100	ASN
38	2g	37	ASN
38	2g	51	GLN
38	2g	86	GLN
39	2h	82	HIS
40	2i	58	HIS
40	2i	89	ASN
41	2j	33	GLN
41	2j	69	ASN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	106	ASN
46	2o	13	GLN
46	2o	50	HIS
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	507 (17%)	27 (0%)
1	2A	2788/2915 (95%)	549 (19%)	23 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	26 (22%)	0
32	1a	1494/1521 (98%)	265 (17%)	0
32	2a	1498/1521 (98%)	330 (22%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	69/76 (90%)	24 (34%)	0
54	2w	66/76 (86%)	20 (30%)	0
55	1x	74/77 (96%)	15 (20%)	0
55	2x	74/77 (96%)	14 (18%)	0
56	1y	71/76 (93%)	27 (38%)	0
56	2y	69/76 (90%)	26 (37%)	0
All	All	9325/9620 (96%)	1816 (19%)	50 (0%)

All (1816) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	27	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	78	A
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	131	G
1	1A	139	G
1	1A	140	G
1	1A	141	A
1	1A	154(A)	C
1	1A	181	A

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Mol	Chain	Res	Type
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	200	U
1	1A	201	C
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	223	A
1	1A	226	G
1	1A	228	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	265	A
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(R)	G
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	380	U
1	1A	386	G

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Mol	Chain	Res	Type
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	442	G
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	455	C
1	1A	481	G
1	1A	489	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	528	A
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	568	U
1	1A	573	G
1	1A	574	C
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(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	621	A
1	1A	627	A
1	1A	637	A

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Mol	Chain	Res	Type
1	1A	645	C
1	1A	646	A
1	1A	648	G
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	719	C
1	1A	730	C
1	1A	749	C
1	1A	762	U
1	1A	764	A
1	1A	765	G
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	790	C
1	1A	792	G
1	1A	802	A
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	861	A
1	1A	866	A
1	1A	879	G
1	1A	880	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

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Mol	Chain	Res	Type
1	1A	890	A
1	1A	892	G
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	914	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	995	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
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	1068	G
1	1A	1070	A
1	1A	1071	G

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Mol	Chain	Res	Type
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1102	C
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G
1	1A	1128	A
1	1A	1130	U
1	1A	1131	G
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
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	1229	G
1	1A	1237	A
1	1A	1244	G
1	1A	1248	G

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Mol	Chain	Res	Type
1	1A	1252	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1289	C
1	1A	1290	C
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1313	U
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1369	G
1	1A	1372	U
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	1427	A
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1473	G
1	1A	1482	G
1	1A	1493	C
1	1A	1507	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C

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Mol	Chain	Res	Type
1	1A	1539	G
1	1A	1540	U
1	1A	1541	G
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1612	C
1	1A	1615	C
1	1A	1648	C
1	1A	1658	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
1	1A	1722	A
1	1A	1740	G
1	1A	1745	C
1	1A	1746	G
1	1A	1756	G
1	1A	1761	C
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	1816	G
1	1A	1828	G
1	1A	1847	A

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Mol	Chain	Res	Type
1	1A	1861	G
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1916	A
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1980	G
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2035	G
1	1A	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	2099	U
1	1A	2100	G
1	1A	2104	G
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G

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Mol	Chain	Res	Type
1	1A	2113	U
1	1A	2116	G
1	1A	2121	G
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
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	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G

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Mol	Chain	Res	Type
1	1A	2239	G
1	1A	2259	G
1	1A	2268	A
1	1A	2269	A
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2358	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2405	G
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2438	U
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A

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Mol	Chain	Res	Type
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2520	C
1	1A	2525	G
1	1A	2529	G
1	1A	2530	A
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	2578	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2675	A
1	1A	2689	U
1	1A	2690	C
1	1A	2703	C
1	1A	2711	A
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2726	U
1	1A	2733	A
1	1A	2739	U
1	1A	2744	G
1	1A	2752	C
1	1A	2757	A
1	1A	2758	A
1	1A	2763	G
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G

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Mol	Chain	Res	Type
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2810	A
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2825	C
1	1A	2833	G
1	1A	2834	G
1	1A	2835	A
1	1A	2836	U
1	1A	2855	C
1	1A	2872	G
1	1A	2875	C
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	12	C
2	1B	15	A
2	1B	35	U
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	65	C
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	5	U
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	50	A
32	1a	51	A
32	1a	52	G

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Mol	Chain	Res	Type
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	92	C
32	1a	93	G
32	1a	98	G
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	151	A
32	1a	153	C
32	1a	161	A
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	175	C
32	1a	180	U
32	1a	182	U
32	1a	189	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	194	C
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	274	A
32	1a	283	C
32	1a	289	G

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Mol	Chain	Res	Type
32	1a	311	C
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	410	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	452	A
32	1a	453	A
32	1a	461	A
32	1a	470	C
32	1a	479	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	531	U
32	1a	532	A

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Mol	Chain	Res	Type
32	1a	536	C
32	1a	545	C
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	672	U
32	1a	684	A
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	721	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	734	G
32	1a	745	C
32	1a	749	C
32	1a	753	A
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	803	G
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	827	U

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Mol	Chain	Res	Type
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	855	G
32	1a	870	U
32	1a	872	A
32	1a	874	G
32	1a	876	G
32	1a	891	U
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	950	U
32	1a	955	U
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1020	U
32	1a	1021	G

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Mol	Chain	Res	Type
32	1a	1022	G
32	1a	1023	G
32	1a	1024	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	1040	U
32	1a	1044	A
32	1a	1051	C
32	1a	1068	G
32	1a	1081	G
32	1a	1085	U
32	1a	1091	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1160	G
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U

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Mol	Chain	Res	Type
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1381	U
32	1a	1394	A
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U

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Mol	Chain	Res	Type
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
54	1w	7	A
54	1w	8	4SU
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	27	G
54	1w	36	A
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	61	C
54	1w	62	C
54	1w	63	G
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
55	1x	3	C
55	1x	7	G
55	1x	8	4SU
55	1x	9	G
55	1x	17(A)	U
55	1x	21	A
55	1x	44	A
55	1x	47	U
55	1x	48	C
55	1x	51	C
55	1x	52	G
55	1x	59	A
55	1x	61	C
55	1x	63	G

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Mol	Chain	Res	Type
55	1x	64	G
56	1y	2	C
56	1y	6	G
56	1y	8	4SU
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	26	A
56	1y	35	A
56	1y	39	PSU
56	1y	40	C
56	1y	44	G
56	1y	45	U
56	1y	46	7MG
56	1y	47	U
56	1y	48	C
56	1y	53	G
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	61	C
56	1y	64	A
56	1y	65	G
56	1y	69	G
56	1y	70	G
1	2A	7	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	38	A
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	76	C
1	2A	79	G

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Mol	Chain	Res	Type
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	120	U
1	2A	121	G
1	2A	141	A
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
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	266	G
1	2A	271(F)	C
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	295	G
1	2A	311	A

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Mol	Chain	Res	Type
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	335	C
1	2A	342	G
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	430	G
1	2A	431	U
1	2A	434	U
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	480	A
1	2A	481	G
1	2A	482	A
1	2A	499	U
1	2A	501	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	527	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C

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Mol	Chain	Res	Type
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(D)	C
1	2A	664	C
1	2A	669	G
1	2A	671	C
1	2A	686	G
1	2A	701	G
1	2A	708	C
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	779	U
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	805	G

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Mol	Chain	Res	Type
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	868	U
1	2A	872	A
1	2A	874	G
1	2A	875	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	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	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	981	A
1	2A	983	A
1	2A	990	A
1	2A	996	A

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Mol	Chain	Res	Type
1	2A	999	U
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	1023	U
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	1042	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1121	C
1	2A	1122	G
1	2A	1126	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1155	A
1	2A	1169	G
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	1221	C
1	2A	1244	G
1	2A	1247	A
1	2A	1248	G
1	2A	1253	A

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Mol	Chain	Res	Type
1	2A	1256	G
1	2A	1264	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1320	C
1	2A	1333	C
1	2A	1341	U
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1392	A
1	2A	1412	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1479	G

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Mol	Chain	Res	Type
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1541	G
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	1588	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G
1	2A	1675	C
1	2A	1680	U
1	2A	1695	G
1	2A	1696	G
1	2A	1698	A
1	2A	1700	A
1	2A	1701	A
1	2A	1707	G
1	2A	1721	G
1	2A	1722	A

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Mol	Chain	Res	Type
1	2A	1739	U
1	2A	1740	G
1	2A	1747	G
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1881	C
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1940	U
1	2A	1955	U
1	2A	1963	U
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A

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Mol	Chain	Res	Type
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2063	C
1	2A	2069	G
1	2A	2093	G
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2115	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	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C

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Mol	Chain	Res	Type
1	2A	2139	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2157	G
1	2A	2158	A
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
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	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	2267	A
1	2A	2269	A
1	2A	2274	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A

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Mol	Chain	Res	Type
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2358	G
1	2A	2366	A
1	2A	2370	G
1	2A	2374	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2403	C
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2426	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2457	U
1	2A	2459	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2477	C
1	2A	2480	C
1	2A	2481	G
1	2A	2490	G
1	2A	2491	U

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Mol	Chain	Res	Type
1	2A	2494	G
1	2A	2497	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2532	G
1	2A	2537	U
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2616	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2636	U
1	2A	2646	C
1	2A	2648	C
1	2A	2654	A
1	2A	2662	A
1	2A	2679	A
1	2A	2686	G
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G

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Mol	Chain	Res	Type
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2779	U
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2805	G
1	2A	2807	G
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2861	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	20	C
2	2B	33	G
2	2B	34	U
2	2B	40	U
2	2B	41	U
2	2B	42	C
2	2B	52	A

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Mol	Chain	Res	Type
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	85	G
2	2B	88	C
2	2B	102	A
2	2B	105	A
2	2B	106	G
2	2B	110	G
2	2B	111	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	27	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	97	G
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	137	C
32	2a	143	A
32	2a	144	G
32	2a	151	A
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U

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Mol	Chain	Res	Type
32	2a	189(A)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(H)	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	217	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	283	C
32	2a	287	U
32	2a	289	G
32	2a	301	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	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	383	A
32	2a	384	G
32	2a	389	A
32	2a	396	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	410	G

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Mol	Chain	Res	Type
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	427	U
32	2a	428	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	441	A
32	2a	442	C
32	2a	447	G
32	2a	452	A
32	2a	457	C
32	2a	470	C
32	2a	476	G
32	2a	484	G
32	2a	485	G
32	2a	487	A
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	549	C
32	2a	559	A
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A

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Mol	Chain	Res	Type
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	598	U
32	2a	601	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	662	G
32	2a	665	A
32	2a	681	C
32	2a	687	A
32	2a	688	G
32	2a	693	G
32	2a	695	A
32	2a	703	G
32	2a	712	A
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	756	C
32	2a	768	A
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	810	C
32	2a	815	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	853	G
32	2a	858	G
32	2a	859	A

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Mol	Chain	Res	Type
32	2a	880	C
32	2a	887	G
32	2a	891	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	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	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1009	G
32	2a	1011	G
32	2a	1019	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G

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Mol	Chain	Res	Type
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1043	C
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1106	G
32	2a	1108	G
32	2a	1109	C
32	2a	1115	C
32	2a	1122	U
32	2a	1123	A
32	2a	1124	G
32	2a	1125	U
32	2a	1126	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A

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Mol	Chain	Res	Type
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1155	G
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1173	G
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C

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Mol	Chain	Res	Type
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1289	A
32	2a	1294	G
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1321	C
32	2a	1323	G
32	2a	1336	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1354	C
32	2a	1359	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1381	U
32	2a	1388	C
32	2a	1400	5MC
32	2a	1404	5MC
32	2a	1405	G
32	2a	1416	G
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	1478	C

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Mol	Chain	Res	Type
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
54	2w	3	C
54	2w	11	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	32	PSU
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	49	C
54	2w	50	U
54	2w	51	U
54	2w	58	A
54	2w	62	C
54	2w	65	G
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	23	C
55	2x	46	G
55	2x	47	U
55	2x	52	G
55	2x	53	G
55	2x	56	C
55	2x	61	C

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Mol	Chain	Res	Type
55	2x	63	G
55	2x	67	C
56	2y	9	A
56	2y	14	A
56	2y	15	G
56	2y	19	G
56	2y	25	C
56	2y	26	A
56	2y	27	G
56	2y	40	C
56	2y	41	C
56	2y	45	U
56	2y	46	7MG
56	2y	48	C
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	56	C
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	65	G
56	2y	67	C
56	2y	68	C
56	2y	69	G
56	2y	70	G
56	2y	73	A

All (50) 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	529	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	1047	G

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Mol	Chain	Res	Type
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1663	C
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2062	A
1	2A	2119	A
1	2A	2126	A
1	2A	2286	A
1	2A	2689	U

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

88 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$
56	7MG	1y	46	56	22,26,27	1.81	3 (13%)	28,39,42	2.81	9 (32%)
54	4SU	2w	8	54	14,21,22	1.26	1 (7%)	15,30,33	1.39	2 (13%)
55	PSU	2x	55	55	17,21,22	1.61	2 (11%)	20,30,33	3.11	6 (30%)
54	PSU	1w	39	54	17,21,22	1.56	2 (11%)	20,30,33	2.92	6 (30%)
56	PSU	1y	55	56	17,21,22	1.36	2 (11%)	20,30,33	3.13	6 (30%)
1	OMU	2A	2552	1,57	14,22,23	0.93	0	14,31,34	1.18	2 (14%)
1	5MU	1A	1939	1,57	15,22,23	1.16	2 (13%)	16,32,35	1.75	2 (12%)
56	PSU	2y	39	56	17,21,22	1.64	2 (11%)	20,30,33	3.42	6 (30%)
56	4SU	2y	8	56	14,21,22	1.22	1 (7%)	15,30,33	1.67	3 (20%)
56	PSU	2y	55	56	17,21,22	1.47	3 (17%)	20,30,33	3.06	5 (25%)
1	4OC	2A	1920	1	15,22,24	0.62	0	17,31,35	1.46	2 (11%)
56	MIA	1y	37	56	18,24,32	1.10	2 (11%)	18,35,47	1.20	2 (11%)
1	5MU	2A	1939	1	15,22,23	1.05	2 (13%)	16,32,35	1.72	2 (12%)
1	2MA	2A	2503	1,57	17,25,26	1.26	2 (11%)	19,37,40	2.13	4 (21%)
54	5MU	1w	54	54	15,22,23	1.06	1 (6%)	16,32,35	1.86	1 (6%)
1	5MC	2A	1942	1	15,22,23	1.32	1 (6%)	19,32,35	1.42	3 (15%)
1	PSU	1A	2605	1,57	17,21,22	1.57	4 (23%)	20,30,33	2.98	6 (30%)
56	PSU	1y	32	56	17,21,22	1.47	2 (11%)	20,30,33	3.26	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.25	1 (6%)	19,32,35	1.43	3 (15%)
32	2MG	1a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.54	8 (38%)
55	31H	2x	76	57,55	28,34,35	1.07	3 (10%)	23,47,50	1.50	3 (13%)
32	7MG	1a	527	57,32	22,26,27	1.76	4 (18%)	28,39,42	2.73	10 (35%)
55	5MC	1x	32	55	15,22,23	1.37	1 (6%)	19,32,35	1.34	3 (15%)
55	5MU	1x	54	55	15,22,23	1.10	2 (13%)	16,32,35	2.11	1 (6%)
54	7MG	1w	46	54	22,26,27	1.75	4 (18%)	28,39,42	2.77	8 (28%)
32	5MC	2a	1404	32	15,22,23	1.35	1 (6%)	19,32,35	1.47	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1915	1	15,22,23	1.01	1 (6%)	16,32,35	1.81	2 (12%)
32	MA6	1a	1518	32	19,26,27	0.79	0	18,38,41	1.50	2 (11%)
1	OMG	1A	2251	55,1,57	18,26,27	1.19	2 (11%)	20,38,41	2.22	6 (30%)
32	UR3	2a	1498	32	14,22,23	0.81	1 (7%)	15,32,35	0.85	1 (6%)
54	MIA	1w	37	54	24,31,32	2.19	3 (12%)	26,44,47	2.65	11 (42%)
43	0TD	2l	92	43	4,9,10	3.17	1 (25%)	3,11,13	1.80	1 (33%)
32	7MG	2a	527	57,32	22,26,27	1.71	4 (18%)	28,39,42	2.67	10 (35%)
1	MA6	1A	2058	1,57	19,26,27	0.83	0	18,38,41	1.75	3 (16%)
32	MA6	1a	1519	32	19,26,27	0.86	0	18,38,41	1.81	3 (16%)
54	5MU	2w	54	54	15,22,23	1.05	2 (13%)	16,32,35	2.30	1 (6%)
55	4SU	2x	8	55	14,21,22	1.45	2 (14%)	15,30,33	2.45	2 (13%)
1	MA6	2A	2058	1	19,26,27	0.81	0	18,38,41	1.57	3 (16%)
54	4SU	1w	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.70	2 (13%)
1	5MU	2A	1915	1	15,22,23	1.05	1 (6%)	16,32,35	1.82	2 (12%)
1	OMU	1A	2552	1	14,22,23	0.96	1 (7%)	14,31,34	0.72	0
1	OMG	2A	2251	1,55	18,26,27	1.08	2 (11%)	20,38,41	2.32	7 (35%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.44	2 (11%)
1	PSU	2A	1911	1	17,21,22	1.59	2 (11%)	20,30,33	3.11	6 (30%)
32	5MC	1a	967	32	15,22,23	1.32	1 (6%)	19,32,35	1.29	2 (10%)
56	5MU	2y	54	56	15,22,23	0.98	1 (6%)	16,32,35	2.07	1 (6%)
56	4SU	1y	8	56	14,21,22	1.23	1 (7%)	15,30,33	1.52	2 (13%)
1	5MC	1A	1962	1,57	15,22,23	1.35	1 (6%)	19,32,35	1.31	1 (5%)
56	MIA	2y	37	56	18,24,32	1.07	2 (11%)	18,35,47	1.38	2 (11%)
32	5MC	2a	1407	32	15,22,23	1.29	1 (6%)	19,32,35	1.40	2 (10%)
55	5MC	2x	32	55	15,22,23	1.38	1 (6%)	19,32,35	1.40	3 (15%)
1	PSU	1A	1911	1	17,21,22	1.57	4 (23%)	20,30,33	3.12	6 (30%)
54	PSU	2w	39	54	17,21,22	1.56	2 (11%)	20,30,33	2.85	6 (30%)
56	PSU	1y	39	56	17,21,22	1.35	2 (11%)	20,30,33	2.96	5 (25%)
43	0TD	1l	92	43	4,9,10	3.24	1 (25%)	3,11,13	2.14	1 (33%)
55	4SU	1x	8	55	14,21,22	1.36	2 (14%)	15,30,33	2.68	2 (13%)
1	5MC	2A	1962	1,57	15,22,23	1.26	1 (6%)	19,32,35	1.51	4 (21%)
32	UR3	1a	1498	32	14,22,23	0.81	1 (7%)	15,32,35	0.71	0
32	5MC	1a	1407	32	15,22,23	1.26	1 (6%)	19,32,35	1.36	2 (10%)
32	5MC	2a	967	57,32	15,22,23	1.38	1 (6%)	19,32,35	1.29	3 (15%)
32	4OC	2a	1402	57,32	16,23,24	0.65	0	17,32,35	1.39	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1404	32	15,22,23	1.40	1 (6%)	19,32,35	1.41	2 (10%)
54	PSU	2w	32	54	17,21,22	1.51	2 (11%)	20,30,33	3.22	6 (30%)
55	PSU	1x	55	55	17,21,22	1.60	2 (11%)	20,30,33	3.21	6 (30%)
55	31H	1x	76	57,55	28,34,35	1.09	3 (10%)	23,47,50	1.62	3 (13%)
32	5MC	2a	1400	32	15,22,23	1.38	1 (6%)	19,32,35	1.37	3 (15%)
54	PSU	1w	32	54	17,21,22	1.44	2 (11%)	20,30,33	3.15	6 (30%)
54	PSU	2w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.43	7 (35%)
1	2MA	1A	2503	1,57	17,25,26	1.35	2 (11%)	19,37,40	1.98	2 (10%)
32	PSU	2a	516	32	17,21,22	1.46	3 (17%)	20,30,33	3.11	6 (30%)
56	PSU	2y	32	56	17,21,22	1.43	2 (11%)	20,30,33	3.03	5 (25%)
32	PSU	1a	516	57,32	17,21,22	1.64	3 (17%)	20,30,33	3.02	6 (30%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.18	6 (27%)
54	7MG	2w	46	54	22,26,27	1.79	4 (18%)	28,39,42	2.61	9 (32%)
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.87	2 (12%)
56	7MG	2y	46	56	22,26,27	1.79	4 (18%)	28,39,42	3.08	11 (39%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.49	2 (11%)
1	PSU	2A	2605	1	17,21,22	1.36	3 (17%)	20,30,33	3.17	6 (30%)
1	5MC	1A	1942	1,57	15,22,23	1.23	1 (6%)	19,32,35	1.40	2 (10%)
32	2MG	2a	1207	32	19,26,27	1.26	2 (10%)	21,38,41	2.08	6 (28%)
1	PSU	1A	1917	1	17,21,22	1.64	3 (17%)	20,30,33	3.27	7 (35%)
32	4OC	1a	1402	32	16,23,24	0.61	0	17,32,35	1.02	1 (5%)
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	2.26	5 (22%)
54	MIA	2w	37	54	20,27,32	1.69	2 (10%)	22,39,47	1.85	7 (31%)
56	5MU	1y	54	56	15,22,23	1.09	1 (6%)	16,32,35	1.97	1 (6%)
1	4OC	1A	1920	1	15,22,24	0.68	0	17,31,35	1.49	2 (11%)
54	PSU	1w	55	54	17,21,22	1.50	2 (11%)	20,30,33	3.35	6 (30%)
1	PSU	2A	1917	1	17,21,22	1.50	3 (17%)	20,30,33	3.02	7 (35%)

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
56	7MG	1y	46	56	-	2/7/37/38	0/3/3/3
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/7/27/28	0/2/2/2
1	5MU	1A	1939	1,57	-	0/5/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/5/25/26	0/2/2/2
56	PSU	2y	55	56	-	3/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
56	MIA	1y	37	56	-	0/3/25/34	0/3/3/3
1	5MU	2A	1939	1	-	2/5/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
55	31H	2x	76	57,55	-	7/18/40/41	0/3/3/3
32	7MG	1a	527	57,32	-	2/7/37/38	0/3/3/3
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
32	5MC	2a	1404	32	-	3/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	OMG	1A	2251	55,1,57	-	0/5/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
43	0TD	2l	92	43	-	1/3/12/14	-
32	7MG	2a	527	57,32	-	3/7/37/38	0/3/3/3
1	MA6	1A	2058	1,57	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
1	MA6	2A	2058	1	-	0/7/29/30	0/3/3/3
54	4SU	1w	8	54	-	1/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/7/27/28	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/5/25/26	0/2/2/2
56	5MU	2y	54	56	-	0/5/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/5/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	2/5/25/26	0/2/2/2
56	MIA	2y	37	56	-	0/3/25/34	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	2/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	57,32	-	0/5/25/26	0/2/2/2
32	4OC	2a	1402	57,32	-	4/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
54	PSU	2w	32	54	-	3/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	31H	1x	76	57,55	-	9/18/40/41	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
54	PSU	1w	32	54	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
56	7MG	2y	46	56	-	6/7/37/38	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,57	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
56	5MU	1y	54	56	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-7.01	1.69	1.75
54	1w	37	MIA	C13-C14	6.84	1.52	1.32
43	1l	92	0TD	CB-SB	-6.16	1.69	1.84
43	2l	92	0TD	CB-SB	-6.08	1.69	1.84
54	2w	37	MIA	C2-S10	-6.05	1.70	1.75
54	2w	46	7MG	C6-C5	5.34	1.48	1.41
32	2a	967	5MC	C5-C4	4.99	1.49	1.41
56	1y	46	7MG	C6-C5	4.94	1.48	1.41
32	1a	1404	5MC	C5-C4	4.92	1.49	1.41
32	2a	1400	5MC	C5-C4	4.91	1.49	1.41
55	2x	32	5MC	C5-C4	4.91	1.49	1.41
32	2a	527	7MG	C6-C5	4.84	1.48	1.41
56	2y	46	7MG	C5-C4	4.79	1.48	1.39
1	2A	1942	5MC	C5-C4	4.78	1.48	1.41
1	1A	1962	5MC	C5-C4	4.77	1.48	1.41
32	2a	1404	5MC	C5-C4	4.76	1.48	1.41
32	1a	527	7MG	C6-C5	4.75	1.48	1.41
55	1x	32	5MC	C5-C4	4.75	1.48	1.41
32	1a	967	5MC	C5-C4	4.74	1.48	1.41
56	1y	46	7MG	C5-C4	4.67	1.48	1.39
56	2y	39	PSU	C5-C1'	-4.66	1.48	1.52
32	1a	516	PSU	C5-C1'	-4.66	1.48	1.52
32	2a	1407	5MC	C5-C4	4.58	1.48	1.41
1	1A	2503	2MA	C6-C5	4.55	1.48	1.41
1	1A	1917	PSU	C5-C1'	-4.54	1.48	1.52
54	1w	46	7MG	C5-C4	4.51	1.48	1.39
55	2x	55	PSU	C5-C1'	-4.49	1.48	1.52
54	1w	46	7MG	C6-C5	4.45	1.47	1.41
32	1a	966	M2G	C6-C5	4.45	1.49	1.41
1	2A	1962	5MC	C5-C4	4.45	1.48	1.41
32	1a	1207	2MG	C6-C5	4.43	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C6-C5	4.42	1.49	1.41
55	1x	55	PSU	C5-C1'	-4.38	1.48	1.52
54	1w	39	PSU	C5-C1'	-4.37	1.48	1.52
32	1a	1400	5MC	C5-C4	4.34	1.48	1.41
1	1A	1942	5MC	C5-C4	4.32	1.48	1.41
32	1a	1407	5MC	C5-C4	4.32	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.31	1.48	1.52
32	2a	966	M2G	C6-C5	4.29	1.48	1.41
54	2w	46	7MG	C5-C4	4.28	1.47	1.39
32	2a	527	7MG	C5-C4	4.28	1.47	1.39
32	1a	527	7MG	C5-C4	4.26	1.47	1.39
1	2A	2503	2MA	C6-C5	4.25	1.47	1.41
56	2y	46	7MG	C6-C5	4.23	1.47	1.41
54	2w	39	PSU	C5-C1'	-4.21	1.48	1.52
1	1A	2605	PSU	C5-C1'	-4.13	1.48	1.52
1	1A	1911	PSU	C5-C1'	-4.10	1.48	1.52
55	2x	8	4SU	C4-S4	-4.07	1.60	1.67
54	2w	8	4SU	C4-S4	-3.91	1.60	1.67
54	1w	8	4SU	C4-S4	-3.89	1.60	1.67
56	1y	39	PSU	C4-C5	3.86	1.49	1.41
1	2A	1917	PSU	C5-C1'	-3.84	1.49	1.52
56	2y	8	4SU	C4-S4	-3.82	1.60	1.67
1	1A	2251	OMG	C6-C5	3.78	1.47	1.41
56	1y	32	PSU	C5-C1'	-3.77	1.49	1.52
56	1y	8	4SU	C4-S4	-3.73	1.60	1.67
55	2x	55	PSU	C4-C5	3.71	1.49	1.41
56	2y	46	7MG	C5-N7	-3.69	1.33	1.39
54	1w	55	PSU	C5-C1'	-3.69	1.49	1.52
54	2w	32	PSU	C4-C5	3.69	1.49	1.41
54	1w	32	PSU	C4-C5	3.69	1.49	1.41
54	2w	32	PSU	C5-C1'	-3.65	1.49	1.52
56	2y	32	PSU	C4-C5	3.64	1.49	1.41
1	2A	2251	OMG	C6-C5	3.63	1.47	1.41
56	2y	55	PSU	C4-C5	3.53	1.49	1.41
54	2w	39	PSU	C4-C5	3.52	1.49	1.41
54	2w	55	PSU	C5-C1'	-3.51	1.49	1.52
32	2a	516	PSU	C4-C5	3.51	1.49	1.41
56	1y	46	7MG	C5-N7	-3.51	1.33	1.39
56	2y	39	PSU	C4-C5	3.47	1.48	1.41
32	1a	966	M2G	C2-N2	3.46	1.40	1.34
56	2y	55	PSU	C5-C1'	-3.45	1.49	1.52
55	2x	54	5MU	C4-C5	3.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	54	5MU	C4-C5	3.44	1.48	1.41
32	1a	527	7MG	C5-N7	-3.43	1.33	1.39
54	1w	55	PSU	C4-C5	3.43	1.48	1.41
32	2a	966	M2G	C2-N2	3.41	1.40	1.34
55	1x	8	4SU	C4-S4	-3.40	1.61	1.67
1	2A	1911	PSU	C4-C5	3.39	1.48	1.41
54	1w	46	7MG	C5-N7	-3.39	1.34	1.39
32	2a	516	PSU	C5-C1'	-3.38	1.49	1.52
1	2A	1917	PSU	C4-C5	3.38	1.48	1.41
1	2A	1915	5MU	C4-C5	3.38	1.48	1.41
55	1x	55	PSU	C4-C5	3.38	1.48	1.41
54	2w	55	PSU	C4-C5	3.37	1.48	1.41
55	1x	8	4SU	C2-N3	-3.36	1.31	1.38
56	1y	32	PSU	C4-C5	3.35	1.48	1.41
1	2A	2605	PSU	C4-C5	3.33	1.48	1.41
54	1w	39	PSU	C4-C5	3.29	1.48	1.41
54	2w	54	5MU	C4-C5	3.25	1.48	1.41
1	1A	1911	PSU	C4-C5	3.23	1.48	1.41
1	1A	1939	5MU	C4-C5	3.21	1.48	1.41
54	1w	54	5MU	C4-C5	3.20	1.48	1.41
1	2A	1939	5MU	C4-C5	3.19	1.48	1.41
55	2x	8	4SU	C2-N3	-3.18	1.31	1.38
56	1y	55	PSU	C4-C5	3.15	1.48	1.41
55	1x	54	5MU	C4-C5	3.14	1.48	1.41
1	1A	1917	PSU	C4-C5	3.13	1.48	1.41
1	1A	1915	5MU	C4-C5	3.11	1.48	1.41
54	1w	32	PSU	C5-C1'	-3.10	1.49	1.52
32	2a	527	7MG	C5-N7	-3.09	1.34	1.39
56	2y	54	5MU	C4-C5	3.03	1.48	1.41
56	2y	32	PSU	C5-C1'	-3.01	1.49	1.52
32	1a	516	PSU	C4-C5	2.95	1.47	1.41
56	1y	55	PSU	C5-C1'	-2.94	1.49	1.52
55	1x	76	31H	C5-C4	-2.92	1.33	1.40
1	1A	2605	PSU	C4-C5	2.90	1.47	1.41
54	2w	46	7MG	C5-N7	-2.87	1.34	1.39
55	2x	76	31H	C5-C4	-2.84	1.33	1.40
54	2w	37	MIA	C5-C4	2.69	1.48	1.40
1	2A	2605	PSU	C5-C1'	-2.63	1.50	1.52
55	2x	76	31H	C6-C5	-2.63	1.33	1.43
56	1y	37	MIA	C5-C4	2.62	1.47	1.40
54	2w	46	7MG	C4-N9	-2.62	1.33	1.38
32	2a	966	M2G	C5-C4	2.60	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C5-C4	2.58	1.47	1.40
55	1x	76	31H	C6-C5	-2.57	1.33	1.43
56	2y	37	MIA	C5-C4	2.55	1.47	1.40
32	2a	527	7MG	C4-N9	-2.54	1.33	1.38
56	1y	37	MIA	C2-N3	2.53	1.36	1.32
32	1a	527	7MG	C4-N9	-2.51	1.33	1.38
54	1w	46	7MG	C4-N9	-2.49	1.33	1.38
32	1a	966	M2G	C5-C4	2.48	1.47	1.40
32	1a	516	PSU	O4'-C1'	-2.48	1.40	1.44
56	2y	37	MIA	C2-N3	2.48	1.36	1.32
1	1A	1939	5MU	C2-N3	-2.47	1.33	1.38
1	1A	2605	PSU	C2-N3	-2.43	1.33	1.38
32	1a	1207	2MG	C5-C4	2.42	1.47	1.40
1	2A	2605	PSU	C2-N3	-2.39	1.33	1.38
1	1A	2251	OMG	C5-C4	2.38	1.47	1.40
54	1w	37	MIA	C5-C4	2.37	1.47	1.40
55	1x	54	5MU	C2-N3	-2.26	1.33	1.38
32	1a	1498	UR3	C4-N3	2.26	1.41	1.38
32	2a	1498	UR3	C4-N3	2.26	1.41	1.38
1	2A	2503	2MA	C5-C4	2.23	1.46	1.40
1	1A	2503	2MA	C5-C4	2.20	1.46	1.40
1	1A	2552	OMU	C2-N3	-2.20	1.33	1.38
1	1A	2605	PSU	O4'-C1'	-2.16	1.41	1.44
1	1A	1917	PSU	O4'-C1'	-2.15	1.41	1.44
56	2y	55	PSU	C2-N1	-2.15	1.33	1.38
56	1y	39	PSU	C5-C1'	-2.14	1.50	1.52
1	2A	1939	5MU	C2-N3	-2.13	1.33	1.38
55	2x	76	31H	C5-N7	-2.10	1.32	1.39
55	1x	76	31H	C3'-N3'	2.09	1.49	1.45
1	1A	1911	PSU	C2-N3	-2.09	1.34	1.38
56	2y	46	7MG	C4-N3	2.08	1.36	1.34
1	2A	1917	PSU	O4'-C1'	-2.08	1.41	1.44
54	2w	54	5MU	C2-N3	-2.06	1.34	1.38
1	1A	1911	PSU	O4'-C1'	-2.06	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.05	1.41	1.44
1	2A	2251	OMG	C5-C4	2.01	1.46	1.40

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	46	7MG	N3-C4-N9	10.16	139.96	126.91
1	1A	1917	PSU	N1-C2-N3	-9.19	121.12	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	N3-C4-N9	9.18	138.71	126.91
56	1y	32	PSU	N1-C2-N3	-9.09	121.21	128.43
56	1y	46	7MG	N3-C4-N9	9.08	138.58	126.91
54	2w	32	PSU	N1-C2-N3	-9.06	121.22	128.43
55	1x	8	4SU	C2-N3-C4	8.91	128.06	115.15
54	1w	46	7MG	N3-C4-N9	8.89	138.33	126.91
54	2w	54	5MU	C4-N3-C2	8.81	122.58	115.14
56	2y	39	PSU	N1-C2-N3	-8.76	121.47	128.43
1	2A	2605	PSU	N1-C2-N3	-8.71	121.50	128.43
32	2a	516	PSU	N1-C2-N3	-8.71	121.50	128.43
32	2a	527	7MG	N3-C4-N9	8.71	138.09	126.91
54	1w	32	PSU	N1-C2-N3	-8.60	121.59	128.43
55	1x	55	PSU	N1-C2-N3	-8.55	121.63	128.43
54	1w	55	PSU	N1-C2-N3	-8.55	121.63	128.43
56	2y	32	PSU	N1-C2-N3	-8.50	121.67	128.43
54	2w	55	PSU	N1-C2-N3	-8.49	121.68	128.43
56	1y	55	PSU	N1-C2-N3	-8.44	121.72	128.43
1	2A	1911	PSU	N1-C2-N3	-8.40	121.75	128.43
54	2w	46	7MG	N3-C4-N9	8.35	137.63	126.91
55	2x	55	PSU	N1-C2-N3	-8.30	121.83	128.43
55	2x	8	4SU	C2-N3-C4	8.28	127.15	115.15
1	1A	1911	PSU	N1-C2-N3	-8.27	121.86	128.43
54	1w	37	MIA	C12-C13-C14	-8.23	111.13	127.14
56	2y	55	PSU	N1-C2-N3	-8.19	121.92	128.43
56	1y	39	PSU	N1-C2-N3	-8.11	121.98	128.43
1	1A	2605	PSU	N1-C2-N3	-8.06	122.02	128.43
54	1w	55	PSU	C4-N3-C2	8.04	121.93	115.14
32	1a	516	PSU	N1-C2-N3	-7.99	122.08	128.43
1	2A	1917	PSU	N1-C2-N3	-7.94	122.12	128.43
55	1x	54	5MU	C4-N3-C2	7.93	121.84	115.14
56	2y	54	5MU	C4-N3-C2	7.73	121.67	115.14
54	2w	39	PSU	N1-C2-N3	-7.57	122.41	128.43
56	1y	55	PSU	C4-N3-C2	7.52	121.50	115.14
56	2y	39	PSU	C4-N3-C2	7.51	121.49	115.14
54	1w	39	PSU	N1-C2-N3	-7.41	122.54	128.43
56	1y	32	PSU	C4-N3-C2	7.36	121.36	115.14
56	1y	54	5MU	C4-N3-C2	7.34	121.34	115.14
56	2y	55	PSU	C4-N3-C2	7.34	121.34	115.14
55	1x	55	PSU	C4-N3-C2	7.13	121.16	115.14
1	1A	1917	PSU	C4-N3-C2	7.12	121.15	115.14
54	2w	55	PSU	C4-N3-C2	7.11	121.14	115.14
1	1A	1911	PSU	C4-N3-C2	7.04	121.09	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	32	PSU	C4-N3-C2	7.00	121.05	115.14
54	1w	32	PSU	C4-N3-C2	6.94	121.00	115.14
32	2a	516	PSU	C4-N3-C2	6.80	120.88	115.14
55	2x	54	5MU	C4-N3-C2	6.77	120.86	115.14
56	2y	32	PSU	C4-N3-C2	6.76	120.85	115.14
1	1A	2503	2MA	C2-N3-C4	6.66	120.93	115.52
54	1w	54	5MU	C4-N3-C2	6.63	120.74	115.14
1	2A	1917	PSU	C4-N3-C2	6.62	120.73	115.14
56	1y	39	PSU	C4-N3-C2	6.60	120.71	115.14
1	2A	1915	5MU	C4-N3-C2	6.57	120.69	115.14
1	2A	2503	2MA	C2-N3-C4	6.57	120.86	115.52
32	1a	516	PSU	C4-N3-C2	6.53	120.66	115.14
1	2A	1911	PSU	C4-N3-C2	6.50	120.63	115.14
55	2x	55	PSU	C4-N3-C2	6.46	120.60	115.14
1	1A	1915	5MU	C4-N3-C2	6.44	120.58	115.14
54	1w	55	PSU	C5-C4-N3	-6.38	117.14	125.36
1	2A	2605	PSU	C4-N3-C2	6.13	120.32	115.14
56	2y	55	PSU	C5-C4-N3	-5.93	117.72	125.36
1	1A	2605	PSU	C4-N3-C2	5.87	120.09	115.14
1	1A	2058	MA6	N3-C2-N1	-5.86	119.53	128.68
55	1x	55	PSU	C5-C4-N3	-5.81	117.87	125.36
54	2w	55	PSU	C5-C1'-C2'	-5.76	105.05	115.32
32	2a	527	7MG	N7-C8-N9	-5.69	95.24	103.38
56	2y	39	PSU	C5-C4-N3	-5.68	118.04	125.36
55	1x	76	31H	N3-C2-N1	-5.67	119.82	128.68
54	2w	46	7MG	N7-C8-N9	-5.66	95.28	103.38
55	2x	76	31H	N3-C2-N1	-5.64	119.86	128.68
54	2w	55	PSU	C5-C4-N3	-5.63	118.11	125.36
56	1y	55	PSU	C5-C4-N3	-5.62	118.12	125.36
54	1w	46	7MG	N7-C8-N9	-5.55	95.44	103.38
32	1a	527	7MG	N7-C8-N9	-5.48	95.55	103.38
56	2y	46	7MG	C5-C4-N3	-5.47	117.57	126.49
1	1A	1911	PSU	C5-C4-N3	-5.41	118.39	125.36
1	1A	1939	5MU	C4-N3-C2	5.38	119.69	115.14
1	2A	1917	PSU	C5-C4-N3	-5.37	118.44	125.36
56	2y	46	7MG	C6-N1-C2	5.37	124.46	115.93
56	1y	32	PSU	C5-C4-N3	-5.35	118.46	125.36
55	2x	55	PSU	C5-C4-N3	-5.35	118.47	125.36
32	2a	966	M2G	C6-N1-C2	5.34	122.54	116.18
54	2w	39	PSU	C4-N3-C2	5.34	119.65	115.14
32	1a	516	PSU	C5-C4-N3	-5.34	118.49	125.36
32	1a	966	M2G	C6-N1-C2	5.32	122.52	116.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	C5-C4-N3	-5.30	118.53	125.36
56	1y	46	7MG	C5-C4-N3	-5.28	117.86	126.49
1	2A	1939	5MU	C4-N3-C2	5.28	119.60	115.14
32	1a	1519	MA6	N3-C2-N1	-5.25	120.47	128.68
54	1w	8	4SU	C2-N3-C4	5.25	122.75	115.15
32	1a	1518	MA6	N3-C2-N1	-5.24	120.49	128.68
1	2A	2058	MA6	N3-C2-N1	-5.22	120.52	128.68
56	2y	32	PSU	C5-C4-N3	-5.20	118.66	125.36
54	2w	32	PSU	C5-C4-N3	-5.19	118.67	125.36
54	1w	32	PSU	C5-C4-N3	-5.17	118.70	125.36
32	2a	516	PSU	C5-C4-N3	-5.17	118.71	125.36
32	2a	1518	MA6	N3-C2-N1	-5.13	120.66	128.68
56	1y	39	PSU	C5-C4-N3	-5.13	118.75	125.36
56	2y	39	PSU	C5-C1'-C2'	-5.12	106.19	115.32
1	2A	1911	PSU	C5-C4-N3	-5.11	118.78	125.36
32	1a	1207	2MG	C6-N1-C2	5.10	124.32	115.18
54	2w	39	PSU	C5-C4-N3	-5.09	118.81	125.36
32	1a	527	7MG	C5-C4-N3	-5.08	118.19	126.49
54	1w	46	7MG	C6-N1-C2	5.05	123.96	115.93
56	2y	46	7MG	N7-C8-N9	-5.04	96.17	103.38
54	1w	39	PSU	C4-N3-C2	5.03	119.39	115.14
54	1w	39	PSU	C5-C4-N3	-5.02	118.90	125.36
32	1a	966	M2G	C2-N3-C4	5.01	120.96	115.28
32	1a	966	M2G	C6-C5-C4	-4.95	116.07	120.80
32	2a	1519	MA6	N3-C2-N1	-4.94	120.95	128.68
56	1y	46	7MG	N7-C8-N9	-4.93	96.33	103.38
54	2w	46	7MG	C5-C4-N3	-4.91	118.47	126.49
32	2a	966	M2G	C2-N3-C4	4.84	120.78	115.28
55	1x	8	4SU	C5-C4-N3	-4.84	117.36	123.83
56	1y	46	7MG	C6-N1-C2	4.77	123.51	115.93
32	1a	1207	2MG	C2-N3-C4	4.76	120.68	115.28
1	2A	2251	OMG	C2-N3-C4	4.75	120.78	115.36
56	2y	8	4SU	C2-N3-C4	4.69	121.95	115.15
54	1w	39	PSU	C5-C6-N1	-4.68	118.68	124.44
1	1A	2251	OMG	C2-N3-C4	4.68	120.70	115.36
1	1A	2605	PSU	C5-C6-N1	-4.67	118.70	124.44
56	2y	46	7MG	C6-C5-C4	4.67	120.21	115.20
54	1w	37	MIA	C15-C14-C13	-4.65	109.20	122.65
32	2a	527	7MG	C5-C4-N3	-4.64	118.91	126.49
1	2A	1920	4OC	C2-N3-C4	4.61	121.01	116.34
54	2w	37	MIA	C2-N3-C4	4.61	121.67	115.32
32	1a	1207	2MG	C5-C6-N1	-4.57	117.18	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	C5-C6-N1	-4.53	118.87	124.44
1	1A	1920	4OC	C2-N3-C4	4.53	120.93	116.34
32	2a	1207	2MG	C5-C6-N1	-4.53	117.24	123.43
32	1a	516	PSU	C5-C6-N1	-4.52	118.89	124.44
56	1y	46	7MG	C6-C5-C4	4.51	120.04	115.20
1	1A	2605	PSU	C5-C4-N3	-4.49	119.58	125.36
1	1A	2251	OMG	C6-N1-C2	4.49	123.06	115.93
32	2a	527	7MG	C6-N1-C2	4.48	123.04	115.93
54	1w	46	7MG	C5-C4-N3	-4.47	119.19	126.49
54	1w	37	MIA	C2-N3-C4	4.46	121.47	115.32
1	2A	2251	OMG	C6-C5-C4	-4.44	116.56	120.80
32	2a	1402	4OC	CM4-N4-C4	-4.44	119.16	122.97
1	2A	2605	PSU	C5-C1'-C2'	-4.43	107.42	115.32
32	1a	1207	2MG	C6-C5-C4	-4.42	116.58	120.80
54	2w	39	PSU	C5-C6-N1	-4.42	119.00	124.44
1	2A	2605	PSU	C6-N1-C2	4.41	122.64	115.36
1	1A	1917	PSU	C6-N1-C2	4.37	122.56	115.36
1	2A	2503	2MA	C5-C6-N1	-4.32	118.53	123.06
54	2w	32	PSU	C6-N1-C2	4.32	122.48	115.36
56	1y	8	4SU	C2-N3-C4	4.29	121.38	115.15
1	1A	1962	5MC	C2-N3-C4	4.23	121.13	116.02
1	1A	2605	PSU	C6-N1-C2	4.23	122.34	115.36
1	1A	1917	PSU	C5-C6-N1	-4.23	119.24	124.44
55	2x	55	PSU	C6-N1-C2	4.23	122.34	115.36
54	1w	39	PSU	C6-N1-C2	4.23	122.33	115.36
1	2A	2251	OMG	C6-N1-C2	4.22	122.63	115.93
32	2a	516	PSU	C6-N1-C2	4.22	122.31	115.36
1	2A	2605	PSU	C5-C4-N3	-4.19	119.96	125.36
54	2w	39	PSU	C6-N1-C2	4.18	122.25	115.36
32	2a	966	M2G	C5-C6-N1	-4.18	117.72	123.43
54	1w	39	PSU	C5-C1'-C2'	-4.18	107.87	115.32
1	2A	1911	PSU	C6-N1-C2	4.18	122.25	115.36
1	2A	2605	PSU	C5-C6-N1	-4.16	119.33	124.44
1	1A	1911	PSU	C5-C6-N1	-4.16	119.33	124.44
32	1a	1404	5MC	C2-N3-C4	4.16	121.03	116.02
1	1A	1942	5MC	C2-N3-C4	4.15	121.03	116.02
54	1w	55	PSU	C5-C1'-C2'	-4.13	107.95	115.32
56	2y	39	PSU	C5-C6-N1	-4.11	119.39	124.44
1	2A	1911	PSU	C5-C6-N1	-4.11	119.39	124.44
32	2a	1207	2MG	C2-N3-C4	4.11	119.94	115.28
32	1a	1407	5MC	C2-N3-C4	4.09	120.95	116.02
1	2A	1917	PSU	C5-C6-N1	-4.07	119.44	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	32	PSU	C6-N1-C2	4.05	122.04	115.36
56	1y	32	PSU	C6-N1-C2	4.04	122.03	115.36
54	1w	32	PSU	C6-N1-C2	4.04	122.02	115.36
32	1a	527	7MG	C6-N1-C2	4.00	122.28	115.93
54	2w	55	PSU	C6-N1-C2	3.99	121.94	115.36
56	2y	39	PSU	C6-N1-C2	3.99	121.93	115.36
55	2x	8	4SU	C5-C4-N3	-3.98	118.50	123.83
1	1A	2251	OMG	C5-C6-N1	-3.98	117.99	123.43
1	1A	1911	PSU	C6-N1-C2	3.97	121.91	115.36
56	1y	39	PSU	C6-N1-C2	3.97	121.90	115.36
54	1w	37	MIA	C16-C14-C13	-3.96	111.19	122.65
32	2a	516	PSU	C5-C6-N1	-3.95	119.59	124.44
32	1a	516	PSU	C6-N1-C2	3.95	121.87	115.36
32	1a	1400	5MC	C2-N3-C4	3.94	120.78	116.02
32	1a	1207	2MG	N2-C2-N3	3.94	120.74	116.96
55	1x	55	PSU	C6-N1-C2	3.93	121.85	115.36
54	2w	32	PSU	C5-C6-N1	-3.93	119.61	124.44
1	1A	2251	OMG	C6-C5-C4	-3.90	117.07	120.80
56	1y	46	7MG	C5-C6-N1	-3.89	115.14	123.14
32	2a	1407	5MC	C2-N3-C4	3.89	120.72	116.02
1	1A	2503	2MA	C5-C6-N1	-3.88	118.99	123.06
54	2w	8	4SU	C2-N3-C4	3.88	120.77	115.15
32	1a	527	7MG	C6-C5-C4	3.86	119.35	115.20
32	1a	967	5MC	C2-N3-C4	3.86	120.68	116.02
1	2A	1917	PSU	C6-N1-C2	3.85	121.71	115.36
56	2y	46	7MG	C5-C6-N1	-3.85	115.24	123.14
1	1A	2251	OMG	N3-C2-N1	-3.84	122.11	127.22
54	2w	55	PSU	C5-C6-N1	-3.83	119.73	124.44
55	1x	55	PSU	C5-C6-N1	-3.83	119.73	124.44
54	1w	46	7MG	C5-C6-N1	-3.83	115.27	123.14
32	2a	1207	2MG	C6-N1-C2	3.82	122.02	115.18
32	2a	967	5MC	C2-N3-C4	3.80	120.60	116.02
1	2A	2251	OMG	C5-C6-N1	-3.79	118.25	123.43
54	1w	46	7MG	C6-C5-C4	3.76	119.23	115.20
56	2y	37	MIA	N3-C2-N1	-3.76	122.80	128.68
1	2A	2251	OMG	N3-C2-N1	-3.74	122.23	127.22
56	1y	32	PSU	C5-C6-N1	-3.73	119.86	124.44
1	2A	1942	5MC	C2-N3-C4	3.72	120.51	116.02
32	1a	966	M2G	C5-C6-N1	-3.72	118.35	123.43
56	1y	39	PSU	C5-C6-N1	-3.64	119.97	124.44
54	2w	37	MIA	C5-C6-N1	-3.63	117.80	120.81
56	2y	32	PSU	C5-C6-N1	-3.62	120.00	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	C5-C6-N1	-3.61	118.31	122.19
55	2x	32	5MC	C2-N3-C4	3.60	120.36	116.02
1	2A	1962	5MC	C2-N3-C4	3.60	120.36	116.02
54	2w	46	7MG	C6-N1-C2	3.60	121.65	115.93
32	1a	1519	MA6	C4-C5-N7	-3.52	105.73	109.40
32	2a	1207	2MG	C6-C5-C4	-3.52	117.44	120.80
54	2w	46	7MG	C6-C5-C4	3.50	118.95	115.20
54	1w	32	PSU	C5-C6-N1	-3.48	120.16	124.44
1	2A	1962	5MC	N4-C4-N3	3.48	121.95	117.03
55	1x	32	5MC	C2-N3-C4	3.44	120.17	116.02
1	2A	1911	PSU	C5-C1'-C2'	-3.44	109.19	115.32
43	1l	92	0TD	CSB-SB-CB	3.43	108.61	101.85
32	2a	527	7MG	C5-C6-N1	-3.43	116.10	123.14
54	1w	37	MIA	C12-N6-C6	-3.42	117.48	122.55
54	1w	55	PSU	C6-N1-C2	3.41	120.99	115.36
56	2y	8	4SU	C5-C4-N3	-3.41	119.27	123.83
54	1w	8	4SU	C5-C4-N3	-3.39	119.29	123.83
56	1y	55	PSU	C6-N1-C2	3.38	120.93	115.36
55	1x	76	31H	CA-N-CN	-3.36	117.65	122.82
56	2y	55	PSU	C6-N1-C2	3.34	120.87	115.36
32	2a	966	M2G	C6-C5-C4	-3.33	117.61	120.80
32	2a	1207	2MG	C4-C5-N7	-3.32	105.94	109.40
56	1y	8	4SU	C5-C4-N3	-3.31	119.40	123.83
1	2A	1939	5MU	C5-C6-N1	-3.30	118.64	122.19
32	2a	1404	5MC	C2-N3-C4	3.29	119.99	116.02
32	2a	527	7MG	C6-C5-C4	3.29	118.73	115.20
32	1a	527	7MG	C5-C6-N1	-3.29	116.39	123.14
32	1a	1207	2MG	C4-C5-N7	-3.27	106.00	109.40
32	2a	1400	5MC	C2-N3-C4	3.26	119.95	116.02
54	2w	46	7MG	C5-C6-N1	-3.26	116.44	123.14
56	1y	37	MIA	N3-C2-N1	-3.26	123.58	128.68
1	1A	2605	PSU	C5-C1'-C2'	-3.20	109.61	115.32
55	1x	55	PSU	C5-C1'-C2'	-3.19	109.62	115.32
32	1a	1519	MA6	C1'-N9-C4	-3.16	121.08	126.64
32	2a	1519	MA6	C4-C5-N7	-3.14	106.13	109.40
54	1w	37	MIA	C5-C6-N1	-3.12	118.22	120.81
32	1a	1402	4OC	CM4-N4-C4	-3.11	120.30	122.97
56	1y	55	PSU	C5-C1'-C2'	-3.06	109.86	115.32
32	2a	1404	5MC	C5-C6-N1	-2.99	118.97	122.19
56	1y	32	PSU	C5-C1'-C2'	-2.98	110.00	115.32
54	1w	32	PSU	C5-C1'-C2'	-2.98	110.00	115.32
32	2a	966	M2G	N3-C2-N2	2.92	120.14	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	8	4SU	C5-C4-N3	-2.91	119.93	123.83
56	2y	46	7MG	C5-C4-N9	-2.86	102.44	106.44
43	2l	92	0TD	CSB-SB-CB	-2.85	96.25	101.85
54	1w	37	MIA	C2-N1-C6	2.85	122.28	117.19
54	1w	46	7MG	C5-C4-N9	-2.84	102.47	106.44
32	1a	1404	5MC	N4-C4-N3	2.83	121.04	117.03
32	2a	1400	5MC	C5-C6-N1	-2.81	119.16	122.19
54	2w	46	7MG	C8-N7-C5	2.80	116.22	108.94
55	1x	32	5MC	C5-C6-N1	-2.79	119.19	122.19
32	2a	527	7MG	C8-N7-C5	2.79	116.18	108.94
1	2A	1917	PSU	C5-C1'-C2'	-2.75	110.42	115.32
32	1a	1518	MA6	C4-C5-N7	-2.74	106.54	109.40
54	1w	55	PSU	C5-C6-N1	-2.74	121.07	124.44
56	1y	37	MIA	C4-C5-N7	-2.73	106.55	109.40
32	1a	527	7MG	C8-N7-C5	2.73	116.04	108.94
1	2A	2503	2MA	C4-C5-N7	-2.72	106.56	109.40
32	2a	1407	5MC	N4-C4-N3	2.71	120.86	117.03
32	1a	1207	2MG	N3-C2-N1	-2.70	121.96	126.23
1	1A	1942	5MC	N4-C4-N3	2.70	120.85	117.03
54	2w	32	PSU	C5-C1'-C2'	-2.67	110.56	115.32
54	1w	37	MIA	C4-C5-N7	-2.66	106.62	109.40
54	1w	37	MIA	N3-C2-N1	-2.66	122.09	126.98
55	2x	32	5MC	N4-C4-N3	2.65	120.78	117.03
56	2y	46	7MG	C8-N7-C5	2.65	115.83	108.94
56	1y	46	7MG	C8-N7-C5	2.64	115.81	108.94
32	1a	1407	5MC	N4-C4-N3	2.64	120.77	117.03
32	1a	1207	2MG	CM2-N2-C2	-2.64	120.41	123.59
55	2x	55	PSU	C5-C1'-C2'	-2.63	110.63	115.32
1	2A	1942	5MC	N4-C4-N3	2.62	120.73	117.03
56	2y	37	MIA	C4-C5-N7	-2.61	106.68	109.40
56	1y	55	PSU	C5-C6-N1	-2.61	121.23	124.44
55	2x	32	5MC	C5-C6-N1	-2.60	119.39	122.19
32	1a	1400	5MC	N4-C4-N3	2.59	120.70	117.03
1	1A	1917	PSU	C5-C1'-C2'	-2.59	110.70	115.32
32	2a	1207	2MG	CM2-N2-C2	-2.59	120.47	123.59
54	1w	46	7MG	C8-N7-C5	2.58	115.66	108.94
54	2w	37	MIA	C2-N1-C6	2.57	121.80	117.19
32	2a	1498	UR3	C3U-N3-C4	2.57	121.53	118.12
32	2a	966	M2G	C4-C5-N7	-2.56	106.73	109.40
1	1A	1911	PSU	C5-C1'-C2'	-2.54	110.78	115.32
32	2a	1518	MA6	C4-C5-N7	-2.54	106.75	109.40
54	2w	37	MIA	C12-N6-C6	-2.53	120.69	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	37	MIA	C4-C5-N7	-2.52	106.77	109.40
32	2a	1400	5MC	N4-C4-N3	2.49	120.55	117.03
1	1A	2058	MA6	C10-N6-C6	-2.48	112.00	119.51
54	2w	55	PSU	O4'-C1'-C5	2.48	113.77	109.93
32	2a	1404	5MC	N4-C4-N3	2.48	120.54	117.03
32	2a	527	7MG	C5-C4-N9	-2.47	102.98	106.44
1	2A	2251	OMG	C4-C5-N7	-2.47	106.83	109.40
55	1x	76	31H	OCN-CN-N	-2.45	118.81	125.27
1	2A	2058	MA6	C10-N6-C6	-2.42	112.17	119.51
32	1a	967	5MC	N4-C4-N3	2.41	120.44	117.03
1	1A	1920	4OC	N4-C4-N3	2.41	120.29	116.49
32	1a	516	PSU	O4'-C1'-C2'	2.41	108.56	104.66
54	2w	37	MIA	N6-C6-N1	2.39	121.49	118.50
32	1a	527	7MG	C5-C4-N9	-2.39	103.09	106.44
32	1a	966	M2G	C4-C5-N7	-2.38	106.92	109.40
54	2w	39	PSU	C5-C1'-C2'	-2.35	111.12	115.32
56	2y	55	PSU	C5-C6-N1	-2.32	121.59	124.44
1	2A	2503	2MA	C1'-N9-C4	-2.31	122.59	126.64
54	2w	46	7MG	C2-N3-C4	2.31	120.26	113.89
1	2A	2251	OMG	CM2-O2'-C2'	-2.29	108.52	114.52
1	2A	2058	MA6	C9-N6-C6	2.28	126.40	119.51
54	2w	37	MIA	N3-C2-N1	-2.27	122.80	126.98
1	1A	2058	MA6	C9-N6-C6	2.27	126.38	119.51
1	2A	1962	5MC	C5-C6-N1	-2.25	119.77	122.19
55	2x	76	31H	OCN-CN-N	-2.24	119.37	125.27
1	2A	2552	OMU	C5-C4-N3	-2.24	118.39	123.31
32	1a	1400	5MC	C5-C6-N1	-2.23	119.79	122.19
1	2A	1915	5MU	C5-C6-N1	-2.23	119.79	122.19
1	2A	1920	4OC	N4-C4-N3	2.21	119.99	116.49
32	2a	967	5MC	C5-C6-N1	-2.21	119.81	122.19
56	1y	46	7MG	C2-N3-C4	2.18	119.93	113.89
32	1a	527	7MG	C2-N3-C4	2.17	119.90	113.89
56	2y	46	7MG	C2-N3-C4	2.16	119.86	113.89
54	1w	37	MIA	C16-C14-C15	-2.16	109.84	114.60
1	2A	1962	5MC	CM5-C5-C4	-2.15	119.55	121.72
55	1x	32	5MC	N4-C4-N3	2.14	120.06	117.03
1	2A	1942	5MC	C5-C6-N1	-2.14	119.89	122.19
56	2y	8	4SU	C6-N1-C2	-2.13	117.81	121.20
54	1w	37	MIA	C11-S10-C2	-2.11	100.69	102.27
32	2a	527	7MG	C2-N3-C4	2.11	119.71	113.89
1	1A	2251	OMG	C4-C5-N7	-2.10	107.21	109.40
55	2x	76	31H	O4'-C1'-C2'	-2.10	103.86	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C5-C6-N1	-2.10	119.93	122.19
32	2a	967	5MC	N4-C4-N3	2.10	120.00	117.03
32	2a	527	7MG	CM7-N7-C5	2.10	132.06	124.01
32	2a	516	PSU	O4'-C1'-C2'	2.09	108.05	104.66
56	2y	46	7MG	O4'-C1'-N9	-2.08	106.54	109.35
56	2y	46	7MG	N2-C2-N3	2.07	120.47	117.25
1	2A	1917	PSU	O4'-C1'-C2'	2.07	108.01	104.66
32	1a	527	7MG	CM7-N7-C5	2.06	131.94	124.01
56	1y	46	7MG	C5-C4-N9	-2.06	103.56	106.44
32	2a	1404	5MC	CM5-C5-C4	-2.04	119.65	121.72
1	1A	1915	5MU	C5-C6-N1	-2.03	120.00	122.19
1	1A	1917	PSU	O4'-C1'-C2'	2.02	107.94	104.66
54	2w	46	7MG	N2-C2-N1	2.02	120.39	117.25
1	2A	2552	OMU	O5'-C5'-C4'	-2.00	102.18	108.99

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	8	4SU	C2'-C1'-N1-C6
56	1y	46	7MG	C4'-C5'-O5'-P
43	2l	92	0TD	CG-CB-SB-CSB
56	2y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C6
1	1A	1920	4OC	C2'-C1'-N1-C6
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	2a	1402	4OC	O4'-C1'-N1-C6
32	2a	1402	4OC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	8	4SU	O4'-C1'-N1-C6
54	2w	32	PSU	C3'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2w	46	7MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	1x	76	31H	CB-CA-N-CN
55	1x	76	31H	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
56	1y	8	4SU	O4'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
55	1x	76	31H	N-CA-CB-CG
1	2A	1917	PSU	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C6
32	2a	1404	5MC	O4'-C4'-C5'-O5'
55	1x	76	31H	CA-CB-CG-SD
55	1x	76	31H	C-CA-CB-CG
56	2y	46	7MG	C2'-C1'-N9-C8
56	2y	46	7MG	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
55	2x	76	31H	O-C-CA-N
1	1A	2503	2MA	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
55	2x	76	31H	N3'-C-CA-N
56	2y	46	7MG	O4'-C1'-N9-C4
55	2x	76	31H	C2'-C3'-N3'-C
32	2a	527	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
32	1a	1402	4OC	C3'-C2'-O2'-CM2
56	1y	55	PSU	O4'-C1'-C5-C4
55	1x	76	31H	O-C-CA-N
56	2y	46	7MG	C3'-C4'-C5'-O5'
55	1x	76	31H	N3'-C-CA-N
54	1w	32	PSU	C2'-C1'-C5-C6
54	2w	32	PSU	C2'-C1'-C5-C6
56	2y	46	7MG	C2'-C1'-N9-C4
56	2y	46	7MG	O4'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
32	1a	1207	2MG	N3-C2-N2-CM2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C4'-C5'-O5'-P
32	1a	967	5MC	O4'-C4'-C5'-O5'
56	1y	46	7MG	C2'-C1'-N9-C8

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 2765 ligands modelled in this entry, 2761 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	$\# Z > 2$
61	SF4	1d	501	35	0,12,12	-	-	-		
59	6IF	1A	4089	-	30,34,34	1.11	2 (6%)	32,49,49	1.93	6 (18%)
59	6IF	2A	3857	-	30,34,34	0.88	2 (6%)	32,49,49	1.59	5 (15%)
61	SF4	2d	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
61	SF4	1d	501	35	-	-	0/6/5/5
59	6IF	1A	4089	-	-	3/22/65/65	0/3/3/3
59	6IF	2A	3857	-	-	2/22/65/65	0/3/3/3
61	SF4	2d	302	35	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4089	6IF	CG-CB	-2.50	1.49	1.53
59	2A	3857	6IF	OAF-CAA	2.47	1.46	1.42
59	1A	4089	6IF	CAA-CAB	-2.35	1.49	1.53
59	2A	3857	6IF	OAV-CB	2.17	1.44	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	4089	6IF	CD1-CG-CB	-7.23	94.86	103.80
59	2A	3857	6IF	CBB-CBA-CAY	-5.02	111.74	116.03
59	1A	4089	6IF	OAF-CAA-SBE	4.10	120.13	110.14
59	2A	3857	6IF	CD2-CAY-CAX	-3.51	108.63	113.89
59	2A	3857	6IF	CAA-OAF-CAE	-3.11	109.91	114.12
59	1A	4089	6IF	CAA-CAB-CAC	2.96	116.43	110.59
59	2A	3857	6IF	CAK-CAI-CAG	-2.90	110.52	114.26
59	1A	4089	6IF	CAK-CAI-CAG	-2.86	110.57	114.26
59	2A	3857	6IF	CD1-CG-CB	-2.79	100.34	103.80
59	1A	4089	6IF	CD2-CG-CB	-2.71	108.58	113.98
59	1A	4089	6IF	C-CA-N	2.01	115.43	111.73

There are no chirality outliers.

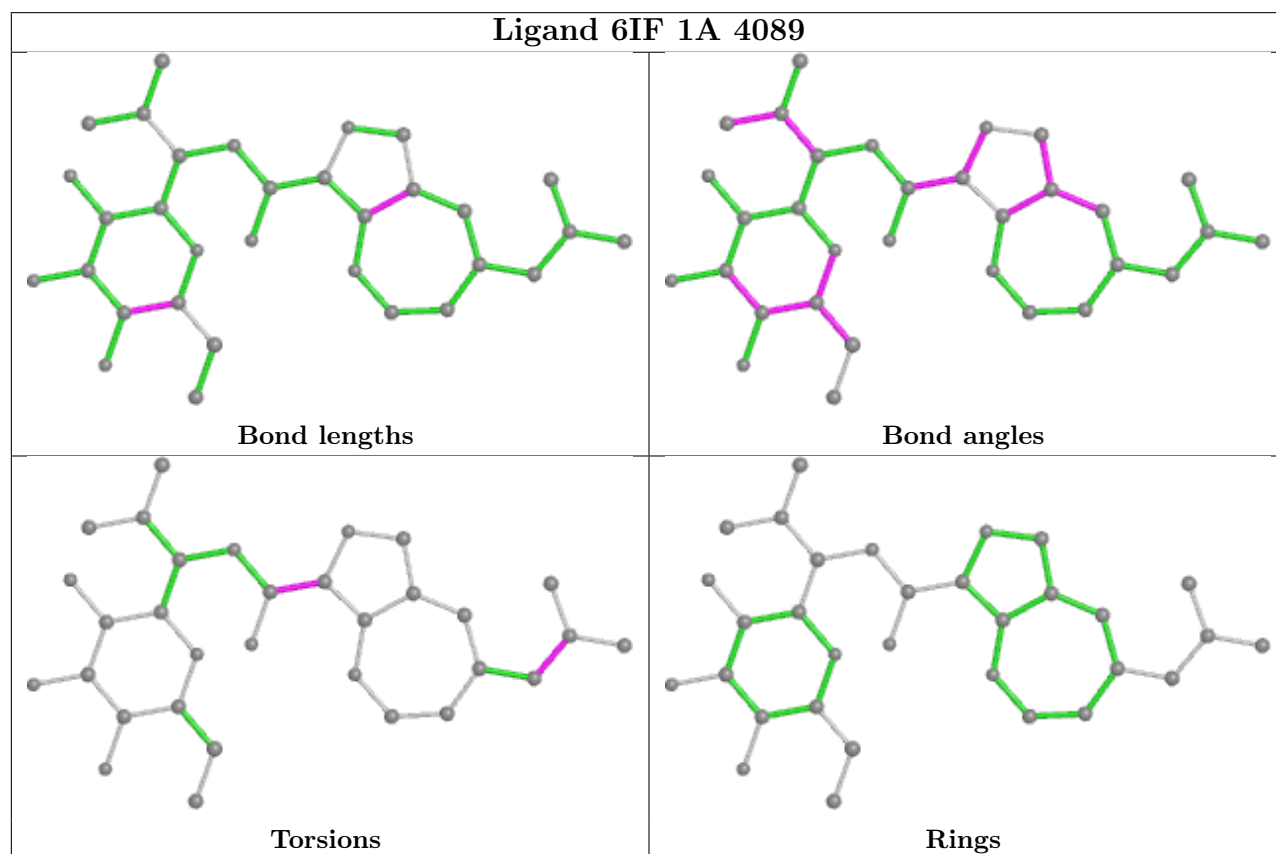
All (5) torsion outliers are listed below:

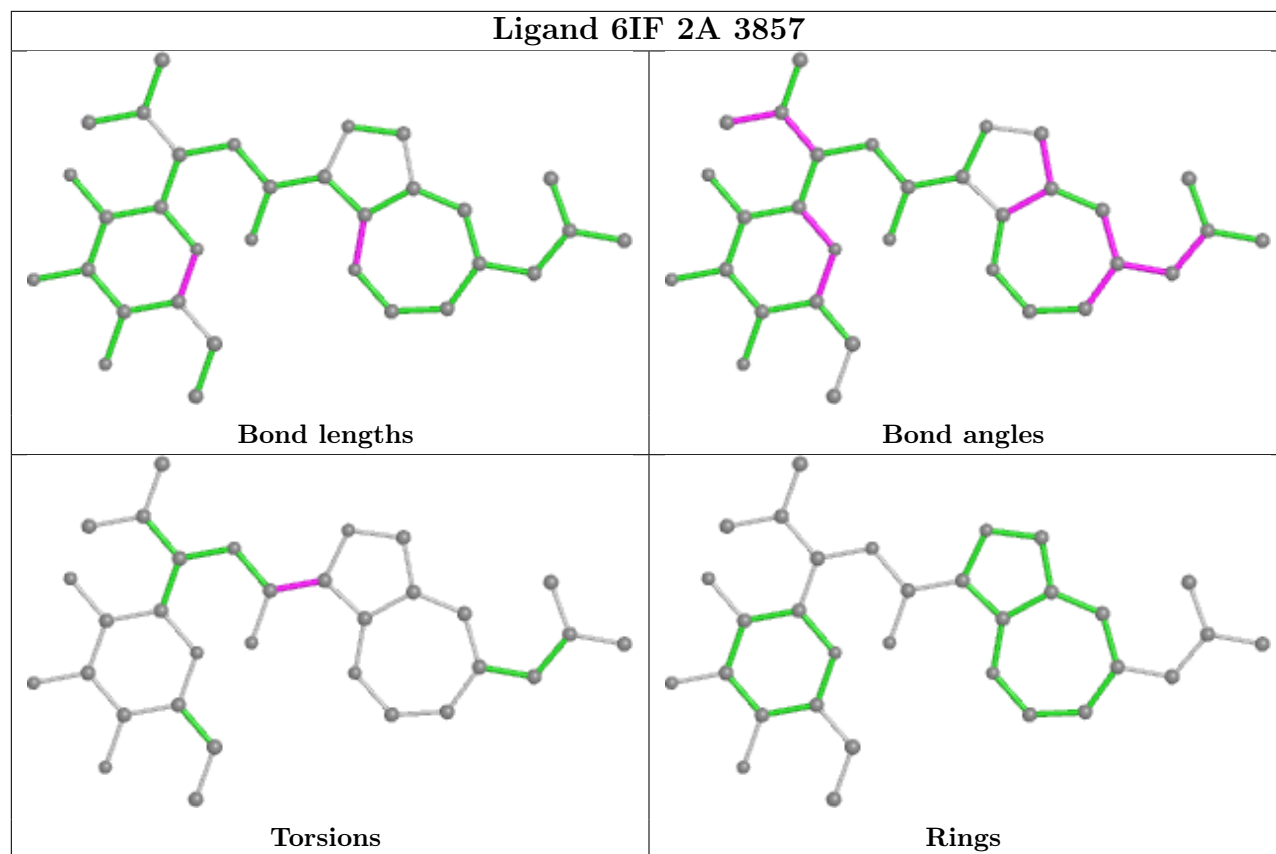
Mol	Chain	Res	Type	Atoms
59	1A	4089	6IF	O-C-CA-CB
59	1A	4089	6IF	NAH-C-CA-CB
59	2A	3857	6IF	O-C-CA-CB
59	2A	3857	6IF	NAH-C-CA-CB
59	1A	4089	6IF	CAY-CBA-CBB-CBC

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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, 95th 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	2859/2915 (98%)	0.38	72 (2%) 57 51	18, 36, 88, 101	0
1	2A	2788/2915 (95%)	0.23	65 (2%) 60 54	34, 57, 87, 98	0
2	1B	120/121 (99%)	0.10	0 100 100	29, 47, 62, 84	0
2	2B	120/121 (99%)	-0.17	1 (0%) 86 84	58, 73, 78, 84	0
3	1D	275/276 (99%)	0.44	2 (0%) 87 86	18, 39, 54, 61	0
3	2D	275/276 (99%)	0.53	4 (1%) 73 70	31, 52, 65, 81	0
4	1E	204/206 (99%)	0.42	1 (0%) 91 89	19, 40, 60, 71	0
4	2E	204/206 (99%)	0.58	14 (6%) 16 12	33, 58, 68, 74	0
5	1F	203/210 (96%)	0.23	0 100 100	19, 42, 60, 76	0
5	2F	203/210 (96%)	0.31	4 (1%) 65 60	36, 63, 72, 77	0
6	1G	181/182 (99%)	0.22	2 (1%) 80 78	39, 57, 69, 76	0
6	2G	181/182 (99%)	0.68	20 (11%) 5 3	64, 73, 78, 84	0
7	1H	174/180 (96%)	0.16	1 (0%) 89 88	37, 52, 64, 68	0
7	2H	174/180 (96%)	2.06	82 (47%) 0 0	62, 77, 85, 89	0
8	1I	146/148 (98%)	-0.06	0 100 100	44, 68, 74, 78	0
8	2I	146/148 (98%)	0.33	5 (3%) 45 38	54, 70, 79, 82	0
9	1N	140/140 (100%)	0.49	1 (0%) 87 86	23, 39, 61, 70	0
9	2N	140/140 (100%)	0.77	10 (7%) 16 11	45, 62, 73, 83	0
10	1O	122/122 (100%)	0.30	0 100 100	28, 43, 57, 62	0
10	2O	122/122 (100%)	0.63	1 (0%) 86 84	47, 59, 69, 78	0
11	1P	149/150 (99%)	0.34	2 (1%) 77 73	20, 45, 67, 71	0
11	2P	149/150 (99%)	0.69	14 (9%) 8 5	40, 63, 79, 84	0
12	1Q	141/141 (100%)	0.40	0 100 100	27, 41, 56, 72	0
12	2Q	141/141 (100%)	1.29	32 (22%) 0 0	50, 64, 72, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.34	0 100 100	24, 34, 48, 58	0
13	2R	118/118 (100%)	0.73	12 (10%) 6 4	42, 51, 61, 72	0
14	1S	110/112 (98%)	0.16	0 100 100	39, 48, 59, 65	0
14	2S	110/112 (98%)	0.73	14 (12%) 3 2	58, 66, 75, 79	0
15	1T	131/146 (89%)	0.27	2 (1%) 73 70	34, 46, 66, 72	0
15	2T	131/146 (89%)	0.36	3 (2%) 60 54	49, 60, 69, 76	0
16	1U	116/118 (98%)	0.57	0 100 100	21, 30, 48, 53	0
16	2U	116/118 (98%)	0.64	10 (8%) 10 7	43, 60, 71, 74	0
17	1V	101/101 (100%)	0.37	0 100 100	21, 38, 54, 72	0
17	2V	101/101 (100%)	0.35	4 (3%) 38 31	42, 66, 75, 85	0
18	1W	112/113 (99%)	0.50	0 100 100	23, 32, 48, 80	0
18	2W	112/113 (99%)	0.49	2 (1%) 68 64	38, 50, 62, 77	0
19	1X	95/96 (98%)	0.34	0 100 100	29, 40, 56, 73	0
19	2X	95/96 (98%)	0.27	1 (1%) 80 78	48, 60, 72, 79	0
20	1Y	107/110 (97%)	0.29	1 (0%) 84 82	34, 48, 61, 71	0
20	2Y	107/110 (97%)	0.40	1 (0%) 84 82	49, 66, 76, 82	0
21	1Z	154/206 (74%)	0.25	2 (1%) 77 73	37, 58, 75, 83	0
21	2Z	160/206 (77%)	1.12	33 (20%) 1 0	59, 74, 84, 88	0
22	10	83/85 (97%)	0.64	6 (7%) 15 11	26, 38, 58, 73	0
22	20	83/85 (97%)	1.37	21 (25%) 0 0	48, 61, 71, 77	0
23	11	97/98 (98%)	0.51	3 (3%) 49 42	28, 46, 66, 72	0
23	21	97/98 (98%)	0.57	2 (2%) 63 58	37, 55, 71, 74	0
24	12	70/72 (97%)	0.44	0 100 100	31, 48, 59, 65	0
24	22	70/72 (97%)	0.18	1 (1%) 75 71	58, 68, 75, 85	0
25	13	59/60 (98%)	0.34	0 100 100	23, 35, 58, 75	0
25	23	59/60 (98%)	1.13	12 (20%) 1 0	56, 63, 70, 73	0
26	14	69/71 (97%)	0.43	5 (7%) 15 11	49, 71, 80, 84	0
26	24	69/71 (97%)	0.31	4 (5%) 23 17	66, 78, 87, 90	0
27	15	59/60 (98%)	0.50	0 100 100	21, 33, 53, 60	0
27	25	59/60 (98%)	0.41	1 (1%) 70 66	37, 51, 69, 74	0
28	16	53/54 (98%)	0.31	1 (1%) 66 62	33, 42, 54, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.92	10 (18%) 1 0	50, 57, 63, 65	0
29	17	48/49 (97%)	0.60	1 (2%) 63 58	22, 27, 47, 57	0
29	27	48/49 (97%)	0.66	1 (2%) 63 58	35, 45, 60, 66	0
30	18	64/65 (98%)	0.60	0 100 100	28, 35, 45, 51	0
30	28	64/65 (98%)	1.64	16 (25%) 0 0	39, 53, 61, 64	0
31	19	37/37 (100%)	0.73	0 100 100	25, 40, 56, 61	0
31	29	37/37 (100%)	1.82	16 (43%) 0 0	54, 66, 71, 79	0
32	1a	1488/1521 (97%)	0.14	29 (1%) 66 62	37, 65, 86, 101	0
32	2a	1491/1521 (98%)	0.10	42 (2%) 53 46	50, 74, 89, 101	0
33	1b	231/256 (90%)	0.23	6 (2%) 56 50	63, 73, 80, 84	0
33	2b	231/256 (90%)	0.55	18 (7%) 13 9	68, 78, 85, 93	0
34	1c	206/239 (86%)	0.59	12 (5%) 23 17	56, 69, 76, 80	0
34	2c	206/239 (86%)	0.94	33 (16%) 1 1	66, 77, 83, 89	0
35	1d	208/209 (99%)	0.39	2 (0%) 82 80	54, 67, 73, 79	0
35	2d	208/209 (99%)	0.47	7 (3%) 45 38	58, 67, 75, 80	0
36	1e	148/162 (91%)	0.30	2 (1%) 75 71	52, 63, 71, 76	0
36	2e	148/162 (91%)	0.67	13 (8%) 10 7	62, 73, 79, 84	0
37	1f	100/101 (99%)	0.10	0 100 100	51, 64, 71, 73	0
37	2f	100/101 (99%)	-0.01	0 100 100	61, 68, 73, 77	0
38	1g	155/156 (99%)	0.87	25 (16%) 1 1	57, 66, 74, 95	0
38	2g	155/156 (99%)	0.81	20 (12%) 3 2	63, 73, 80, 89	0
39	1h	137/138 (99%)	0.45	5 (3%) 42 35	55, 65, 72, 82	0
39	2h	137/138 (99%)	0.95	22 (16%) 1 1	64, 73, 79, 84	0
40	1i	127/128 (99%)	1.42	35 (27%) 0 0	50, 72, 79, 81	0
40	2i	127/128 (99%)	2.33	72 (56%) 0 0	68, 76, 81, 85	0
41	1j	97/105 (92%)	0.83	19 (19%) 1 0	59, 71, 80, 85	0
41	2j	96/105 (91%)	1.56	33 (34%) 0 0	70, 78, 83, 86	0
42	1k	114/129 (88%)	0.59	4 (3%) 44 36	47, 64, 71, 73	0
42	2k	114/129 (88%)	0.37	1 (0%) 84 82	54, 70, 77, 80	0
43	1l	121/132 (91%)	0.54	6 (4%) 28 23	44, 55, 64, 65	0
43	2l	121/132 (91%)	0.71	9 (7%) 14 10	56, 66, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.79	10 (8%) 12 8	52, 66, 74, 78	0
44	2m	122/126 (96%)	0.98	25 (20%) 1 0	64, 75, 80, 82	0
45	1n	60/61 (98%)	1.79	24 (40%) 0 0	59, 65, 72, 73	0
45	2n	60/61 (98%)	2.86	41 (68%) 0 0	71, 79, 86, 88	0
46	1o	88/89 (98%)	0.53	3 (3%) 45 38	48, 61, 71, 74	0
46	2o	88/89 (98%)	0.49	5 (5%) 23 18	60, 70, 77, 85	0
47	1p	82/88 (93%)	1.15	22 (26%) 0 0	59, 68, 72, 76	0
47	2p	82/88 (93%)	0.74	6 (7%) 15 11	55, 66, 73, 77	0
48	1q	99/105 (94%)	1.13	15 (15%) 2 1	56, 63, 72, 78	0
48	2q	99/105 (94%)	0.76	11 (11%) 5 3	59, 68, 76, 80	0
49	1r	68/88 (77%)	0.33	2 (2%) 51 45	51, 64, 72, 74	0
49	2r	68/88 (77%)	0.17	0 100 100	63, 70, 77, 83	0
50	1s	83/93 (89%)	0.88	10 (12%) 4 2	58, 67, 73, 77	0
50	2s	83/93 (89%)	1.60	31 (37%) 0 0	69, 79, 83, 87	0
51	1t	96/106 (90%)	1.27	27 (28%) 0 0	56, 65, 76, 80	0
51	2t	96/106 (90%)	1.23	27 (28%) 0 0	55, 66, 75, 84	0
52	1u	23/27 (85%)	1.64	8 (34%) 0 0	59, 63, 67, 69	0
52	2u	23/27 (85%)	2.47	14 (60%) 0 0	70, 75, 78, 81	0
53	1v	13/24 (54%)	1.42	5 (38%) 0 0	49, 61, 78, 90	0
53	2v	13/24 (54%)	1.88	5 (38%) 0 0	67, 77, 86, 93	0
54	1w	65/76 (85%)	1.01	11 (16%) 1 1	59, 81, 93, 98	0
54	2w	63/76 (82%)	1.30	17 (26%) 0 0	75, 86, 96, 100	0
55	1x	71/77 (92%)	0.09	0 100 100	27, 59, 74, 86	0
55	2x	71/77 (92%)	-0.11	1 (1%) 75 71	47, 73, 84, 87	0
56	1y	67/76 (88%)	0.57	6 (8%) 9 6	37, 82, 92, 95	0
56	2y	66/76 (86%)	0.81	4 (6%) 21 16	56, 89, 93, 96	0
All	All	20867/21748 (95%)	0.47	1263 (6%) 21 16	18, 62, 83, 101	0

All (1263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	1g	81	GLY	11.0
22	20	2	ALA	9.7

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	8.6
44	2m	123	ALA	8.6
45	2n	34	TYR	7.5
44	2m	124	PRO	7.3
39	2h	83	ILE	7.3
54	2w	73	A	7.2
7	2H	105	LEU	7.2
44	1m	123	ALA	7.1
41	2j	47	PHE	7.1
50	2s	80	TYR	6.8
41	2j	63	PHE	6.6
40	2i	114	TYR	6.5
38	1g	79	ARG	6.4
54	1w	71	G	6.4
1	2A	652(C)	G	6.2
7	2H	113	VAL	6.2
22	10	3	HIS	6.1
41	2j	62	HIS	6.1
41	2j	59	SER	6.1
1	1A	652(C)	G	5.9
38	1g	80	VAL	5.9
53	2v	24	A	5.9
21	2Z	144	LEU	5.9
1	2A	654	A	5.9
40	2i	19	LEU	5.8
40	2i	82	ALA	5.8
1	1A	652(V)	C	5.8
40	2i	79	LEU	5.7
30	28	23	VAL	5.7
38	1g	154	TYR	5.6
1	2A	2146	C	5.5
7	2H	165	ALA	5.5
38	2g	80	VAL	5.5
52	2u	16	GLY	5.5
1	2A	652(T)	C	5.4
40	2i	65	VAL	5.4
1	1A	652(U)	G	5.4
45	2n	39	LEU	5.4
41	2j	55	LYS	5.4
7	2H	100	GLY	5.4
41	2j	65	LEU	5.3
38	1g	85	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	1A	652(S)	C	5.3
34	2c	200	ALA	5.3
1	1A	653	A	5.3
33	2b	165	VAL	5.3
40	2i	80	GLY	5.2
40	1i	117	HIS	5.2
41	1j	59	SER	5.2
34	2c	8	ILE	5.2
1	2A	653	A	5.2
7	2H	35	VAL	5.2
21	2Z	170	THR	5.1
21	2Z	149	SER	5.1
29	27	1	MET	5.1
32	1a	1001(A)	G	5.1
38	2g	40	ALA	5.1
38	2g	81	GLY	5.0
45	2n	2	ALA	5.0
51	2t	83	ARG	5.0
40	2i	102	LEU	5.0
40	2i	115	GLY	5.0
35	1d	2	GLY	5.0
54	2w	4	C	4.9
40	2i	127	LYS	4.9
40	1i	113	LYS	4.9
7	2H	107	VAL	4.9
1	2A	2112	G	4.9
34	2c	157	ILE	4.8
45	2n	61	TRP	4.8
44	2m	102	ARG	4.8
1	2A	652(U)	G	4.8
39	2h	111	ILE	4.8
45	2n	42	ILE	4.8
40	2i	9	ARG	4.8
45	2n	38	GLY	4.8
21	2Z	145	GLU	4.8
32	2a	1001(A)	G	4.8
32	2a	1032	G	4.8
7	2H	24	VAL	4.7
38	1g	83	ALA	4.7
47	1p	1	MET	4.7
32	1a	1286	A	4.7
7	2H	128	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1033	G	4.7
31	29	19	ARG	4.7
7	2H	121	ILE	4.7
32	1a	1002	G	4.7
32	2a	1034	G	4.6
22	20	7	LEU	4.6
22	20	75	LEU	4.6
40	1i	65	VAL	4.6
34	2c	6	HIS	4.6
50	1s	40	ILE	4.6
32	2a	1030(B)	C	4.6
40	2i	17	VAL	4.5
38	1g	87	VAL	4.5
40	2i	81	ILE	4.5
38	1g	156	TRP	4.5
40	1i	106	ALA	4.5
45	2n	10	ALA	4.5
1	1A	2151	G	4.5
38	1g	78	ARG	4.5
39	2h	134	ILE	4.5
40	2i	125	TYR	4.5
44	2m	4	ILE	4.5
45	1n	10	ALA	4.5
53	2v	23	A	4.5
34	2c	198	VAL	4.5
45	2n	12	ARG	4.4
40	1i	109	VAL	4.4
54	2w	71	G	4.4
7	2H	169	VAL	4.4
7	2H	141	VAL	4.4
34	2c	4	LYS	4.4
51	2t	63	ILE	4.4
44	2m	97	PRO	4.4
1	1A	654	A	4.4
47	1p	19	ILE	4.4
34	2c	189	ALA	4.3
40	1i	115	GLY	4.3
7	2H	72	ILE	4.3
52	2u	17	THR	4.3
40	2i	72	GLY	4.3
45	2n	44	LEU	4.3
39	2h	86	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
50	2s	82	GLY	4.3
50	2s	38	SER	4.3
45	1n	2	ALA	4.3
45	2n	58	LYS	4.3
34	2c	159	GLY	4.3
50	2s	79	THR	4.2
38	2g	4	ARG	4.2
54	2w	74	C	4.2
1	2A	652(V)	C	4.2
1	2A	229	A	4.2
40	2i	109	VAL	4.2
13	2R	69	ASP	4.2
52	2u	14	TRP	4.2
53	1v	12	A	4.2
32	1a	1257	U	4.2
39	2h	133	LEU	4.2
39	2h	136	GLU	4.2
12	2Q	114	ALA	4.2
41	2j	27	ALA	4.2
1	1A	885	C	4.2
54	1w	72	C	4.2
45	1n	59	ALA	4.1
45	2n	11	LYS	4.1
48	1q	36	ILE	4.1
12	2Q	109	VAL	4.1
1	2A	883	G	4.1
22	10	2	ALA	4.1
47	1p	30	GLY	4.1
34	2c	182	ILE	4.1
36	2e	20	GLN	4.1
7	2H	45	VAL	4.1
54	2w	67	C	4.1
39	2h	135	CYS	4.1
50	2s	71	LEU	4.1
50	2s	63	THR	4.1
32	2a	1220	G	4.1
1	1A	2117	A	4.1
40	2i	117	HIS	4.0
45	2n	15	LYS	4.0
52	2u	11	GLY	4.0
7	2H	133	VAL	4.0
41	2j	44	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
45	1n	61	TRP	4.0
45	2n	55	GLY	4.0
34	2c	184	TYR	4.0
40	2i	4	TYR	4.0
33	1b	213	LEU	4.0
40	1i	8	GLY	4.0
40	1i	81	ILE	4.0
45	2n	25	VAL	4.0
40	1i	114	TYR	4.0
51	2t	26	ASN	4.0
6	2G	133	LEU	3.9
45	2n	53	LEU	3.9
50	2s	13	ASP	3.9
23	11	2	SER	3.9
50	2s	35	SER	3.9
54	2w	3	C	3.9
6	2G	157	ILE	3.9
14	2S	58	LEU	3.9
31	29	17	ILE	3.9
41	2j	49	VAL	3.9
50	1s	71	LEU	3.9
35	2d	122	ARG	3.9
38	2g	154	TYR	3.9
40	2i	5	TYR	3.9
40	2i	36	TYR	3.9
40	2i	62	TYR	3.9
40	2i	83	ARG	3.9
22	20	6	GLY	3.9
34	2c	5	ILE	3.9
1	1A	652(T)	C	3.9
1	1A	2111	C	3.9
21	2Z	153	SER	3.8
50	2s	69	HIS	3.8
32	1a	1036	G	3.8
30	28	41	ILE	3.8
16	2U	20	LEU	3.8
34	1c	196	LEU	3.8
34	2c	160	ALA	3.8
32	2a	1257	U	3.8
34	2c	14	ILE	3.8
51	1t	63	ILE	3.8
36	2e	90	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
34	1c	8	ILE	3.8
1	2A	2115	G	3.8
32	2a	1030(A)	G	3.8
40	2i	78	LYS	3.8
54	1w	1	G	3.8
4	1E	195	LEU	3.8
50	1s	67	VAL	3.8
44	1m	122	LYS	3.8
44	2m	103	THR	3.8
51	1t	9	ASN	3.8
45	2n	16	PHE	3.8
7	2H	148	ILE	3.7
12	2Q	66	ILE	3.7
40	2i	122	ALA	3.7
22	20	4	LYS	3.7
43	2l	39	VAL	3.7
45	2n	14	PRO	3.7
33	2b	34	ALA	3.7
45	2n	7	ILE	3.7
45	2n	35	ARG	3.7
39	2h	112	LEU	3.7
51	1t	84	LEU	3.7
40	2i	116	LYS	3.7
7	2H	166	GLY	3.7
51	1t	72	LEU	3.7
42	1k	126	ARG	3.7
46	2o	61	GLY	3.7
40	2i	73	GLN	3.7
50	2s	49	ILE	3.7
54	2w	72	C	3.7
56	2y	36	A	3.6
40	2i	76	ALA	3.6
4	2E	196	VAL	3.6
40	2i	14	VAL	3.6
52	1u	3	LYS	3.6
38	2g	38	LEU	3.6
39	2h	9	MET	3.6
4	2E	116	VAL	3.6
7	2H	94	TYR	3.6
44	2m	120	LYS	3.6
21	2Z	125	LEU	3.6
34	2c	10	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
44	2m	96	LEU	3.6
34	2c	178	LEU	3.6
41	1j	60	ARG	3.6
1	1A	888	C	3.6
1	2A	1026	U	3.6
32	1a	1003	G	3.6
21	2Z	148	ASP	3.6
12	2Q	33	GLY	3.6
7	2H	41	MET	3.6
45	2n	19	ARG	3.6
48	1q	28	PRO	3.6
40	1i	116	LYS	3.6
33	2b	71	VAL	3.5
52	2u	13	ILE	3.5
1	1A	2159	G	3.5
32	2a	1002	G	3.5
51	1t	47	GLY	3.5
40	2i	43	ALA	3.5
7	2H	161	GLY	3.5
26	24	51	ASP	3.5
40	2i	18	PHE	3.5
56	1y	34	G	3.5
1	2A	885	C	3.5
33	2b	187	LEU	3.5
1	1A	2141	G	3.5
52	2u	22	ARG	3.5
26	14	52	THR	3.5
23	11	98	LEU	3.5
31	29	16	VAL	3.5
1	1A	2115	G	3.5
32	2a	1116	C	3.5
40	2i	45	ALA	3.5
22	10	4	LYS	3.5
41	1j	93	GLY	3.5
7	2H	29	PRO	3.5
7	2H	114	VAL	3.5
40	1i	14	VAL	3.5
47	1p	6	LEU	3.5
38	1g	4	ARG	3.5
32	2a	1150	U	3.4
47	1p	28	ARG	3.4
45	2n	49	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
45	2n	57	ARG	3.4
56	1y	35	A	3.4
7	2H	99	VAL	3.4
7	2H	89	ILE	3.4
33	1b	61	LEU	3.4
52	1u	17	THR	3.4
45	2n	50	LYS	3.4
41	2j	51	ARG	3.4
28	26	11	LEU	3.4
45	2n	36	PHE	3.4
54	2w	70	G	3.4
1	1A	2132	U	3.4
6	2G	160	VAL	3.4
35	2d	162	LEU	3.4
40	2i	63	ILE	3.4
50	2s	68	GLY	3.4
45	2n	37	PHE	3.4
11	2P	65	ARG	3.4
50	2s	50	ALA	3.4
21	2Z	139	VAL	3.4
51	2t	72	LEU	3.4
40	2i	77	ILE	3.4
40	1i	37	PHE	3.4
1	1A	2145	C	3.4
45	2n	59	ALA	3.4
1	2A	2154	G	3.4
22	20	38	VAL	3.4
4	2E	134	ILE	3.4
1	2A	2174	C	3.4
1	1A	896	A	3.4
12	2Q	79	LEU	3.4
14	2S	32	LEU	3.4
13	2R	68	ARG	3.4
21	2Z	96	VAL	3.4
8	2I	1	MET	3.3
1	1A	2108	C	3.3
45	2n	31	ARG	3.3
6	2G	39	ILE	3.3
41	2j	50	ILE	3.3
48	1q	27	PHE	3.3
7	2H	145	ALA	3.3
56	1y	20	U	3.3

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Mol	Chain	Res	Type	RSRZ
45	1n	15	LYS	3.3
4	2E	106	GLY	3.3
1	2A	2123	G	3.3
31	29	24	TYR	3.3
43	2l	55	VAL	3.3
30	28	15	LYS	3.3
32	2a	1021	G	3.3
13	2R	83	ILE	3.3
27	25	29	THR	3.3
7	2H	159	GLU	3.3
16	2U	16	LYS	3.3
4	2E	105	THR	3.3
40	2i	7	THR	3.3
9	2N	116	LEU	3.3
45	2n	6	LEU	3.3
54	1w	70	G	3.3
1	2A	888	C	3.2
1	1A	2109	U	3.2
38	2g	79	ARG	3.2
41	2j	58	ASP	3.2
52	2u	5	ASP	3.2
40	2i	126	SER	3.2
1	2A	2133	G	3.2
14	2S	34	HIS	3.2
41	2j	48	THR	3.2
51	2t	57	ARG	3.2
52	2u	9	ARG	3.2
34	1c	33	LEU	3.2
28	26	52	VAL	3.2
1	1A	2129	C	3.2
44	2m	88	ARG	3.2
17	2V	79	VAL	3.2
41	1j	68	HIS	3.2
32	2a	1035	A	3.2
40	2i	33	PHE	3.2
1	1A	1059	G	3.2
6	2G	159	VAL	3.2
25	23	6	VAL	3.2
41	1j	48	THR	3.2
30	28	18	ALA	3.2
13	2R	65	LEU	3.2
48	2q	30	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
38	1g	77	SER	3.2
9	2N	69	GLN	3.2
40	1i	10	ARG	3.2
7	2H	4	ILE	3.2
34	2c	201	TYR	3.2
11	2P	15	ARG	3.2
40	2i	121	ARG	3.2
1	2A	884	C	3.2
41	1j	62	HIS	3.2
41	1j	47	PHE	3.2
47	1p	4	ILE	3.2
50	2s	40	ILE	3.2
28	26	20	ASN	3.2
38	2g	33	ASP	3.1
50	2s	77	THR	3.1
51	2t	41	ILE	3.1
51	1t	20	LEU	3.1
51	1t	69	GLY	3.1
52	2u	18	TYR	3.1
4	2E	195	LEU	3.1
32	2a	1031	G	3.1
32	2a	1061	G	3.1
40	2i	10	ARG	3.1
1	1A	2118	U	3.1
25	23	47	VAL	3.1
50	2s	84	GLY	3.1
9	2N	23	LEU	3.1
40	1i	19	LEU	3.1
7	2H	90	LYS	3.1
21	2Z	151	HIS	3.1
7	2H	23	ARG	3.1
40	1i	120	ARG	3.1
51	1t	83	ARG	3.1
1	1A	2152	G	3.1
34	2c	155	GLY	3.1
56	1y	19	G	3.1
1	1A	1060	U	3.1
54	1w	74	C	3.1
19	2X	1	MET	3.1
46	2o	59	MET	3.1
40	1i	108	VAL	3.1
46	2o	60	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
44	2m	122	LYS	3.1
12	2Q	47	ILE	3.1
33	2b	118	LEU	3.1
34	2c	7	PRO	3.1
1	2A	2169	A	3.1
50	2s	70	LYS	3.1
40	2i	119	ALA	3.1
7	2H	25	LYS	3.1
45	1n	50	LYS	3.1
4	2E	51	PHE	3.1
40	1i	28	VAL	3.1
12	2Q	28	ALA	3.1
51	2t	62	LEU	3.1
30	28	16	ILE	3.1
30	28	25	MET	3.0
7	2H	19	VAL	3.0
7	2H	73	ALA	3.0
40	2i	112	LYS	3.0
1	1A	1080	C	3.0
1	2A	2119	A	3.0
45	1n	56	VAL	3.0
22	10	7	LEU	3.0
40	2i	105	ASP	3.0
52	2u	6	ARG	3.0
50	2s	31	ILE	3.0
45	1n	34	TYR	3.0
1	1A	2119	A	3.0
32	2a	1001	A	3.0
1	2A	2118	U	3.0
47	1p	60	LEU	3.0
21	2Z	57	ILE	3.0
1	2A	2802	G	3.0
40	2i	11	LYS	3.0
51	1t	68	LYS	3.0
1	1A	1092	C	3.0
34	2c	3	ASN	3.0
1	1A	1095	A	3.0
48	1q	60	ILE	3.0
40	1i	110	GLU	3.0
48	1q	75	ARG	3.0
1	1A	652(D)	C	3.0
1	1A	2149	G	3.0

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Mol	Chain	Res	Type	RSRZ
32	1a	1367	C	3.0
39	2h	2	LEU	3.0
44	1m	98	VAL	3.0
44	2m	17	VAL	3.0
30	28	55	ALA	3.0
22	20	44	ARG	3.0
38	2g	156	TRP	3.0
54	2w	2	C	3.0
7	2H	151	ILE	3.0
14	2S	3	ARG	3.0
36	2e	45	PHE	3.0
6	1G	139	LEU	3.0
40	2i	26	VAL	3.0
47	2p	2	VAL	3.0
50	2s	15	LEU	3.0
6	2G	29	TRP	3.0
22	20	22	GLY	3.0
34	1c	197	GLY	3.0
1	1A	2112	G	2.9
32	1a	1368	G	2.9
32	1a	1447	A	2.9
7	2H	48	GLY	2.9
38	2g	16	LEU	2.9
40	1i	121	ARG	2.9
40	2i	28	VAL	2.9
40	2i	90	PRO	2.9
40	2i	74	ILE	2.9
32	2a	1030	C	2.9
11	2P	45	LEU	2.9
12	2Q	15	GLY	2.9
56	2y	34	G	2.9
1	1A	1057	A	2.9
9	2N	8	GLN	2.9
7	2H	96	ALA	2.9
7	2H	124	GLU	2.9
1	2A	2111	C	2.9
1	2A	2113	U	2.9
54	1w	2	C	2.9
34	1c	193	TYR	2.9
51	1t	13	LEU	2.9
6	2G	37	VAL	2.9
1	2A	2162	G	2.9

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Mol	Chain	Res	Type	RSRZ
32	2a	1117	G	2.9
33	2b	120	ALA	2.9
22	20	3	HIS	2.9
45	1n	7	ILE	2.9
52	2u	15	ARG	2.9
7	2H	78	GLY	2.9
1	1A	2130	U	2.9
45	1n	39	LEU	2.9
53	2v	22	U	2.9
1	1A	2174	C	2.9
39	2h	95	VAL	2.9
36	2e	129	ILE	2.9
1	1A	2170	A	2.9
41	2j	54	PHE	2.9
53	1v	24	A	2.9
14	2S	5	THR	2.9
30	28	17	THR	2.9
40	2i	103	THR	2.9
41	2j	60	ARG	2.9
4	2E	115	GLY	2.9
7	2H	87	LEU	2.9
10	2O	1	MET	2.9
50	2s	14	HIS	2.9
1	1A	884	C	2.9
51	1t	33	ILE	2.9
22	10	5	LYS	2.9
7	2H	125	VAL	2.9
12	2Q	96	VAL	2.9
21	2Z	152	ALA	2.9
50	2s	78	ARG	2.9
54	2w	5	G	2.9
38	1g	34	GLY	2.8
20	2Y	31	LEU	2.8
26	14	56	VAL	2.8
1	1A	2131	G	2.8
32	1a	1287	A	2.8
48	2q	38	ARG	2.8
3	1D	2	ALA	2.8
7	2H	115	VAL	2.8
45	1n	58	LYS	2.8
47	2p	51	VAL	2.8
42	1k	25	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
7	2H	2	SER	2.8
12	2Q	104	PHE	2.8
1	2A	2159	G	2.8
44	2m	90	LEU	2.8
1	1A	2146	C	2.8
7	2H	36	PRO	2.8
41	2j	26	ALA	2.8
31	29	15	LYS	2.8
45	2n	4	LYS	2.8
7	2H	106	THR	2.8
47	1p	22	THR	2.8
32	1a	1035	A	2.8
32	2a	965	A	2.8
21	2Z	98	MET	2.8
45	2n	56	VAL	2.8
1	2A	2128	C	2.8
40	1i	36	TYR	2.8
51	1t	15	ARG	2.8
39	1h	100	ILE	2.8
48	1q	6	LEU	2.8
51	2t	33	ILE	2.8
32	2a	1040	U	2.8
40	2i	123	PRO	2.8
32	2a	1003	G	2.8
32	2a	1016	A	2.8
54	1w	44	G	2.8
7	2H	162	ILE	2.8
51	1t	75	ASN	2.8
7	2H	122	THR	2.8
52	1u	11	GLY	2.8
21	2Z	172	ALA	2.8
38	1g	32	ARG	2.8
40	2i	111	ARG	2.8
47	1p	39	TYR	2.8
28	26	10	LEU	2.8
41	2j	40	LEU	2.8
51	2t	10	LEU	2.8
25	23	56	VAL	2.7
28	26	5	VAL	2.7
45	1n	18	VAL	2.7
45	1n	20	ALA	2.7
1	1A	1094	U	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	2.7
13	2R	10	LEU	2.7
31	29	37	GLY	2.7
1	1A	2110	G	2.7
12	2Q	132	VAL	2.7
1	1A	2113	U	2.7
30	28	39	LYS	2.7
34	2c	196	LEU	2.7
33	2b	214	ILE	2.7
50	1s	49	ILE	2.7
44	2m	101	GLN	2.7
21	1Z	149	SER	2.7
40	1i	82	ALA	2.7
40	2i	108	VAL	2.7
16	2U	40	PHE	2.7
40	2i	124	GLN	2.7
51	1t	41	ILE	2.7
23	21	2	SER	2.7
29	17	46	VAL	2.7
36	2e	33	VAL	2.7
1	2A	652(D)	C	2.7
32	2a	1369	C	2.7
53	2v	21	C	2.7
12	2Q	2	LEU	2.7
38	1g	38	LEU	2.7
9	2N	83	LYS	2.7
32	1a	204	U	2.7
47	1p	67	THR	2.7
40	1i	119	ALA	2.7
43	2l	56	ALA	2.7
51	2t	77	ALA	2.7
5	2F	37	VAL	2.7
51	1t	80	ARG	2.7
32	1a	1030(B)	C	2.7
34	1c	201	TYR	2.7
39	2h	100	ILE	2.7
40	2i	75	ASP	2.7
40	1i	26	VAL	2.7
40	1i	33	PHE	2.7
12	2Q	32	TYR	2.7
33	2b	92	TYR	2.7
33	2b	201	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
36	2e	13	ILE	2.7
41	2j	74	ILE	2.7
1	1A	887	A	2.7
7	2H	16	SER	2.7
32	1a	1532	U	2.7
39	2h	4	ASP	2.7
41	2j	66	ARG	2.7
32	2a	1030(D)	A	2.7
40	2i	44	VAL	2.7
46	1o	60	VAL	2.7
26	24	49	PHE	2.7
41	2j	11	PHE	2.7
25	23	12	PRO	2.6
25	23	25	ALA	2.6
32	1a	1029	C	2.6
32	2a	1219	U	2.6
31	29	25	VAL	2.6
45	1n	36	PHE	2.6
12	2Q	5	ARG	2.6
4	2E	77	ILE	2.6
30	28	35	GLN	2.6
42	1k	89	ALA	2.6
47	1p	24	ALA	2.6
9	2N	9	VAL	2.6
30	28	22	VAL	2.6
33	2b	69	LEU	2.6
7	2H	123	PHE	2.6
22	20	45	PHE	2.6
41	1j	58	ASP	2.6
51	1t	67	ALA	2.6
51	2t	73	HIS	2.6
38	1g	84	ASN	2.6
7	2H	103	LEU	2.6
41	1j	46	ARG	2.6
41	2j	46	ARG	2.6
50	2s	36	ARG	2.6
33	2b	70	PHE	2.6
1	1A	2173	A	2.6
43	2l	64	TYR	2.6
43	2l	65	GLU	2.6
12	2Q	94	VAL	2.6
7	2H	171	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
43	1l	27	LEU	2.6
1	2A	2122	U	2.6
1	2A	2144	U	2.6
41	2j	61	GLU	2.6
52	1u	14	TRP	2.6
40	2i	49	PRO	2.6
32	2a	1251	A	2.6
45	2n	18	VAL	2.6
21	2Z	91	LEU	2.6
21	2Z	102	LEU	2.6
1	1A	1058	G	2.6
1	2A	2147	G	2.6
7	2H	13	LYS	2.6
41	1j	44	VAL	2.6
48	1q	9	VAL	2.6
7	2H	77	LYS	2.6
21	2Z	155	LEU	2.6
31	29	12	ASP	2.6
26	14	53	GLU	2.6
33	2b	203	GLY	2.6
41	1j	50	ILE	2.6
47	1p	7	ALA	2.6
4	2E	198	VAL	2.6
32	2a	1043	C	2.6
48	2q	21	VAL	2.6
25	23	26	LEU	2.6
50	1s	74	PHE	2.6
1	1A	2171	A	2.6
22	20	55	ARG	2.6
40	1i	9	ARG	2.6
16	2U	17	ILE	2.5
41	1j	57	LYS	2.5
52	2u	12	LYS	2.5
12	2Q	36	ALA	2.5
34	2c	167	TRP	2.5
1	2A	2131	G	2.5
34	1c	66	VAL	2.5
38	2g	101	LEU	2.5
44	1m	48	LEU	2.5
44	2m	60	VAL	2.5
51	2t	64	ASP	2.5
32	2a	1027	C	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	80	GLY	2.5
12	2Q	59	ARG	2.5
45	2n	45	ARG	2.5
47	1p	5	ARG	2.5
40	1i	112	LYS	2.5
48	2q	37	LYS	2.5
30	28	63	PRO	2.5
38	2g	152	ALA	2.5
54	2w	14	A	2.5
7	2H	144	VAL	2.5
50	2s	67	VAL	2.5
40	2i	104	ARG	2.5
43	1l	23	LYS	2.5
1	1A	1064	C	2.5
1	1A	1509	C	2.5
9	2N	10	GLU	2.5
12	2Q	99	PRO	2.5
36	2e	131	ILE	2.5
40	1i	122	ALA	2.5
1	2A	2171	A	2.5
11	2P	79	ARG	2.5
35	1d	120	LEU	2.5
40	2i	30	GLY	2.5
48	1q	77	VAL	2.5
1	1A	1087	G	2.5
1	1A	2116	G	2.5
32	2a	1149	C	2.5
16	2U	2	PRO	2.5
44	2m	80	ARG	2.5
51	2t	69	GLY	2.5
4	2E	52	LEU	2.5
39	2h	94	TYR	2.5
44	1m	56	LEU	2.5
52	1u	18	TYR	2.5
1	1A	2158	A	2.5
2	2B	90	A	2.5
7	2H	18	GLU	2.5
40	2i	113	LYS	2.5
51	1t	64	ASP	2.5
51	2t	30	LYS	2.5
41	1j	43	ARG	2.5
45	2n	13	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2160	G	2.5
39	2h	132	GLU	2.5
46	2o	27	VAL	2.5
50	2s	56	GLN	2.5
7	2H	109	PHE	2.5
15	1T	106	SER	2.5
7	2H	85	LYS	2.5
51	1t	14	LYS	2.5
38	1g	3	ARG	2.5
53	2v	12	A	2.5
35	2d	160	GLN	2.5
40	1i	50	LEU	2.5
16	2U	63	VAL	2.5
32	2a	1115	C	2.5
1	1A	1063	G	2.5
40	2i	128	ARG	2.5
41	1j	45	ARG	2.5
41	2j	29	ARG	2.5
6	2G	134	GLY	2.5
13	2R	39	PRO	2.5
50	2s	62	ILE	2.5
11	2P	115	LEU	2.5
44	1m	96	LEU	2.5
32	1a	1037	C	2.5
32	1a	1032	G	2.5
32	1a	1034	G	2.5
33	1b	68	ILE	2.4
14	2S	12	PHE	2.4
44	2m	104	ARG	2.4
7	2H	74	ASN	2.4
7	2H	34	GLU	2.4
40	2i	67	GLY	2.4
1	1A	652(F)	G	2.4
1	1A	1093	G	2.4
1	2A	2319	G	2.4
22	20	10	THR	2.4
32	1a	1353	G	2.4
51	2t	66	ALA	2.4
28	26	34	LEU	2.4
40	2i	120	ARG	2.4
52	2u	10	ARG	2.4
7	2H	163	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
46	1o	61	GLY	2.4
31	29	11	CYS	2.4
43	1l	94	PRO	2.4
6	2G	73	ALA	2.4
40	2i	61	ALA	2.4
51	2t	24	LEU	2.4
1	2A	1114	G	2.4
40	2i	110	GLU	2.4
7	2H	30	LYS	2.4
45	1n	16	PHE	2.4
51	2t	29	LYS	2.4
44	2m	119	GLY	2.4
32	2a	1363(A)	A	2.4
11	2P	32	THR	2.4
33	2b	121	LEU	2.4
36	2e	132	ALA	2.4
38	2g	83	ALA	2.4
39	2h	10	LEU	2.4
40	1i	47	LEU	2.4
50	1s	48	THR	2.4
1	1A	897	C	2.4
45	2n	46	GLU	2.4
48	1q	59	ILE	2.4
56	2y	4	C	2.4
1	2A	2127	G	2.4
1	2A	2160	G	2.4
12	2Q	103	MET	2.4
7	2H	152	ARG	2.4
45	2n	23	ARG	2.4
12	2Q	112	GLU	2.4
21	2Z	69	THR	2.4
40	2i	27	THR	2.4
47	2p	74	LEU	2.4
28	26	54	ILE	2.4
34	1c	39	ILE	2.4
39	2h	6	ILE	2.4
13	2R	66	VAL	2.4
44	2m	98	VAL	2.4
7	1H	170	ARG	2.4
21	2Z	4	ARG	2.4
25	23	29	ARG	2.4
42	2k	25	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
43	1l	91	LYS	2.4
51	2t	86	ARG	2.4
1	2A	2155	G	2.4
7	2H	33	LEU	2.4
34	2c	87	LEU	2.4
42	1k	57	THR	2.4
43	2l	9	GLN	2.4
46	1o	57	LEU	2.4
49	1r	31	LEU	2.4
51	1t	76	ALA	2.4
4	2E	153	GLY	2.4
8	2I	13	GLY	2.4
7	2H	49	VAL	2.4
7	2H	52	VAL	2.4
33	1b	136	VAL	2.4
1	1A	2161	C	2.4
1	2A	2145	C	2.4
40	1i	66	ARG	2.4
55	2x	34	C	2.4
43	2l	5	PRO	2.4
11	2P	59	LEU	2.4
21	2Z	93	ASP	2.4
28	26	23	THR	2.4
36	1e	48	ALA	2.4
36	2e	125	SER	2.4
40	2i	52	ALA	2.4
47	2p	49	LEU	2.4
51	1t	77	ALA	2.4
1	1A	2162	G	2.4
31	29	26	ILE	2.4
32	1a	1030(A)	G	2.4
38	1g	82	GLY	2.4
6	2G	35	GLU	2.4
30	28	65	GLU	2.4
1	2A	2132	U	2.3
1	1A	2135	A	2.3
1	1A	2143	C	2.3
1	2A	2170	A	2.3
32	1a	1288	A	2.3
34	1c	184	TYR	2.3
51	1t	16	HIS	2.3
7	2H	71	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
30	28	12	LYS	2.3
31	29	33	LYS	2.3
39	2h	131	GLY	2.3
43	1l	13	LYS	2.3
50	2s	53	ASN	2.3
34	2c	186	PHE	2.3
45	2n	33	VAL	2.3
1	1A	2150	U	2.3
41	2j	77	PRO	2.3
48	2q	42	TYR	2.3
6	2G	34	LEU	2.3
11	2P	28	GLY	2.3
54	1w	73	A	2.3
3	2D	271	ILE	2.3
15	2T	110	ILE	2.3
41	2j	38	ILE	2.3
6	2G	141	PHE	2.3
31	29	3	VAL	2.3
6	1G	26	GLN	2.3
45	2n	40	CYS	2.3
1	2A	652(E)	G	2.3
1	2A	882	G	2.3
25	23	28	LEU	2.3
30	28	45	GLY	2.3
32	2a	1030(C)	G	2.3
46	2o	56	LEU	2.3
54	2w	15	G	2.3
51	2t	12	ALA	2.3
54	2w	68	C	2.3
12	2Q	113	GLN	2.3
17	2V	72	VAL	2.3
26	14	49	PHE	2.3
8	2I	12	LEU	2.3
30	28	61	LEU	2.3
44	1m	87	TYR	2.3
51	1t	59	ALA	2.3
52	2u	21	TYR	2.3
41	2j	57	LYS	2.3
1	1A	889	C	2.3
6	2G	92	VAL	2.3
32	2a	1018	C	2.3
38	1g	105	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	1A	1847	A	2.3
35	2d	49	ARG	2.3
40	2i	20	ARG	2.3
3	2D	210	GLY	2.3
6	2G	76	SER	2.3
11	2P	62	LEU	2.3
23	2I	98	LEU	2.3
7	2H	146	ALA	2.3
51	1t	55	ILE	2.3
54	1w	20	U	2.3
11	2P	149	GLU	2.3
21	2Z	71	VAL	2.3
33	2b	17	PHE	2.3
36	2e	84	PHE	2.3
43	2l	18	VAL	2.3
45	1n	37	PHE	2.3
50	2s	81	ARG	2.3
32	1a	1038	C	2.3
12	2Q	3	MET	2.3
21	2Z	33	LEU	2.3
36	2e	16	THR	2.3
28	16	54	ILE	2.3
44	2m	99	ARG	2.3
47	1p	2	VAL	2.3
50	1s	81	ARG	2.3
22	10	6	GLY	2.3
40	1i	118	LYS	2.3
40	2i	57	GLY	2.3
32	1a	1371	G	2.3
33	2b	37	ASN	2.3
40	2i	85	LEU	2.3
12	2Q	53	ALA	2.3
38	2g	145	ALA	2.3
40	2i	84	ALA	2.3
56	1y	56	C	2.3
7	2H	167	GLU	2.3
39	1h	3	THR	2.3
15	2T	22	PHE	2.3
36	2e	76	ILE	2.3
1	2A	2109	U	2.2
7	2H	82	GLY	2.2
6	2G	142	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	10	PRO	2.2
28	26	42	TRP	2.2
23	11	97	LEU	2.2
38	1g	2	ALA	2.2
51	1t	28	ALA	2.2
12	2Q	110	THR	2.2
1	2A	2161	C	2.2
22	20	5	LYS	2.2
32	1a	1006	C	2.2
32	2a	1452	C	2.2
18	2W	112	GLY	2.2
21	2Z	106	GLY	2.2
39	1h	93	VAL	2.2
40	2i	8	GLY	2.2
56	1y	36	A	2.2
31	29	34	GLN	2.2
33	2b	94	ASN	2.2
31	29	22	ARG	2.2
38	2g	128	ALA	2.2
45	1n	3	ARG	2.2
45	2n	3	ARG	2.2
7	2H	157	TYR	2.2
1	2A	2143	C	2.2
13	2R	47	PHE	2.2
7	2H	17	VAL	2.2
14	2S	82	ILE	2.2
40	1i	17	VAL	2.2
3	2D	275	LYS	2.2
32	2a	1092	A	2.2
47	1p	73	LEU	2.2
32	1a	1040	U	2.2
34	2c	53	ALA	2.2
11	1P	149	GLU	2.2
21	1Z	104	PHE	2.2
34	2c	205	GLY	2.2
38	1g	86	GLN	2.2
39	2h	128	GLY	2.2
40	2i	101	PHE	2.2
43	2l	72	GLY	2.2
14	2S	35	ILE	2.2
41	1j	64	GLU	2.2
1	1A	2140	C	2.2

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Mol	Chain	Res	Type	RSRZ
15	1T	104	ASN	2.2
32	2a	1060	C	2.2
41	1j	40	LEU	2.2
51	2t	80	ARG	2.2
1	1A	1081	U	2.2
14	2S	6	ALA	2.2
32	1a	1001	A	2.2
51	1t	12	ALA	2.2
53	1v	13	A	2.2
53	1v	14	A	2.2
50	2s	12	ASP	2.2
25	23	48	GLU	2.2
33	1b	133	LYS	2.2
34	2c	124	ILE	2.2
35	2d	70	ILE	2.2
41	2j	24	VAL	2.2
26	14	55	ARG	2.2
7	2H	7	LEU	2.2
7	2H	39	PRO	2.2
22	20	21	LEU	2.2
50	2s	57	HIS	2.2
32	2a	1226	C	2.2
8	2I	46	ALA	2.2
41	1j	20	ALA	2.2
47	2p	1	MET	2.2
1	2A	2148	G	2.2
41	1j	10	GLY	2.2
41	2j	67	THR	2.2
47	1p	27	LYS	2.2
54	2w	66	U	2.2
1	2A	896	A	2.2
11	2P	101	VAL	2.2
14	2S	14	VAL	2.2
14	2S	31	SER	2.2
21	2Z	58	VAL	2.2
22	20	74	ARG	2.2
41	2j	6	ILE	2.2
45	1n	23	ARG	2.2
51	2t	9	ASN	2.2
4	2E	182	LEU	2.2
6	2G	139	LEU	2.2
13	2R	20	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
31	29	20	HIS	2.2
44	2m	66	LEU	2.2
50	2s	30	LEU	2.2
6	2G	75	LYS	2.2
21	2Z	50	GLN	2.2
48	1q	37	LYS	2.2
16	2U	48	ALA	2.2
22	20	53	MET	2.2
41	2j	18	ALA	2.2
49	1r	73	ALA	2.2
52	1u	2	GLY	2.2
1	2A	2897	U	2.2
11	2P	51	PHE	2.2
51	2t	17	ARG	2.2
1	2A	1112	G	2.2
1	2A	2110	G	2.2
1	2A	2120	G	2.2
1	2A	2125	G	2.2
52	1u	21	TYR	2.2
38	2g	30	ILE	2.2
1	2A	2114	A	2.2
12	2Q	39	PRO	2.2
39	1h	112	LEU	2.2
45	2n	8	GLU	2.2
22	20	73	GLY	2.2
40	2i	46	ALA	2.2
34	2c	177	THR	2.2
7	2H	83	TYR	2.1
11	2P	64	LYS	2.1
25	23	49	LYS	2.1
4	2E	167	VAL	2.1
7	2H	26	VAL	2.1
26	24	50	VAL	2.1
38	1g	141	VAL	2.1
40	1i	126	SER	2.1
9	2N	112	LEU	2.1
45	1n	49	HIS	2.1
45	2n	47	LEU	2.1
32	2a	1224	G	2.1
1	2A	2753	A	2.1
11	2P	22	GLY	2.1
5	2F	80	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
25	23	51	ALA	2.1
39	2h	84	ARG	2.1
3	2D	38	LYS	2.1
14	2S	29	PHE	2.1
1	1A	1079	C	2.1
47	1p	17	TYR	2.1
21	2Z	5	LEU	2.1
24	22	60	LEU	2.1
7	2H	142	GLY	2.1
21	2Z	22	GLY	2.1
44	2m	94	ARG	2.1
44	2m	72	ALA	2.1
47	1p	64	ALA	2.1
1	1A	1099	G	2.1
1	1A	1077	A	2.1
41	1j	11	PHE	2.1
7	2H	67	LEU	2.1
7	2H	92	ILE	2.1
34	1c	23	TYR	2.1
34	1c	207	VAL	2.1
1	2A	1043	C	2.1
1	2A	2129	C	2.1
22	20	62	LEU	2.1
7	2H	126	PRO	2.1
21	2Z	68	PRO	2.1
41	2j	56	HIS	2.1
54	1w	13	C	2.1
21	2Z	21	ALA	2.1
36	1e	134	ALA	2.1
40	2i	13	ALA	2.1
6	2G	161	THR	2.1
31	29	29	ASN	2.1
1	1A	892	G	2.1
1	1A	2166	G	2.1
1	2A	100	G	2.1
9	2N	85	ILE	2.1
21	2Z	143	GLY	2.1
34	2c	39	ILE	2.1
48	1q	31	LEU	2.1
48	1q	81	ARG	2.1
48	2q	33	GLY	2.1
48	2q	36	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
51	2t	27	LYS	2.1
32	1a	1352	C	2.1
32	2a	981	U	2.1
41	2j	32	ALA	2.1
13	2R	71	GLN	2.1
26	24	66	SER	2.1
35	2d	75	PHE	2.1
45	1n	60	SER	2.1
3	1D	273	ARG	2.1
14	2S	20	ARG	2.1
39	2h	92	ARG	2.1
13	2R	48	VAL	2.1
16	2U	90	VAL	2.1
34	2c	173	VAL	2.1
41	2j	36	GLY	2.1
12	2Q	9	TYR	2.1
38	1g	153	HIS	2.1
47	1p	32	TYR	2.1
48	2q	32	TYR	2.1
48	2q	84	LEU	2.1
25	23	16	PRO	2.1
53	1v	23	A	2.1
54	2w	6	G	2.1
1	2A	2646	C	2.1
12	2Q	6	ARG	2.1
22	20	72	ARG	2.1
38	1g	43	PHE	2.1
22	20	54	GLY	2.1
9	2N	82	LEU	2.1
12	2Q	37	LEU	2.1
16	2U	60	LEU	2.1
33	2b	185	ILE	2.1
47	1p	33	ILE	2.1
48	1q	19	VAL	2.1
1	2A	2310	A	2.1
12	2Q	20	ALA	2.1
56	2y	64	A	2.1
1	1A	1082	U	2.1
7	2H	84	SER	2.1
47	1p	9	PHE	2.1
1	2A	1509	C	2.1
54	1w	3	C	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	98	LEU	2.1
8	2I	68	LEU	2.1
9	1N	140	VAL	2.1
15	2T	48	ILE	2.1
36	2e	109	ILE	2.1
38	1g	42	ILE	2.1
38	2g	42	ILE	2.1
38	2g	153	HIS	2.1
40	2i	86	VAL	2.1
48	2q	65	ILE	2.1
44	2m	87	TYR	2.1
12	2Q	121	ALA	2.1
50	1s	66	MET	2.1
51	2t	56	MET	2.1
1	2A	6	A	2.1
1	2A	2149	G	2.0
17	2V	75	PHE	2.1
32	1a	1350	A	2.1
32	2a	969	A	2.1
33	2b	163	PHE	2.1
34	1c	41	GLY	2.1
48	2q	98	LEU	2.0
43	1l	18	VAL	2.0
16	2U	44	ASN	2.0
20	1Y	36	ALA	2.0
44	1m	30	ALA	2.0
44	1m	103	THR	2.0
48	1q	14	LYS	2.0
51	2t	68	LYS	2.0
38	1g	99	LEU	2.0
45	1n	6	LEU	2.0
51	2t	20	LEU	2.0
5	2F	114	VAL	2.0
5	2F	193	VAL	2.0
6	2G	149	VAL	2.0
17	2V	50	PRO	2.0
18	2W	17	VAL	2.0
32	1a	1026	G	2.0
32	2a	1036	G	2.0
35	2d	112	VAL	2.0
39	2h	137	VAL	2.0
40	1i	77	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
54	2w	69	G	2.0
45	1n	31	ARG	2.0
51	2t	25	ARG	2.0
34	2c	193	TYR	2.0
44	2m	5	ALA	2.0
7	2H	129	THR	2.0
11	1P	109	GLY	2.0
34	2c	199	LYS	2.0
51	1t	70	SER	2.0
12	2Q	1	MET	2.0
7	2H	132	ARG	2.0
12	2Q	57	HIS	2.0
13	2R	61	HIS	2.0
21	2Z	49	ARG	2.0
22	20	77	ARG	2.0
34	2c	206	GLU	2.0
38	2g	32	ARG	2.0
38	2g	78	ARG	2.0
39	1h	26	VAL	2.0
44	2m	15	VAL	2.0
45	1n	33	VAL	2.0
47	2p	20	VAL	2.0
52	1u	10	ARG	2.0
28	26	7	ILE	2.0
40	1i	63	ILE	2.0
14	2S	33	LYS	2.0
1	1A	886	C	2.0
1	2A	2142	C	2.0
33	1b	188	ALA	2.0
45	2n	5	ALA	2.0
51	1t	32	ALA	2.0
54	2w	10	G	2.0
45	1n	13	THR	2.0
6	2G	178	PHE	2.0
21	2Z	44	PHE	2.0
7	2H	130	ARG	2.0
47	1p	49	LEU	2.0
50	1s	30	LEU	2.0
50	2s	16	LEU	2.0
21	2Z	167	PRO	2.0
48	1q	34	LYS	2.0
50	1s	58	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
50	2s	59	PRO	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	1y	55	20/21	0.77	0.23	76,88,98,107	0
54	7MG	2w	46	24/25	0.80	0.19	73,84,97,109	0
56	PSU	2y	55	20/21	0.81	0.30	82,89,98,99	0
56	4SU	2y	8	20/21	0.81	0.13	79,91,105,109	0
54	PSU	2w	55	20/21	0.82	0.23	65,83,91,93	0
56	7MG	1y	46	24/25	0.84	0.20	77,89,97,101	0
54	7MG	1w	46	24/25	0.84	0.18	73,83,99,115	0
56	PSU	2y	32	20/21	0.84	0.24	77,84,94,100	0
56	7MG	2y	46	24/25	0.84	0.20	81,93,98,108	0
54	PSU	2w	32	20/21	0.86	0.23	74,81,91,101	0
56	5MU	1y	54	21/22	0.87	0.21	69,78,89,89	0
54	4SU	2w	8	20/21	0.87	0.16	79,89,97,102	0
32	5MC	2a	967	21/22	0.88	0.23	61,70,76,83	0
56	5MU	2y	54	21/22	0.88	0.26	78,88,95,104	0
56	4SU	1y	8	20/21	0.88	0.15	81,85,89,89	0
54	4SU	1w	8	20/21	0.89	0.16	68,80,88,90	0
56	PSU	1y	32	20/21	0.89	0.24	70,76,82,88	0
56	PSU	2y	39	20/21	0.89	0.22	70,79,93,96	0
54	PSU	1w	55	20/21	0.90	0.20	62,73,80,84	0
55	4SU	2x	8	20/21	0.90	0.14	64,72,82,83	0
56	PSU	1y	39	20/21	0.91	0.23	64,72,79,80	0
32	2MG	2a	1207	24/25	0.91	0.16	73,80,84,86	0
55	PSU	2x	55	20/21	0.91	0.14	63,70,80,81	0
54	5MU	2w	54	21/22	0.92	0.18	62,74,79,82	0
56	MIA	2y	37	22/30	0.92	0.18	75,80,90,95	0
54	PSU	2w	39	20/21	0.92	0.32	67,78,83,83	0
32	PSU	2a	516	20/21	0.92	0.19	67,74,79,80	0
55	5MU	2x	54	21/22	0.92	0.15	68,72,77,85	0
43	0TD	1l	92	10/11	0.92	0.21	43,51,56,57	0
54	MIA	2w	37	25/30	0.93	0.23	70,77,83,90	0
32	7MG	2a	527	24/25	0.93	0.21	55,65,70,76	0
1	4OC	2A	1920	21/23	0.93	0.18	59,65,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	1w	32	20/21	0.93	0.23	59,70,75,76	0
43	0TD	2l	92	10/11	0.93	0.24	63,66,70,80	0
32	M2G	2a	966	25/26	0.94	0.27	62,70,82,86	0
56	MIA	1y	37	22/30	0.94	0.19	69,74,80,86	0
1	PSU	2A	1911	20/21	0.94	0.19	53,65,73,74	0
32	5MC	2a	1400	21/22	0.94	0.28	62,71,78,80	0
55	4SU	1x	8	20/21	0.94	0.20	50,67,71,71	0
54	PSU	1w	39	20/21	0.94	0.27	64,69,75,76	0
55	5MC	2x	32	21/22	0.94	0.19	60,65,73,75	0
32	4OC	2a	1402	22/23	0.94	0.18	56,65,69,73	0
55	PSU	1x	55	20/21	0.94	0.16	51,59,66,75	0
1	5MU	2A	1915	21/22	0.94	0.16	63,70,78,85	0
1	MA6	2A	2058	24/25	0.95	0.24	32,43,47,49	0
54	MIA	1w	37	29/30	0.95	0.25	45,59,66,67	0
1	OMU	2A	2552	21/22	0.95	0.18	40,47,53,58	0
32	5MC	2a	1407	21/22	0.95	0.20	53,59,68,71	0
32	MA6	2a	1518	24/25	0.95	0.24	53,68,73,74	0
32	PSU	1a	516	20/21	0.95	0.14	52,59,63,65	0
32	2MG	1a	1207	24/25	0.95	0.15	57,65,70,77	0
1	5MU	1A	1915	21/22	0.95	0.15	40,47,52,65	0
32	MA6	2a	1519	24/25	0.96	0.22	53,66,71,74	0
54	5MU	1w	54	21/22	0.96	0.17	59,66,71,74	0
1	PSU	1A	1917	20/21	0.96	0.18	41,46,48,55	0
1	5MC	2A	1942	21/22	0.96	0.17	52,58,65,68	0
32	M2G	1a	966	25/26	0.96	0.19	47,55,60,65	0
1	PSU	2A	2605	20/21	0.96	0.19	37,44,48,49	0
32	5MC	1a	1404	21/22	0.96	0.26	38,43,47,48	0
55	5MC	1x	32	21/22	0.96	0.18	46,55,61,65	0
32	5MC	2a	1404	21/22	0.96	0.24	52,61,65,67	0
55	5MU	1x	54	21/22	0.96	0.17	51,60,65,73	0
32	5MC	1a	967	21/22	0.96	0.20	46,58,60,63	0
32	UR3	2a	1498	21/22	0.96	0.23	57,61,67,68	0
1	5MC	2A	1962	21/22	0.96	0.20	47,53,58,75	0
55	31H	2x	76	32/33	0.96	0.23	32,50,60,68	0
32	5MC	1a	1400	21/22	0.97	0.19	44,52,56,59	0
1	PSU	1A	1911	20/21	0.97	0.20	41,50,54,57	0
32	4OC	1a	1402	22/23	0.97	0.19	42,47,55,57	0
1	OMG	2A	2251	24/25	0.97	0.22	31,39,45,48	0
1	5MU	2A	1939	21/22	0.97	0.18	37,45,51,53	0
1	5MC	1A	1942	21/22	0.97	0.16	34,41,47,52	0
32	5MC	1a	1407	21/22	0.97	0.21	29,42,47,49	0
1	PSU	2A	1917	20/21	0.97	0.14	57,68,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	UR3	1a	1498	21/22	0.97	0.20	38,44,46,47	0
1	4OC	1A	1920	21/23	0.97	0.17	37,45,50,54	0
32	7MG	1a	527	24/25	0.97	0.20	42,51,59,64	0
55	31H	1x	76	32/33	0.97	0.24	19,32,42,42	10
32	MA6	1a	1519	24/25	0.97	0.22	38,44,49,54	0
1	OMU	1A	2552	21/22	0.98	0.22	22,30,34,36	0
1	MA6	1A	2058	24/25	0.98	0.21	17,30,37,39	0
1	PSU	1A	2605	20/21	0.98	0.20	24,27,33,34	0
1	5MC	1A	1962	21/22	0.98	0.19	25,34,38,44	0
1	OMG	1A	2251	24/25	0.98	0.21	22,27,31,35	0
1	5MU	1A	1939	21/22	0.98	0.22	24,31,35,49	0
1	2MA	1A	2503	23/24	0.98	0.22	14,22,29,32	0
1	2MA	2A	2503	23/24	0.98	0.21	31,39,46,54	0
32	MA6	1a	1518	24/25	0.98	0.21	36,44,47,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1680	1/1	0.43	0.54	70,70,70,70	0
57	MG	1a	1703	1/1	0.45	0.26	62,62,62,62	0
57	MG	2A	3073	1/1	0.51	0.28	65,65,65,65	0
57	MG	1A	3867	1/1	0.53	0.22	47,47,47,47	0
57	MG	2A	3404	1/1	0.58	0.27	57,57,57,57	0
57	MG	2a	1789	1/1	0.58	0.17	78,78,78,78	0
57	MG	1a	1789	1/1	0.59	0.10	52,52,52,52	0
57	MG	1B	227	1/1	0.61	0.43	75,75,75,75	0
57	MG	2A	3158	1/1	0.61	0.22	51,51,51,51	0
57	MG	1a	1744	1/1	0.62	0.08	69,69,69,69	0
57	MG	1A	3951	1/1	0.62	0.51	50,50,50,50	0
57	MG	1a	1601	1/1	0.62	0.20	68,68,68,68	0
57	MG	1Q	204	1/1	0.63	0.20	72,72,72,72	0
57	MG	2R	201	1/1	0.63	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1653	1/1	0.63	0.27	55,55,55,55	0
57	MG	1A	3516	1/1	0.63	0.21	67,67,67,67	0
57	MG	1A	3463	1/1	0.64	0.20	59,59,59,59	0
57	MG	2A	3354	1/1	0.65	0.20	63,63,63,63	0
57	MG	1A	3230	1/1	0.66	0.30	64,64,64,64	0
57	MG	1A	3541	1/1	0.66	0.19	53,53,53,53	0
57	MG	2A	3327	1/1	0.67	0.16	67,67,67,67	0
57	MG	1a	1603	1/1	0.68	0.25	67,67,67,67	0
57	MG	2A	3554	1/1	0.68	0.09	46,46,46,46	0
57	MG	2A	3159	1/1	0.68	0.21	62,62,62,62	0
57	MG	1A	3965	1/1	0.68	0.14	62,62,62,62	0
57	MG	1A	3960	1/1	0.68	0.12	61,61,61,61	0
57	MG	1A	3603	1/1	0.69	0.18	31,31,31,31	0
57	MG	2A	3456	1/1	0.69	0.29	71,71,71,71	0
57	MG	2a	1761	1/1	0.69	0.13	67,67,67,67	0
57	MG	1A	3593	1/1	0.69	0.19	39,39,39,39	0
57	MG	2A	3791	1/1	0.70	0.12	58,58,58,58	0
57	MG	2A	3853	1/1	0.70	0.26	62,62,62,62	0
57	MG	2A	3281	1/1	0.70	0.20	61,61,61,61	0
57	MG	2a	1806	1/1	0.70	0.13	69,69,69,69	0
57	MG	2A	3591	1/1	0.71	0.12	39,39,39,39	0
60	ZN	24	501	1/1	0.71	0.10	134,134,134,134	0
57	MG	1a	1636	1/1	0.72	0.16	51,51,51,51	0
57	MG	2a	1626	1/1	0.72	0.19	68,68,68,68	0
57	MG	2A	3528	1/1	0.72	0.15	68,68,68,68	0
57	MG	1A	3709	1/1	0.72	0.30	59,59,59,59	0
57	MG	10	107	1/1	0.72	0.09	42,42,42,42	0
57	MG	1a	1607	1/1	0.72	0.21	66,66,66,66	0
57	MG	2w	107	1/1	0.72	0.13	54,54,54,54	0
57	MG	2A	3443	1/1	0.72	0.11	60,60,60,60	0
57	MG	2A	3205	1/1	0.73	0.16	61,61,61,61	0
57	MG	2A	3777	1/1	0.73	0.17	48,48,48,48	0
57	MG	2a	1627	1/1	0.73	0.28	58,58,58,58	0
57	MG	2B	201	1/1	0.73	0.14	56,56,56,56	0
57	MG	2a	1723	1/1	0.73	0.24	65,65,65,65	0
57	MG	1A	3981	1/1	0.74	0.12	44,44,44,44	0
57	MG	2A	3099	1/1	0.74	0.26	73,73,73,73	0
57	MG	2w	106	1/1	0.74	0.63	66,66,66,66	0
57	MG	2A	3469	1/1	0.74	0.14	57,57,57,57	0
57	MG	1A	3357	1/1	0.74	0.24	45,45,45,45	0
57	MG	1A	3830	1/1	0.75	0.16	69,69,69,69	0
57	MG	1A	3317	1/1	0.75	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3939	1/1	0.75	0.14	66,66,66,66	0
57	MG	1A	3090	1/1	0.75	0.11	73,73,73,73	0
57	MG	1A	3378	1/1	0.75	0.19	64,64,64,64	0
57	MG	1a	1766	1/1	0.75	0.24	67,67,67,67	0
57	MG	2A	3761	1/1	0.75	0.11	52,52,52,52	0
57	MG	1A	3797	1/1	0.75	0.13	56,56,56,56	0
57	MG	1x	103	1/1	0.75	0.19	49,49,49,49	0
57	MG	2A	3385	1/1	0.75	0.11	66,66,66,66	0
57	MG	2A	3058	1/1	0.75	0.29	58,58,58,58	0
57	MG	1A	3664	1/1	0.76	0.16	34,34,34,34	0
57	MG	2a	1679	1/1	0.76	0.16	75,75,75,75	0
57	MG	1a	1650	1/1	0.76	0.20	62,62,62,62	0
57	MG	2A	3479	1/1	0.76	0.21	66,66,66,66	0
57	MG	1A	4004	1/1	0.76	0.10	60,60,60,60	0
57	MG	1A	3928	1/1	0.76	0.13	52,52,52,52	0
57	MG	2A	3441	1/1	0.76	0.14	64,64,64,64	0
57	MG	1A	3437	1/1	0.76	0.27	65,65,65,65	0
57	MG	2a	1651	1/1	0.76	0.14	82,82,82,82	0
57	MG	1A	3938	1/1	0.77	0.12	41,41,41,41	0
57	MG	1A	3913	1/1	0.77	0.09	54,54,54,54	0
57	MG	1A	3460	1/1	0.77	0.21	79,79,79,79	0
57	MG	2A	3181	1/1	0.77	0.29	52,52,52,52	0
57	MG	1a	1671	1/1	0.77	0.30	62,62,62,62	0
57	MG	2A	3085	1/1	0.77	0.30	58,58,58,58	0
57	MG	2A	3486	1/1	0.78	0.27	61,61,61,61	0
57	MG	2A	3373	1/1	0.78	0.26	47,47,47,47	0
57	MG	2A	3383	1/1	0.78	0.12	59,59,59,59	0
57	MG	2A	3577	1/1	0.78	0.15	55,55,55,55	0
57	MG	2a	1657	1/1	0.78	0.09	72,72,72,72	0
57	MG	1A	3097	1/1	0.78	0.13	53,53,53,53	0
57	MG	2a	1705	1/1	0.78	0.19	74,74,74,74	0
57	MG	1A	3451	1/1	0.78	0.26	73,73,73,73	0
57	MG	2a	1744	1/1	0.78	0.23	69,69,69,69	0
57	MG	2a	1757	1/1	0.78	0.19	63,63,63,63	0
57	MG	2A	3229	1/1	0.78	0.20	51,51,51,51	0
57	MG	1A	3418	1/1	0.78	0.26	45,45,45,45	0
57	MG	2A	3282	1/1	0.78	0.14	65,65,65,65	0
57	MG	2g	201	1/1	0.78	0.13	66,66,66,66	0
57	MG	2A	3001	1/1	0.78	0.21	46,46,46,46	0
57	MG	1A	3589	1/1	0.78	0.22	58,58,58,58	0
57	MG	2x	102	1/1	0.78	0.24	71,71,71,71	0
57	MG	2a	1620	1/1	0.78	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3368	1/1	0.79	0.27	65,65,65,65	0
57	MG	2A	3838	1/1	0.79	0.22	70,70,70,70	0
57	MG	2a	1714	1/1	0.79	0.11	73,73,73,73	0
57	MG	2A	3369	1/1	0.79	0.30	52,52,52,52	0
57	MG	1A	3392	1/1	0.79	0.26	58,58,58,58	0
57	MG	1A	3730	1/1	0.79	0.13	49,49,49,49	0
57	MG	1A	3947	1/1	0.79	0.09	39,39,39,39	0
57	MG	1A	3755	1/1	0.79	0.09	49,49,49,49	0
57	MG	1A	3253	1/1	0.79	0.22	47,47,47,47	0
57	MG	2a	1650	1/1	0.79	0.15	77,77,77,77	0
57	MG	2A	3162	1/1	0.79	0.12	52,52,52,52	0
57	MG	2a	1652	1/1	0.79	0.18	67,67,67,67	0
57	MG	2A	3163	1/1	0.79	0.20	65,65,65,65	0
57	MG	2A	3779	1/1	0.79	0.20	62,62,62,62	0
57	MG	1a	1793	1/1	0.80	0.18	64,64,64,64	0
57	MG	2A	3629	1/1	0.80	0.17	46,46,46,46	0
57	MG	2A	3660	1/1	0.80	0.19	65,65,65,65	0
57	MG	1a	1664	1/1	0.80	0.17	49,49,49,49	0
57	MG	2a	1692	1/1	0.80	0.30	59,59,59,59	0
57	MG	2A	3179	1/1	0.80	0.14	68,68,68,68	0
57	MG	1A	3140	1/1	0.80	0.18	33,33,33,33	0
57	MG	1a	1673	1/1	0.80	0.27	68,68,68,68	0
57	MG	1A	3293	1/1	0.80	0.14	45,45,45,45	0
57	MG	2A	3280	1/1	0.80	0.18	52,52,52,52	0
57	MG	1A	3892	1/1	0.80	0.26	65,65,65,65	0
57	MG	1A	4083	1/1	0.80	0.21	56,56,56,56	0
57	MG	2a	1614	1/1	0.80	0.23	56,56,56,56	0
57	MG	2A	3302	1/1	0.80	0.18	55,55,55,55	0
57	MG	2j	201	1/1	0.80	0.19	70,70,70,70	0
57	MG	2A	3304	1/1	0.80	0.32	76,76,76,76	0
57	MG	2A	3107	1/1	0.80	0.12	64,64,64,64	0
57	MG	1A	3590	1/1	0.80	0.36	77,77,77,77	0
57	MG	1A	3672	1/1	0.80	0.15	28,28,28,28	0
57	MG	2a	1612	1/1	0.81	0.20	59,59,59,59	0
57	MG	1A	3488	1/1	0.81	0.30	51,51,51,51	0
57	MG	1A	3943	1/1	0.81	0.12	51,51,51,51	0
57	MG	2A	3172	1/1	0.81	0.15	52,52,52,52	0
57	MG	1a	1751	1/1	0.81	0.10	50,50,50,50	0
57	MG	1V	206	1/1	0.81	0.25	61,61,61,61	0
57	MG	1A	3399	1/1	0.81	0.18	46,46,46,46	0
57	MG	2A	3207	1/1	0.81	0.19	60,60,60,60	0
57	MG	1A	3611	1/1	0.81	0.20	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3659	1/1	0.81	0.11	44,44,44,44	0
57	MG	1A	3225	1/1	0.81	0.23	32,32,32,32	0
57	MG	1A	3571	1/1	0.81	0.27	45,45,45,45	0
57	MG	2A	3070	1/1	0.81	0.21	54,54,54,54	0
57	MG	2A	3609	1/1	0.81	0.10	73,73,73,73	0
57	MG	1A	3994	1/1	0.81	0.15	42,42,42,42	0
57	MG	2A	3321	1/1	0.81	0.16	56,56,56,56	0
57	MG	2A	3727	1/1	0.81	0.24	74,74,74,74	0
57	MG	2A	3325	1/1	0.81	0.19	63,63,63,63	0
57	MG	1A	3055	1/1	0.81	0.23	35,35,35,35	0
57	MG	1A	4079	1/1	0.81	0.37	55,55,55,55	0
57	MG	2A	3367	1/1	0.81	0.29	58,58,58,58	0
57	MG	2A	3100	1/1	0.81	0.13	62,62,62,62	0
57	MG	2I	204	1/1	0.81	0.22	70,70,70,70	0
57	MG	1A	3477	1/1	0.81	0.17	52,52,52,52	0
57	MG	1B	204	1/1	0.81	0.34	68,68,68,68	0
57	MG	1a	1695	1/1	0.81	0.15	48,48,48,48	0
57	MG	2x	103	1/1	0.81	0.12	71,71,71,71	0
57	MG	2X	101	1/1	0.81	0.25	61,61,61,61	0
57	MG	2A	3510	1/1	0.82	0.34	61,61,61,61	0
57	MG	1A	3687	1/1	0.82	0.18	24,24,24,24	0
57	MG	2A	3536	1/1	0.82	0.17	47,47,47,47	0
57	MG	2a	1649	1/1	0.82	0.25	58,58,58,58	0
57	MG	2A	3541	1/1	0.82	0.09	46,46,46,46	0
57	MG	2A	3548	1/1	0.82	0.21	38,38,38,38	0
57	MG	2A	3305	1/1	0.82	0.15	50,50,50,50	0
57	MG	1O	204	1/1	0.82	0.26	55,55,55,55	0
57	MG	1A	3827	1/1	0.82	0.15	58,58,58,58	0
57	MG	1a	1679	1/1	0.82	0.34	63,63,63,63	0
57	MG	1A	4034	1/1	0.82	0.28	61,61,61,61	0
57	MG	2A	3648	1/1	0.82	0.11	69,69,69,69	0
57	MG	2a	1712	1/1	0.82	0.14	70,70,70,70	0
57	MG	2A	3203	1/1	0.82	0.34	70,70,70,70	0
57	MG	1a	1681	1/1	0.82	0.14	64,64,64,64	0
57	MG	1A	4047	1/1	0.82	0.15	30,30,30,30	0
57	MG	1A	3263	1/1	0.82	0.14	37,37,37,37	0
57	MG	2A	3235	1/1	0.82	0.37	53,53,53,53	0
57	MG	2a	1769	1/1	0.82	0.10	73,73,73,73	0
57	MG	2A	3238	1/1	0.82	0.13	47,47,47,47	0
57	MG	2A	3257	1/1	0.82	0.37	66,66,66,66	0
57	MG	2A	3278	1/1	0.82	0.14	66,66,66,66	0
57	MG	2A	3855	1/1	0.82	0.36	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3002	1/1	0.82	0.29	60,60,60,60	0
57	MG	2D	305	1/1	0.82	0.55	60,60,60,60	0
57	MG	1B	203	1/1	0.82	0.18	33,33,33,33	0
57	MG	1A	3565	1/1	0.82	0.18	23,23,23,23	0
57	MG	1B	222	1/1	0.82	0.14	54,54,54,54	0
57	MG	2A	3303	1/1	0.82	0.10	54,54,54,54	0
57	MG	2a	1619	1/1	0.83	0.17	63,63,63,63	0
57	MG	1R	202	1/1	0.83	0.19	41,41,41,41	0
57	MG	2A	3607	1/1	0.83	0.17	42,42,42,42	0
57	MG	1a	1711	1/1	0.83	0.25	69,69,69,69	0
57	MG	2a	1645	1/1	0.83	0.21	62,62,62,62	0
57	MG	1A	3302	1/1	0.83	0.24	55,55,55,55	0
57	MG	2A	3633	1/1	0.83	0.38	49,49,49,49	0
57	MG	2A	3642	1/1	0.83	0.08	79,79,79,79	0
57	MG	2A	3645	1/1	0.83	0.29	71,71,71,71	0
57	MG	2A	3079	1/1	0.83	0.25	59,59,59,59	0
57	MG	2A	3416	1/1	0.83	0.12	57,57,57,57	0
57	MG	2a	1658	1/1	0.83	0.18	67,67,67,67	0
57	MG	2A	3680	1/1	0.83	0.18	67,67,67,67	0
57	MG	2A	3689	1/1	0.83	0.10	54,54,54,54	0
57	MG	1B	219	1/1	0.83	0.26	57,57,57,57	0
57	MG	2A	3088	1/1	0.83	0.15	41,41,41,41	0
57	MG	14	101	1/1	0.83	0.11	57,57,57,57	0
57	MG	1A	3844	1/1	0.83	0.10	55,55,55,55	0
57	MG	2A	3218	1/1	0.83	0.12	60,60,60,60	0
57	MG	2A	3793	1/1	0.83	0.20	68,68,68,68	0
57	MG	2A	3825	1/1	0.83	0.13	43,43,43,43	0
57	MG	1A	3506	1/1	0.83	0.24	50,50,50,50	0
57	MG	2A	3326	1/1	0.83	0.10	57,57,57,57	0
57	MG	2A	3142	1/1	0.83	0.16	54,54,54,54	0
57	MG	2A	3353	1/1	0.83	0.12	67,67,67,67	0
57	MG	2B	213	1/1	0.83	0.11	65,65,65,65	0
57	MG	1A	3511	1/1	0.83	0.28	54,54,54,54	0
57	MG	2q	201	1/1	0.83	0.17	61,61,61,61	0
57	MG	2P	201	1/1	0.83	0.17	55,55,55,55	0
57	MG	1A	4014	1/1	0.83	0.22	46,46,46,46	0
57	MG	2A	3549	1/1	0.83	0.09	48,48,48,48	0
57	MG	2A	3259	1/1	0.83	0.25	60,60,60,60	0
57	MG	2A	3264	1/1	0.83	0.18	59,59,59,59	0
57	MG	1A	3404	1/1	0.84	0.20	58,58,58,58	0
57	MG	1A	3879	1/1	0.84	0.17	40,40,40,40	0
57	MG	1A	3148	1/1	0.84	0.26	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4087	1/1	0.84	0.22	53,53,53,53	0
57	MG	2A	3370	1/1	0.84	0.24	41,41,41,41	0
57	MG	2a	1641	1/1	0.84	0.12	59,59,59,59	0
57	MG	2A	3098	1/1	0.84	0.12	59,59,59,59	0
57	MG	1A	3763	1/1	0.84	0.16	56,56,56,56	0
57	MG	1a	1722	1/1	0.84	0.38	71,71,71,71	0
57	MG	2A	3260	1/1	0.84	0.24	50,50,50,50	0
57	MG	1A	3194	1/1	0.84	0.35	48,48,48,48	0
57	MG	2A	3431	1/1	0.84	0.26	59,59,59,59	0
57	MG	2A	3730	1/1	0.84	0.11	73,73,73,73	0
57	MG	2A	3739	1/1	0.84	0.15	47,47,47,47	0
57	MG	2A	3119	1/1	0.84	0.17	53,53,53,53	0
57	MG	2A	3762	1/1	0.84	0.09	61,61,61,61	0
57	MG	1a	1610	1/1	0.84	0.16	54,54,54,54	0
57	MG	2A	3145	1/1	0.84	0.11	68,68,68,68	0
57	MG	1A	3518	1/1	0.84	0.10	66,66,66,66	0
57	MG	2A	3299	1/1	0.84	0.14	71,71,71,71	0
57	MG	2A	3821	1/1	0.84	0.19	78,78,78,78	0
57	MG	1A	4001	1/1	0.84	0.14	47,47,47,47	0
57	MG	2A	3494	1/1	0.84	0.42	54,54,54,54	0
57	MG	1a	1663	1/1	0.84	0.14	40,40,40,40	0
57	MG	1A	3526	1/1	0.84	0.09	64,64,64,64	0
57	MG	1x	110	1/1	0.84	0.10	71,71,71,71	0
57	MG	2B	202	1/1	0.84	0.29	48,48,48,48	0
57	MG	2A	3174	1/1	0.84	0.15	48,48,48,48	0
57	MG	1A	4006	1/1	0.84	0.10	69,69,69,69	0
57	MG	2A	3047	1/1	0.84	0.14	51,51,51,51	0
57	MG	1A	3942	1/1	0.84	0.12	49,49,49,49	0
57	MG	2T	201	1/1	0.84	0.10	56,56,56,56	0
57	MG	2A	3352	1/1	0.84	0.23	49,49,49,49	0
57	MG	2a	1603	1/1	0.84	0.12	61,61,61,61	0
57	MG	1A	3244	1/1	0.84	0.20	40,40,40,40	0
57	MG	1A	3370	1/1	0.85	0.29	43,43,43,43	0
57	MG	2P	203	1/1	0.85	0.46	63,63,63,63	0
57	MG	2A	3318	1/1	0.85	0.15	62,62,62,62	0
57	MG	1A	3223	1/1	0.85	0.20	37,37,37,37	0
57	MG	1A	4063	1/1	0.85	0.27	53,53,53,53	0
57	MG	26	101	1/1	0.85	0.14	39,39,39,39	0
57	MG	2A	3567	1/1	0.85	0.15	51,51,51,51	0
57	MG	1A	3520	1/1	0.85	0.19	43,43,43,43	0
57	MG	1A	3944	1/1	0.85	0.13	52,52,52,52	0
57	MG	2A	3330	1/1	0.85	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1613	1/1	0.85	0.13	59,59,59,59	0
57	MG	1a	1620	1/1	0.85	0.11	50,50,50,50	0
57	MG	1A	3655	1/1	0.85	0.16	29,29,29,29	0
57	MG	2a	1629	1/1	0.85	0.24	62,62,62,62	0
57	MG	1A	3037	1/1	0.85	0.21	57,57,57,57	0
57	MG	1A	3475	1/1	0.85	0.22	38,38,38,38	0
57	MG	2A	3064	1/1	0.85	0.20	53,53,53,53	0
57	MG	1A	3143	1/1	0.85	0.14	29,29,29,29	0
57	MG	2A	3072	1/1	0.85	0.14	42,42,42,42	0
57	MG	1a	1665	1/1	0.85	0.16	52,52,52,52	0
57	MG	2A	3078	1/1	0.85	0.15	47,47,47,47	0
57	MG	2A	3399	1/1	0.85	0.20	50,50,50,50	0
57	MG	1A	3870	1/1	0.85	0.34	38,38,38,38	0
57	MG	2A	3747	1/1	0.85	0.22	42,42,42,42	0
57	MG	1A	3677	1/1	0.85	0.28	48,48,48,48	0
57	MG	2a	1696	1/1	0.85	0.14	77,77,77,77	0
57	MG	2A	3422	1/1	0.85	0.37	55,55,55,55	0
57	MG	2A	3086	1/1	0.85	0.16	36,36,36,36	0
57	MG	1A	3207	1/1	0.85	0.22	67,67,67,67	0
57	MG	2A	3788	1/1	0.85	0.13	51,51,51,51	0
57	MG	2A	3790	1/1	0.85	0.11	42,42,42,42	0
57	MG	2A	3442	1/1	0.85	0.26	47,47,47,47	0
57	MG	2A	3792	1/1	0.85	0.10	55,55,55,55	0
57	MG	1A	3335	1/1	0.85	0.14	53,53,53,53	0
57	MG	2a	1780	1/1	0.85	0.18	65,65,65,65	0
57	MG	2A	3795	1/1	0.85	0.18	46,46,46,46	0
57	MG	2a	1792	1/1	0.85	0.32	76,76,76,76	0
57	MG	2a	1793	1/1	0.85	0.17	54,54,54,54	0
57	MG	1A	3724	1/1	0.85	0.16	43,43,43,43	0
57	MG	2a	1829	1/1	0.85	0.14	63,63,63,63	0
57	MG	2A	3823	1/1	0.85	0.18	42,42,42,42	0
57	MG	1A	3213	1/1	0.85	0.19	46,46,46,46	0
57	MG	2A	3473	1/1	0.85	0.12	57,57,57,57	0
57	MG	1a	1698	1/1	0.85	0.12	53,53,53,53	0
57	MG	2A	3297	1/1	0.85	0.14	62,62,62,62	0
57	MG	1W	203	1/1	0.85	0.38	38,38,38,38	0
57	MG	10	102	1/1	0.85	0.20	60,60,60,60	0
57	MG	1A	4027	1/1	0.85	0.20	32,32,32,32	0
57	MG	2A	3148	1/1	0.85	0.14	61,61,61,61	0
57	MG	2A	3093	1/1	0.86	0.15	36,36,36,36	0
57	MG	2A	3358	1/1	0.86	0.12	53,53,53,53	0
57	MG	2A	3094	1/1	0.86	0.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1635	1/1	0.86	0.31	51,51,51,51	0
57	MG	1A	3476	1/1	0.86	0.24	41,41,41,41	0
57	MG	2A	3829	1/1	0.86	0.21	49,49,49,49	0
57	MG	1A	4045	1/1	0.86	0.08	49,49,49,49	0
57	MG	1A	3676	1/1	0.86	0.11	24,24,24,24	0
57	MG	1A	3554	1/1	0.86	0.23	31,31,31,31	0
57	MG	1A	3177	1/1	0.86	0.39	38,38,38,38	0
57	MG	1A	3916	1/1	0.86	0.12	63,63,63,63	0
57	MG	1A	3693	1/1	0.86	0.17	36,36,36,36	0
57	MG	2A	3411	1/1	0.86	0.21	63,63,63,63	0
57	MG	1A	3125	1/1	0.86	0.21	45,45,45,45	0
57	MG	1A	3490	1/1	0.86	0.20	52,52,52,52	0
57	MG	1A	3495	1/1	0.86	0.23	50,50,50,50	0
57	MG	1a	1685	1/1	0.86	0.14	52,52,52,52	0
57	MG	2A	3167	1/1	0.86	0.07	66,66,66,66	0
57	MG	1A	3735	1/1	0.86	0.14	60,60,60,60	0
57	MG	1A	3743	1/1	0.86	0.13	54,54,54,54	0
57	MG	2a	1605	1/1	0.86	0.12	68,68,68,68	0
57	MG	1N	204	1/1	0.86	0.20	41,41,41,41	0
57	MG	1A	3361	1/1	0.86	0.43	53,53,53,53	0
57	MG	1a	1718	1/1	0.86	0.15	41,41,41,41	0
57	MG	1A	3759	1/1	0.86	0.15	32,32,32,32	0
57	MG	2a	1621	1/1	0.86	0.25	71,71,71,71	0
57	MG	2a	1622	1/1	0.86	0.14	60,60,60,60	0
57	MG	2A	3492	1/1	0.86	0.12	62,62,62,62	0
57	MG	1A	3251	1/1	0.86	0.13	58,58,58,58	0
57	MG	2A	3495	1/1	0.86	0.15	61,61,61,61	0
57	MG	2A	3208	1/1	0.86	0.15	63,63,63,63	0
57	MG	1R	203	1/1	0.86	0.53	52,52,52,52	0
57	MG	1a	1763	1/1	0.86	0.10	75,75,75,75	0
57	MG	2A	3234	1/1	0.86	0.22	54,54,54,54	0
57	MG	1A	3375	1/1	0.86	0.27	35,35,35,35	0
57	MG	1a	1787	1/1	0.86	0.15	49,49,49,49	0
57	MG	2A	3251	1/1	0.86	0.16	44,44,44,44	0
57	MG	2A	3255	1/1	0.86	0.13	60,60,60,60	0
57	MG	1A	3972	1/1	0.86	0.12	28,28,28,28	0
57	MG	1Z	303	1/1	0.86	0.29	64,64,64,64	0
57	MG	1a	1794	1/1	0.86	0.09	53,53,53,53	0
57	MG	1t	201	1/1	0.86	0.15	62,62,62,62	0
57	MG	1v	101	1/1	0.86	0.15	67,67,67,67	0
57	MG	2A	3632	1/1	0.86	0.23	51,51,51,51	0
57	MG	1w	106	1/1	0.86	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3804	1/1	0.86	0.24	25,25,25,25	0
57	MG	1x	108	1/1	0.86	0.11	68,68,68,68	0
57	MG	2a	1754	1/1	0.86	0.28	62,62,62,62	0
57	MG	10	105	1/1	0.86	0.23	54,54,54,54	0
57	MG	2a	1758	1/1	0.86	0.25	57,57,57,57	0
57	MG	1A	3805	1/1	0.86	0.15	39,39,39,39	0
57	MG	2a	1766	1/1	0.86	0.08	64,64,64,64	0
57	MG	2A	3300	1/1	0.86	0.25	54,54,54,54	0
57	MG	2A	3025	1/1	0.86	0.13	51,51,51,51	0
57	MG	2A	3719	1/1	0.86	0.22	66,66,66,66	0
57	MG	13	105	1/1	0.86	0.21	38,38,38,38	0
57	MG	1A	3822	1/1	0.86	0.20	51,51,51,51	0
57	MG	2a	1803	1/1	0.86	0.12	56,56,56,56	0
57	MG	18	103	1/1	0.86	0.46	47,47,47,47	0
57	MG	1A	3633	1/1	0.86	0.14	38,38,38,38	0
57	MG	2A	3320	1/1	0.86	0.38	52,52,52,52	0
57	MG	1A	3079	1/1	0.86	0.32	35,35,35,35	0
57	MG	2A	3766	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3387	1/1	0.86	0.47	43,43,43,43	0
57	MG	1A	4022	1/1	0.86	0.24	40,40,40,40	0
57	MG	1a	1612	1/1	0.86	0.11	54,54,54,54	0
57	MG	1A	3324	1/1	0.86	0.28	56,56,56,56	0
57	MG	1A	4030	1/1	0.86	0.19	43,43,43,43	0
57	MG	1a	1629	1/1	0.86	0.20	49,49,49,49	0
57	MG	1a	1624	1/1	0.87	0.13	51,51,51,51	0
57	MG	1a	1761	1/1	0.87	0.15	57,57,57,57	0
57	MG	1A	4017	1/1	0.87	0.18	57,57,57,57	0
57	MG	1A	3216	1/1	0.87	0.20	40,40,40,40	0
57	MG	2A	3096	1/1	0.87	0.10	48,48,48,48	0
57	MG	1A	3858	1/1	0.87	0.25	56,56,56,56	0
57	MG	1A	3218	1/1	0.87	0.21	43,43,43,43	0
57	MG	1a	1790	1/1	0.87	0.09	74,74,74,74	0
57	MG	2A	3699	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3707	1/1	0.87	0.18	61,61,61,61	0
57	MG	2A	3105	1/1	0.87	0.07	57,57,57,57	0
57	MG	2a	1640	1/1	0.87	0.25	63,63,63,63	0
57	MG	2A	3407	1/1	0.87	0.32	42,42,42,42	0
57	MG	2a	1644	1/1	0.87	0.13	50,50,50,50	0
57	MG	1A	3004	1/1	0.87	0.14	29,29,29,29	0
57	MG	1A	3132	1/1	0.87	0.11	46,46,46,46	0
57	MG	1a	1811	1/1	0.87	0.20	63,63,63,63	0
57	MG	2A	3284	1/1	0.87	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3438	1/1	0.87	0.18	40,40,40,40	0
57	MG	2A	3765	1/1	0.87	0.41	60,60,60,60	0
57	MG	2A	3286	1/1	0.87	0.27	52,52,52,52	0
57	MG	2A	3295	1/1	0.87	0.15	46,46,46,46	0
57	MG	2a	1678	1/1	0.87	0.14	57,57,57,57	0
57	MG	1Z	304	1/1	0.87	0.25	57,57,57,57	0
57	MG	1A	3780	1/1	0.87	0.10	40,40,40,40	0
57	MG	2A	3462	1/1	0.87	0.28	43,43,43,43	0
57	MG	2a	1703	1/1	0.87	0.20	69,69,69,69	0
57	MG	1A	3480	1/1	0.87	0.18	42,42,42,42	0
57	MG	1A	3973	1/1	0.87	0.19	33,33,33,33	0
57	MG	1A	3133	1/1	0.87	0.15	26,26,26,26	0
57	MG	1A	3987	1/1	0.87	0.12	40,40,40,40	0
57	MG	2a	1733	1/1	0.87	0.11	63,63,63,63	0
57	MG	1A	3992	1/1	0.87	0.14	38,38,38,38	0
57	MG	1a	1686	1/1	0.87	0.12	62,62,62,62	0
57	MG	2A	3033	1/1	0.87	0.16	43,43,43,43	0
57	MG	2A	3496	1/1	0.87	0.21	57,57,57,57	0
57	MG	1a	1690	1/1	0.87	0.12	61,61,61,61	0
57	MG	1A	3922	1/1	0.87	0.09	39,39,39,39	0
57	MG	1A	3713	1/1	0.87	0.13	46,46,46,46	0
57	MG	1A	4003	1/1	0.87	0.15	71,71,71,71	0
57	MG	2A	3328	1/1	0.87	0.13	76,76,76,76	0
57	MG	2B	204	1/1	0.87	0.22	61,61,61,61	0
57	MG	2A	3329	1/1	0.87	0.20	61,61,61,61	0
57	MG	2B	219	1/1	0.87	0.08	66,66,66,66	0
57	MG	1A	3159	1/1	0.87	0.28	46,46,46,46	0
57	MG	2a	1815	1/1	0.87	0.27	61,61,61,61	0
57	MG	2F	303	1/1	0.87	0.17	57,57,57,57	0
57	MG	2F	304	1/1	0.87	0.20	45,45,45,45	0
57	MG	2A	3351	1/1	0.87	0.37	49,49,49,49	0
57	MG	1a	1715	1/1	0.87	0.28	52,52,52,52	0
57	MG	1F	315	1/1	0.87	0.18	50,50,50,50	0
57	MG	1A	3318	1/1	0.87	0.20	24,24,24,24	0
57	MG	1A	3385	1/1	0.87	0.16	29,29,29,29	0
57	MG	25	104	1/1	0.87	0.19	55,55,55,55	0
57	MG	2A	3363	1/1	0.87	0.35	59,59,59,59	0
60	ZN	14	102	1/1	0.87	0.12	122,122,122,122	0
57	MG	28	102	1/1	0.87	0.18	55,55,55,55	0
60	ZN	2n	501	1/1	0.87	0.07	91,91,91,91	0
57	MG	2A	3258	1/1	0.88	0.25	56,56,56,56	0
57	MG	2E	301	1/1	0.88	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1660	1/1	0.88	0.11	50,50,50,50	0
57	MG	1A	3474	1/1	0.88	0.21	47,47,47,47	0
57	MG	2G	201	1/1	0.88	0.09	67,67,67,67	0
57	MG	1B	206	1/1	0.88	0.17	47,47,47,47	0
57	MG	1A	3584	1/1	0.88	0.25	42,42,42,42	0
57	MG	1A	3058	1/1	0.88	0.09	55,55,55,55	0
57	MG	1A	3247	1/1	0.88	0.23	50,50,50,50	0
57	MG	1F	311	1/1	0.88	0.17	38,38,38,38	0
57	MG	2I	102	1/1	0.88	0.22	51,51,51,51	0
57	MG	1A	3307	1/1	0.88	0.14	40,40,40,40	0
57	MG	2A	3511	1/1	0.88	0.13	42,42,42,42	0
57	MG	2A	3514	1/1	0.88	0.17	48,48,48,48	0
57	MG	2a	1601	1/1	0.88	0.17	59,59,59,59	0
57	MG	1A	3963	1/1	0.88	0.28	65,65,65,65	0
57	MG	1A	3597	1/1	0.88	0.15	38,38,38,38	0
57	MG	1A	3379	1/1	0.88	0.22	37,37,37,37	0
57	MG	1A	3482	1/1	0.88	0.39	46,46,46,46	0
57	MG	1A	3309	1/1	0.88	0.20	44,44,44,44	0
57	MG	2A	3301	1/1	0.88	0.19	52,52,52,52	0
57	MG	1A	3023	1/1	0.88	0.24	45,45,45,45	0
57	MG	1A	3989	1/1	0.88	0.12	51,51,51,51	0
57	MG	1a	1710	1/1	0.88	0.17	51,51,51,51	0
57	MG	1A	3991	1/1	0.88	0.20	35,35,35,35	0
57	MG	1A	3826	1/1	0.88	0.19	37,37,37,37	0
57	MG	1A	3492	1/1	0.88	0.21	42,42,42,42	0
57	MG	2A	3630	1/1	0.88	0.15	41,41,41,41	0
57	MG	1a	1721	1/1	0.88	0.17	52,52,52,52	0
57	MG	10	103	1/1	0.88	0.25	38,38,38,38	0
57	MG	1a	1733	1/1	0.88	0.17	39,39,39,39	0
57	MG	2A	3131	1/1	0.88	0.26	57,57,57,57	0
57	MG	1A	3389	1/1	0.88	0.17	58,58,58,58	0
57	MG	1A	3670	1/1	0.88	0.13	25,25,25,25	0
57	MG	1A	3855	1/1	0.88	0.17	37,37,37,37	0
57	MG	2A	3688	1/1	0.88	0.10	65,65,65,65	0
57	MG	2A	3331	1/1	0.88	0.17	52,52,52,52	0
57	MG	2a	1672	1/1	0.88	0.15	53,53,53,53	0
57	MG	2a	1676	1/1	0.88	0.10	73,73,73,73	0
57	MG	2A	3694	1/1	0.88	0.10	63,63,63,63	0
57	MG	2A	3336	1/1	0.88	0.16	54,54,54,54	0
57	MG	2a	1687	1/1	0.88	0.12	50,50,50,50	0
57	MG	2A	3704	1/1	0.88	0.12	51,51,51,51	0
57	MG	2A	3342	1/1	0.88	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3151	1/1	0.88	0.22	53,53,53,53	0
57	MG	1A	3025	1/1	0.88	0.23	58,58,58,58	0
57	MG	1A	3258	1/1	0.88	0.22	28,28,28,28	0
57	MG	1a	1767	1/1	0.88	0.24	66,66,66,66	0
57	MG	2a	1717	1/1	0.88	0.21	53,53,53,53	0
57	MG	2A	3740	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3746	1/1	0.88	0.12	59,59,59,59	0
57	MG	2a	1737	1/1	0.88	0.15	61,61,61,61	0
57	MG	1A	3325	1/1	0.88	0.18	38,38,38,38	0
57	MG	2a	1748	1/1	0.88	0.13	52,52,52,52	0
57	MG	2A	3758	1/1	0.88	0.16	55,55,55,55	0
57	MG	2a	1755	1/1	0.88	0.24	74,74,74,74	0
57	MG	1A	3877	1/1	0.88	0.16	34,34,34,34	0
57	MG	1A	3679	1/1	0.88	0.09	43,43,43,43	0
57	MG	1A	3883	1/1	0.88	0.24	34,34,34,34	0
57	MG	1A	3056	1/1	0.88	0.27	38,38,38,38	0
57	MG	1a	1802	1/1	0.88	0.24	66,66,66,66	0
57	MG	2A	3372	1/1	0.88	0.17	51,51,51,51	0
57	MG	2A	3186	1/1	0.88	0.20	59,59,59,59	0
57	MG	2A	3194	1/1	0.88	0.20	51,51,51,51	0
57	MG	1A	3434	1/1	0.88	0.22	56,56,56,56	0
57	MG	2a	1801	1/1	0.88	0.33	78,78,78,78	0
57	MG	1b	301	1/1	0.88	0.11	62,62,62,62	0
57	MG	2a	1804	1/1	0.88	0.20	60,60,60,60	0
57	MG	1A	3356	1/1	0.88	0.13	39,39,39,39	0
57	MG	1A	3273	1/1	0.88	0.13	43,43,43,43	0
57	MG	2A	3217	1/1	0.88	0.25	63,63,63,63	0
57	MG	2A	3412	1/1	0.88	0.24	58,58,58,58	0
57	MG	2A	3413	1/1	0.88	0.26	42,42,42,42	0
57	MG	1w	101	1/1	0.88	0.18	53,53,53,53	0
57	MG	1A	3274	1/1	0.88	0.13	39,39,39,39	0
57	MG	2w	105	1/1	0.88	0.10	75,75,75,75	0
57	MG	1x	102	1/1	0.88	0.15	56,56,56,56	0
57	MG	1a	1632	1/1	0.88	0.14	54,54,54,54	0
57	MG	1x	105	1/1	0.88	0.10	49,49,49,49	0
57	MG	2A	3243	1/1	0.88	0.17	58,58,58,58	0
57	MG	1A	3366	1/1	0.88	0.36	50,50,50,50	0
57	MG	1A	3732	1/1	0.88	0.08	32,32,32,32	0
57	MG	1A	3733	1/1	0.88	0.20	38,38,38,38	0
57	MG	2A	3522	1/1	0.89	0.11	49,49,49,49	0
57	MG	2A	3527	1/1	0.89	0.29	66,66,66,66	0
57	MG	1A	3688	1/1	0.89	0.25	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3530	1/1	0.89	0.11	50,50,50,50	0
57	MG	1A	3161	1/1	0.89	0.45	39,39,39,39	0
57	MG	2A	3111	1/1	0.89	0.14	63,63,63,63	0
57	MG	2X	103	1/1	0.89	0.18	49,49,49,49	0
57	MG	2A	3117	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3306	1/1	0.89	0.16	45,45,45,45	0
57	MG	1B	202	1/1	0.89	0.33	50,50,50,50	0
57	MG	2A	3125	1/1	0.89	0.40	60,60,60,60	0
57	MG	1A	3369	1/1	0.89	0.11	46,46,46,46	0
57	MG	2A	3580	1/1	0.89	0.13	64,64,64,64	0
57	MG	2A	3582	1/1	0.89	0.31	77,77,77,77	0
57	MG	2a	1609	1/1	0.89	0.08	73,73,73,73	0
57	MG	2A	3140	1/1	0.89	0.19	40,40,40,40	0
57	MG	2A	3603	1/1	0.89	0.09	41,41,41,41	0
57	MG	2A	3604	1/1	0.89	0.09	41,41,41,41	0
57	MG	1a	1619	1/1	0.89	0.28	61,61,61,61	0
57	MG	1A	3268	1/1	0.89	0.25	52,52,52,52	0
57	MG	2A	3611	1/1	0.89	0.19	68,68,68,68	0
57	MG	2A	3628	1/1	0.89	0.13	45,45,45,45	0
57	MG	1a	1622	1/1	0.89	0.24	55,55,55,55	0
57	MG	2a	1628	1/1	0.89	0.27	57,57,57,57	0
57	MG	1A	3155	1/1	0.89	0.19	23,23,23,23	0
57	MG	2a	1636	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3631	1/1	0.89	0.14	46,46,46,46	0
57	MG	1B	214	1/1	0.89	0.21	56,56,56,56	0
57	MG	1A	3866	1/1	0.89	0.12	40,40,40,40	0
57	MG	2A	3334	1/1	0.89	0.49	63,63,63,63	0
57	MG	1A	3976	1/1	0.89	0.13	25,25,25,25	0
57	MG	1A	3729	1/1	0.89	0.16	49,49,49,49	0
57	MG	2A	3654	1/1	0.89	0.15	70,70,70,70	0
57	MG	1a	1638	1/1	0.89	0.18	48,48,48,48	0
57	MG	2A	3667	1/1	0.89	0.14	57,57,57,57	0
57	MG	1a	1640	1/1	0.89	0.12	46,46,46,46	0
57	MG	1f	201	1/1	0.89	0.15	39,39,39,39	0
57	MG	2A	3176	1/1	0.89	0.12	38,38,38,38	0
57	MG	1a	1649	1/1	0.89	0.17	48,48,48,48	0
57	MG	1D	307	1/1	0.89	0.14	38,38,38,38	0
57	MG	1E	313	1/1	0.89	0.09	51,51,51,51	0
57	MG	2a	1680	1/1	0.89	0.15	64,64,64,64	0
57	MG	1A	3453	1/1	0.89	0.14	43,43,43,43	0
57	MG	1A	3604	1/1	0.89	0.14	58,58,58,58	0
57	MG	2a	1694	1/1	0.89	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1695	1/1	0.89	0.30	66,66,66,66	0
57	MG	2A	3721	1/1	0.89	0.11	57,57,57,57	0
57	MG	1A	3455	1/1	0.89	0.17	30,30,30,30	0
57	MG	1A	3459	1/1	0.89	0.15	34,34,34,34	0
57	MG	2A	3735	1/1	0.89	0.09	46,46,46,46	0
57	MG	2a	1713	1/1	0.89	0.12	69,69,69,69	0
57	MG	1A	3651	1/1	0.89	0.20	40,40,40,40	0
57	MG	2A	3379	1/1	0.89	0.32	55,55,55,55	0
57	MG	1A	3906	1/1	0.89	0.20	22,22,22,22	0
57	MG	1x	112	1/1	0.89	0.14	66,66,66,66	0
57	MG	2A	3754	1/1	0.89	0.12	61,61,61,61	0
57	MG	1A	3911	1/1	0.89	0.18	57,57,57,57	0
57	MG	2A	3023	1/1	0.89	0.14	64,64,64,64	0
57	MG	2a	1752	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3252	1/1	0.89	0.21	45,45,45,45	0
57	MG	1W	202	1/1	0.89	0.28	43,43,43,43	0
57	MG	1A	3029	1/1	0.89	0.28	37,37,37,37	0
57	MG	2A	3248	1/1	0.89	0.25	49,49,49,49	0
57	MG	1a	1688	1/1	0.89	0.07	56,56,56,56	0
57	MG	1A	3349	1/1	0.89	0.21	45,45,45,45	0
57	MG	2A	3066	1/1	0.89	0.07	71,71,71,71	0
57	MG	2a	1778	1/1	0.89	0.14	67,67,67,67	0
57	MG	1a	1692	1/1	0.89	0.20	56,56,56,56	0
57	MG	2a	1784	1/1	0.89	0.16	55,55,55,55	0
57	MG	2a	1788	1/1	0.89	0.12	68,68,68,68	0
57	MG	1A	3766	1/1	0.89	0.13	20,20,20,20	0
57	MG	1A	3934	1/1	0.89	0.10	60,60,60,60	0
57	MG	2A	3263	1/1	0.89	0.23	63,63,63,63	0
57	MG	2A	3810	1/1	0.89	0.27	53,53,53,53	0
57	MG	2A	3074	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3275	1/1	0.89	0.18	52,52,52,52	0
57	MG	1A	3354	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1704	1/1	0.89	0.30	56,56,56,56	0
57	MG	2a	1827	1/1	0.89	0.19	55,55,55,55	0
57	MG	1A	3206	1/1	0.89	0.28	54,54,54,54	0
57	MG	2A	3852	1/1	0.89	0.20	45,45,45,45	0
57	MG	1A	3260	1/1	0.89	0.19	39,39,39,39	0
57	MG	1a	1713	1/1	0.89	0.25	44,44,44,44	0
57	MG	1A	3360	1/1	0.89	0.75	51,51,51,51	0
57	MG	1A	3261	1/1	0.89	0.16	52,52,52,52	0
57	MG	1A	3946	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3499	1/1	0.89	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3500	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	4073	1/1	0.89	0.13	38,38,38,38	0
57	MG	2y	106	1/1	0.89	0.10	64,64,64,64	0
57	MG	1A	3588	1/1	0.89	0.40	45,45,45,45	0
57	MG	1a	1736	1/1	0.89	0.12	59,59,59,59	0
57	MG	2A	3520	1/1	0.89	0.20	65,65,65,65	0
57	MG	2A	3782	1/1	0.90	0.15	66,66,66,66	0
57	MG	2A	3785	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3975	1/1	0.90	0.17	32,32,32,32	0
57	MG	2A	3121	1/1	0.90	0.12	52,52,52,52	0
57	MG	1a	1705	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3127	1/1	0.90	0.11	42,42,42,42	0
57	MG	1a	1709	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3135	1/1	0.90	0.16	60,60,60,60	0
57	MG	2A	3378	1/1	0.90	0.20	62,62,62,62	0
57	MG	1A	3027	1/1	0.90	0.20	24,24,24,24	0
57	MG	1Q	203	1/1	0.90	0.18	42,42,42,42	0
57	MG	2A	3824	1/1	0.90	0.16	54,54,54,54	0
57	MG	1A	3977	1/1	0.90	0.12	29,29,29,29	0
57	MG	2A	3146	1/1	0.90	0.21	51,51,51,51	0
57	MG	1A	3515	1/1	0.90	0.23	38,38,38,38	0
57	MG	1A	3217	1/1	0.90	0.30	30,30,30,30	0
57	MG	2A	3410	1/1	0.90	0.27	49,49,49,49	0
57	MG	2A	3154	1/1	0.90	0.11	44,44,44,44	0
57	MG	1S	202	1/1	0.90	0.26	63,63,63,63	0
57	MG	1U	202	1/1	0.90	0.42	49,49,49,49	0
57	MG	2A	3414	1/1	0.90	0.14	56,56,56,56	0
57	MG	2A	3160	1/1	0.90	0.20	46,46,46,46	0
57	MG	2A	3418	1/1	0.90	0.29	51,51,51,51	0
57	MG	2D	301	1/1	0.90	0.23	48,48,48,48	0
57	MG	1a	1723	1/1	0.90	0.12	69,69,69,69	0
57	MG	2A	3425	1/1	0.90	0.20	47,47,47,47	0
57	MG	2A	3429	1/1	0.90	0.19	50,50,50,50	0
57	MG	1A	3255	1/1	0.90	0.17	31,31,31,31	0
57	MG	2F	308	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3433	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3108	1/1	0.90	0.17	28,28,28,28	0
57	MG	1a	1741	1/1	0.90	0.12	41,41,41,41	0
57	MG	2Q	201	1/1	0.90	0.39	49,49,49,49	0
57	MG	1A	3184	1/1	0.90	0.49	42,42,42,42	0
57	MG	1a	1745	1/1	0.90	0.08	55,55,55,55	0
57	MG	2T	203	1/1	0.90	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3531	1/1	0.90	0.15	45,45,45,45	0
57	MG	1A	3082	1/1	0.90	0.70	34,34,34,34	0
57	MG	1a	1762	1/1	0.90	0.09	62,62,62,62	0
57	MG	2A	3191	1/1	0.90	0.11	61,61,61,61	0
57	MG	2A	3476	1/1	0.90	0.10	64,64,64,64	0
57	MG	2A	3192	1/1	0.90	0.27	59,59,59,59	0
57	MG	10	101	1/1	0.90	0.15	35,35,35,35	0
57	MG	2A	3197	1/1	0.90	0.19	43,43,43,43	0
57	MG	1a	1765	1/1	0.90	0.14	51,51,51,51	0
57	MG	2a	1607	1/1	0.90	0.11	51,51,51,51	0
57	MG	1A	3869	1/1	0.90	0.14	33,33,33,33	0
57	MG	1A	3464	1/1	0.90	0.13	49,49,49,49	0
57	MG	1a	1776	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3212	1/1	0.90	0.17	49,49,49,49	0
57	MG	2A	3501	1/1	0.90	0.07	72,72,72,72	0
57	MG	2A	3215	1/1	0.90	0.43	55,55,55,55	0
57	MG	1A	3466	1/1	0.90	0.21	27,27,27,27	0
57	MG	1A	3326	1/1	0.90	0.21	35,35,35,35	0
57	MG	1A	3720	1/1	0.90	0.13	52,52,52,52	0
57	MG	2A	3231	1/1	0.90	0.16	56,56,56,56	0
57	MG	2A	3524	1/1	0.90	0.33	64,64,64,64	0
57	MG	1A	3576	1/1	0.90	0.16	40,40,40,40	0
57	MG	15	109	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3236	1/1	0.90	0.17	69,69,69,69	0
57	MG	17	107	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3537	1/1	0.90	0.09	50,50,50,50	0
57	MG	2A	3241	1/1	0.90	0.14	42,42,42,42	0
57	MG	1A	4023	1/1	0.90	0.07	49,49,49,49	0
57	MG	18	105	1/1	0.90	0.16	53,53,53,53	0
57	MG	1A	3070	1/1	0.90	0.18	48,48,48,48	0
57	MG	2A	3563	1/1	0.90	0.07	47,47,47,47	0
57	MG	1a	1602	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3909	1/1	0.90	0.18	31,31,31,31	0
57	MG	1a	1604	1/1	0.90	0.24	53,53,53,53	0
57	MG	2A	3581	1/1	0.90	0.23	50,50,50,50	0
57	MG	1A	3235	1/1	0.90	0.58	35,35,35,35	0
57	MG	2A	3586	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	4037	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3593	1/1	0.90	0.17	44,44,44,44	0
57	MG	1A	3352	1/1	0.90	0.19	48,48,48,48	0
57	MG	1A	3096	1/1	0.90	0.11	40,40,40,40	0
57	MG	1A	4058	1/1	0.90	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3591	1/1	0.90	0.12	42,42,42,42	0
57	MG	1A	4069	1/1	0.90	0.17	59,59,59,59	0
57	MG	2a	1704	1/1	0.90	0.46	75,75,75,75	0
57	MG	2A	3614	1/1	0.90	0.18	49,49,49,49	0
57	MG	1a	1623	1/1	0.90	0.10	57,57,57,57	0
57	MG	2A	3006	1/1	0.90	0.18	61,61,61,61	0
57	MG	2A	3018	1/1	0.90	0.22	45,45,45,45	0
57	MG	1A	3737	1/1	0.90	0.27	15,15,15,15	0
57	MG	2A	3292	1/1	0.90	0.16	41,41,41,41	0
57	MG	2a	1729	1/1	0.90	0.29	49,49,49,49	0
57	MG	1A	4074	1/1	0.90	0.17	58,58,58,58	0
57	MG	1A	4076	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3644	1/1	0.90	0.14	59,59,59,59	0
57	MG	2a	1746	1/1	0.90	0.20	49,49,49,49	0
57	MG	2A	3045	1/1	0.90	0.15	61,61,61,61	0
57	MG	2A	3046	1/1	0.90	0.16	59,59,59,59	0
57	MG	1A	3208	1/1	0.90	0.18	26,26,26,26	0
57	MG	2A	3659	1/1	0.90	0.47	66,66,66,66	0
57	MG	2A	3053	1/1	0.90	0.20	45,45,45,45	0
57	MG	1A	4082	1/1	0.90	0.15	46,46,46,46	0
57	MG	1A	3747	1/1	0.90	0.15	34,34,34,34	0
57	MG	1A	4085	1/1	0.90	0.18	58,58,58,58	0
57	MG	1A	3283	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	4088	1/1	0.90	0.29	45,45,45,45	0
57	MG	2A	3696	1/1	0.90	0.10	37,37,37,37	0
57	MG	1A	3599	1/1	0.90	0.16	25,25,25,25	0
57	MG	2a	1787	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3700	1/1	0.90	0.50	72,72,72,72	0
57	MG	1A	3762	1/1	0.90	0.22	19,19,19,19	0
57	MG	2A	3705	1/1	0.90	0.20	61,61,61,61	0
57	MG	1A	3489	1/1	0.90	0.13	51,51,51,51	0
57	MG	2a	1799	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3713	1/1	0.90	0.08	42,42,42,42	0
57	MG	1A	3427	1/1	0.90	0.18	38,38,38,38	0
57	MG	1B	209	1/1	0.90	0.29	46,46,46,46	0
57	MG	1A	3777	1/1	0.90	0.16	38,38,38,38	0
57	MG	2a	1807	1/1	0.90	0.18	61,61,61,61	0
57	MG	2a	1808	1/1	0.90	0.14	67,67,67,67	0
57	MG	1A	3778	1/1	0.90	0.49	62,62,62,62	0
57	MG	2a	1822	1/1	0.90	0.18	62,62,62,62	0
57	MG	1A	3957	1/1	0.90	0.18	52,52,52,52	0
57	MG	2A	3736	1/1	0.90	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	225	1/1	0.90	0.18	49,49,49,49	0
57	MG	1A	3248	1/1	0.90	0.37	32,32,32,32	0
57	MG	1B	230	1/1	0.90	0.20	57,57,57,57	0
57	MG	1A	3494	1/1	0.90	0.24	32,32,32,32	0
57	MG	2w	103	1/1	0.90	0.44	65,65,65,65	0
57	MG	2A	3344	1/1	0.90	0.15	53,53,53,53	0
57	MG	1A	3160	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3104	1/1	0.90	0.14	54,54,54,54	0
57	MG	1A	3440	1/1	0.90	0.26	31,31,31,31	0
57	MG	1A	3510	1/1	0.90	0.35	36,36,36,36	0
57	MG	2A	3356	1/1	0.90	0.11	67,67,67,67	0
57	MG	2A	3773	1/1	0.90	0.17	62,62,62,62	0
57	MG	1G	203	1/1	0.90	0.10	61,61,61,61	0
57	MG	1I	201	1/1	0.90	0.18	55,55,55,55	0
57	MG	2B	205	1/1	0.91	0.12	48,48,48,48	0
57	MG	2A	3271	1/1	0.91	0.22	50,50,50,50	0
57	MG	2B	216	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	3896	1/1	0.91	0.15	42,42,42,42	0
57	MG	1A	3373	1/1	0.91	0.32	37,37,37,37	0
57	MG	1A	3447	1/1	0.91	0.13	39,39,39,39	0
57	MG	10	104	1/1	0.91	0.17	37,37,37,37	0
57	MG	1A	3739	1/1	0.91	0.14	33,33,33,33	0
57	MG	1a	1717	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3449	1/1	0.91	0.39	43,43,43,43	0
57	MG	2A	3288	1/1	0.91	0.19	58,58,58,58	0
57	MG	11	104	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3288	1/1	0.91	0.25	41,41,41,41	0
57	MG	2A	3540	1/1	0.91	0.11	37,37,37,37	0
57	MG	1A	3496	1/1	0.91	0.31	33,33,33,33	0
57	MG	1a	1725	1/1	0.91	0.17	49,49,49,49	0
57	MG	1A	4071	1/1	0.91	0.09	63,63,63,63	0
57	MG	2A	3108	1/1	0.91	0.07	43,43,43,43	0
57	MG	2A	3110	1/1	0.91	0.25	50,50,50,50	0
57	MG	2Z	301	1/1	0.91	0.16	62,62,62,62	0
57	MG	17	105	1/1	0.91	0.31	50,50,50,50	0
57	MG	2A	3570	1/1	0.91	0.11	57,57,57,57	0
57	MG	2A	3114	1/1	0.91	0.19	41,41,41,41	0
57	MG	1A	3927	1/1	0.91	0.13	41,41,41,41	0
57	MG	1a	1742	1/1	0.91	0.12	73,73,73,73	0
57	MG	1A	3757	1/1	0.91	0.14	20,20,20,20	0
57	MG	1A	3932	1/1	0.91	0.19	22,22,22,22	0
57	MG	2a	1606	1/1	0.91	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4078	1/1	0.91	0.14	41,41,41,41	0
57	MG	2a	1608	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3340	1/1	0.91	0.17	41,41,41,41	0
57	MG	2A	3601	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3761	1/1	0.91	0.10	32,32,32,32	0
57	MG	2A	3138	1/1	0.91	0.26	45,45,45,45	0
57	MG	1A	3341	1/1	0.91	0.17	48,48,48,48	0
57	MG	1a	1764	1/1	0.91	0.17	47,47,47,47	0
57	MG	1A	3940	1/1	0.91	0.08	72,72,72,72	0
57	MG	1A	4086	1/1	0.91	0.15	53,53,53,53	0
57	MG	1A	3380	1/1	0.91	0.25	38,38,38,38	0
57	MG	1A	3644	1/1	0.91	0.11	57,57,57,57	0
57	MG	2A	3341	1/1	0.91	0.12	70,70,70,70	0
57	MG	2a	1631	1/1	0.91	0.15	66,66,66,66	0
57	MG	2a	1634	1/1	0.91	0.22	63,63,63,63	0
57	MG	1A	3179	1/1	0.91	0.17	38,38,38,38	0
57	MG	2A	3343	1/1	0.91	0.20	47,47,47,47	0
57	MG	2A	3157	1/1	0.91	0.13	66,66,66,66	0
57	MG	2A	3350	1/1	0.91	0.19	61,61,61,61	0
57	MG	1A	3945	1/1	0.91	0.09	40,40,40,40	0
57	MG	1A	3241	1/1	0.91	0.23	25,25,25,25	0
57	MG	1A	3116	1/1	0.91	0.17	30,30,30,30	0
57	MG	2A	3650	1/1	0.91	0.26	47,47,47,47	0
57	MG	2A	3651	1/1	0.91	0.12	66,66,66,66	0
57	MG	2A	3161	1/1	0.91	0.15	39,39,39,39	0
57	MG	2a	1654	1/1	0.91	0.06	48,48,48,48	0
57	MG	2A	3656	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3785	1/1	0.91	0.15	33,33,33,33	0
57	MG	2a	1669	1/1	0.91	0.20	62,62,62,62	0
57	MG	1a	1800	1/1	0.91	0.10	64,64,64,64	0
57	MG	2A	3662	1/1	0.91	0.08	51,51,51,51	0
57	MG	2A	3665	1/1	0.91	0.15	55,55,55,55	0
57	MG	2A	3359	1/1	0.91	0.17	44,44,44,44	0
57	MG	2A	3679	1/1	0.91	0.20	63,63,63,63	0
57	MG	2a	1681	1/1	0.91	0.15	59,59,59,59	0
57	MG	2a	1683	1/1	0.91	0.21	55,55,55,55	0
57	MG	1a	1627	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	3796	1/1	0.91	0.09	37,37,37,37	0
57	MG	1A	3519	1/1	0.91	0.10	58,58,58,58	0
57	MG	1A	3669	1/1	0.91	0.15	22,22,22,22	0
57	MG	2A	3177	1/1	0.91	0.23	50,50,50,50	0
57	MG	1f	202	1/1	0.91	0.23	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1m	3001	1/1	0.91	0.08	62,62,62,62	0
57	MG	2A	3183	1/1	0.91	0.11	62,62,62,62	0
57	MG	2a	1711	1/1	0.91	0.11	63,63,63,63	0
57	MG	1n	101	1/1	0.91	0.13	56,56,56,56	0
57	MG	2A	3190	1/1	0.91	0.20	51,51,51,51	0
57	MG	1A	3390	1/1	0.91	0.15	37,37,37,37	0
57	MG	2A	3388	1/1	0.91	0.12	50,50,50,50	0
57	MG	2a	1720	1/1	0.91	0.21	62,62,62,62	0
57	MG	1A	3806	1/1	0.91	0.17	50,50,50,50	0
57	MG	2A	3402	1/1	0.91	0.19	51,51,51,51	0
57	MG	1A	3813	1/1	0.91	0.19	51,51,51,51	0
57	MG	2A	3196	1/1	0.91	0.14	45,45,45,45	0
57	MG	2a	1739	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3467	1/1	0.91	0.20	39,39,39,39	0
57	MG	1A	3185	1/1	0.91	0.28	55,55,55,55	0
57	MG	1a	1654	1/1	0.91	0.22	53,53,53,53	0
57	MG	1a	1658	1/1	0.91	0.12	48,48,48,48	0
57	MG	1F	306	1/1	0.91	0.14	24,24,24,24	0
57	MG	1A	3105	1/1	0.91	0.19	25,25,25,25	0
57	MG	2A	3757	1/1	0.91	0.39	61,61,61,61	0
57	MG	1A	3546	1/1	0.91	0.11	45,45,45,45	0
57	MG	1A	3843	1/1	0.91	0.18	56,56,56,56	0
57	MG	2a	1762	1/1	0.91	0.09	64,64,64,64	0
57	MG	2a	1765	1/1	0.91	0.14	77,77,77,77	0
57	MG	2A	3424	1/1	0.91	0.07	57,57,57,57	0
57	MG	1A	3549	1/1	0.91	0.12	39,39,39,39	0
57	MG	2a	1772	1/1	0.91	0.07	61,61,61,61	0
57	MG	2A	3426	1/1	0.91	0.17	44,44,44,44	0
57	MG	2A	3772	1/1	0.91	0.09	37,37,37,37	0
57	MG	2A	3221	1/1	0.91	0.16	48,48,48,48	0
57	MG	2A	3227	1/1	0.91	0.28	45,45,45,45	0
57	MG	2A	3432	1/1	0.91	0.22	35,35,35,35	0
57	MG	1a	1672	1/1	0.91	0.08	77,77,77,77	0
57	MG	2A	3783	1/1	0.91	0.36	76,76,76,76	0
57	MG	1A	3846	1/1	0.91	0.15	59,59,59,59	0
57	MG	1a	1676	1/1	0.91	0.20	35,35,35,35	0
57	MG	1A	3250	1/1	0.91	0.25	27,27,27,27	0
57	MG	2a	1802	1/1	0.91	0.18	49,49,49,49	0
57	MG	1A	3411	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3451	1/1	0.91	0.26	62,62,62,62	0
57	MG	1A	3860	1/1	0.91	0.17	37,37,37,37	0
57	MG	1A	3568	1/1	0.91	0.20	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3796	1/1	0.91	0.20	39,39,39,39	0
57	MG	2a	1811	1/1	0.91	0.24	58,58,58,58	0
57	MG	2a	1814	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3800	1/1	0.91	0.10	35,35,35,35	0
57	MG	2A	3804	1/1	0.91	0.14	32,32,32,32	0
57	MG	2A	3809	1/1	0.91	0.10	74,74,74,74	0
57	MG	1A	3057	1/1	0.91	0.17	46,46,46,46	0
57	MG	1R	204	1/1	0.91	0.41	38,38,38,38	0
57	MG	1A	3163	1/1	0.91	0.24	33,33,33,33	0
57	MG	1A	3484	1/1	0.91	0.28	53,53,53,53	0
57	MG	2A	3256	1/1	0.91	0.16	38,38,38,38	0
57	MG	2A	3827	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3587	1/1	0.91	0.28	32,32,32,32	0
57	MG	1A	3487	1/1	0.91	0.16	41,41,41,41	0
57	MG	2A	3842	1/1	0.91	0.18	48,48,48,48	0
57	MG	1a	1700	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3113	1/1	0.91	0.20	29,29,29,29	0
57	MG	2x	104	1/1	0.91	0.10	67,67,67,67	0
57	MG	2y	104	1/1	0.91	0.13	73,73,73,73	0
57	MG	2A	3498	1/1	0.91	0.15	55,55,55,55	0
57	MG	1A	3333	1/1	0.91	0.19	45,45,45,45	0
60	ZN	2Y	501	1/1	0.91	0.16	100,100,100,100	0
57	MG	1A	3894	1/1	0.91	0.09	44,44,44,44	0
57	MG	2A	3270	1/1	0.91	0.19	53,53,53,53	0
57	MG	2A	3799	1/1	0.92	0.09	45,45,45,45	0
57	MG	2A	3173	1/1	0.92	0.12	61,61,61,61	0
57	MG	1A	3900	1/1	0.92	0.18	24,24,24,24	0
57	MG	2A	3805	1/1	0.92	0.08	56,56,56,56	0
57	MG	1A	3902	1/1	0.92	0.24	34,34,34,34	0
57	MG	1A	3736	1/1	0.92	0.13	36,36,36,36	0
57	MG	2A	3812	1/1	0.92	0.13	42,42,42,42	0
57	MG	1a	1769	1/1	0.92	0.13	68,68,68,68	0
57	MG	2A	3822	1/1	0.92	0.13	42,42,42,42	0
57	MG	1A	3249	1/1	0.92	0.15	47,47,47,47	0
57	MG	1a	1781	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3358	1/1	0.92	0.18	44,44,44,44	0
57	MG	1A	3047	1/1	0.92	0.23	35,35,35,35	0
57	MG	2A	3427	1/1	0.92	0.23	42,42,42,42	0
57	MG	2A	3428	1/1	0.92	0.44	50,50,50,50	0
57	MG	1A	3491	1/1	0.92	0.30	25,25,25,25	0
57	MG	2A	3849	1/1	0.92	0.24	44,44,44,44	0
57	MG	1A	3920	1/1	0.92	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3592	1/1	0.92	0.14	66,66,66,66	0
57	MG	1a	1796	1/1	0.92	0.06	48,48,48,48	0
57	MG	2A	3856	1/1	0.92	0.13	49,49,49,49	0
57	MG	1a	1615	1/1	0.92	0.19	56,56,56,56	0
57	MG	1a	1618	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	3924	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3127	1/1	0.92	0.17	70,70,70,70	0
57	MG	2B	207	1/1	0.92	0.13	47,47,47,47	0
57	MG	2B	209	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	3596	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3128	1/1	0.92	0.28	34,34,34,34	0
57	MG	2A	3459	1/1	0.92	0.11	44,44,44,44	0
57	MG	1l	202	1/1	0.92	0.08	64,64,64,64	0
57	MG	1A	3443	1/1	0.92	0.14	37,37,37,37	0
57	MG	1A	3445	1/1	0.92	0.24	58,58,58,58	0
57	MG	2E	303	1/1	0.92	0.24	53,53,53,53	0
57	MG	2E	307	1/1	0.92	0.16	51,51,51,51	0
57	MG	2F	301	1/1	0.92	0.28	44,44,44,44	0
57	MG	2A	3475	1/1	0.92	0.14	30,30,30,30	0
57	MG	1A	3314	1/1	0.92	0.25	57,57,57,57	0
57	MG	2F	305	1/1	0.92	0.18	59,59,59,59	0
57	MG	2A	3477	1/1	0.92	0.23	32,32,32,32	0
57	MG	2A	3222	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3226	1/1	0.92	0.34	51,51,51,51	0
57	MG	1A	3774	1/1	0.92	0.16	25,25,25,25	0
57	MG	2A	3228	1/1	0.92	0.54	76,76,76,76	0
57	MG	1A	3077	1/1	0.92	0.23	39,39,39,39	0
57	MG	1w	103	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3232	1/1	0.92	0.14	53,53,53,53	0
57	MG	2V	202	1/1	0.92	0.16	66,66,66,66	0
57	MG	2A	3233	1/1	0.92	0.15	34,34,34,34	0
57	MG	1w	105	1/1	0.92	0.19	60,60,60,60	0
57	MG	1A	3628	1/1	0.92	0.14	23,23,23,23	0
57	MG	2A	3504	1/1	0.92	0.23	47,47,47,47	0
57	MG	25	103	1/1	0.92	0.15	47,47,47,47	0
57	MG	1a	1637	1/1	0.92	0.19	52,52,52,52	0
57	MG	1A	3174	1/1	0.92	0.11	32,32,32,32	0
57	MG	27	101	1/1	0.92	0.17	38,38,38,38	0
57	MG	27	102	1/1	0.92	0.29	53,53,53,53	0
57	MG	2A	3512	1/1	0.92	0.09	63,63,63,63	0
57	MG	2A	3239	1/1	0.92	0.16	45,45,45,45	0
57	MG	2A	3519	1/1	0.92	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3634	1/1	0.92	0.18	51,51,51,51	0
57	MG	2A	3242	1/1	0.92	0.19	62,62,62,62	0
57	MG	1x	106	1/1	0.92	0.13	54,54,54,54	0
57	MG	2A	3245	1/1	0.92	0.68	62,62,62,62	0
57	MG	1a	1645	1/1	0.92	0.14	49,49,49,49	0
57	MG	2a	1610	1/1	0.92	0.21	50,50,50,50	0
57	MG	2A	3250	1/1	0.92	0.18	49,49,49,49	0
57	MG	2A	3533	1/1	0.92	0.07	55,55,55,55	0
57	MG	1a	1646	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3253	1/1	0.92	0.20	53,53,53,53	0
57	MG	1x	111	1/1	0.92	0.08	51,51,51,51	0
57	MG	1B	215	1/1	0.92	0.13	32,32,32,32	0
57	MG	2A	3542	1/1	0.92	0.17	49,49,49,49	0
57	MG	1A	3637	1/1	0.92	0.15	59,59,59,59	0
57	MG	2A	3005	1/1	0.92	0.20	47,47,47,47	0
57	MG	1a	1653	1/1	0.92	0.08	48,48,48,48	0
57	MG	2A	3561	1/1	0.92	0.43	63,63,63,63	0
57	MG	2a	1632	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3013	1/1	0.92	0.24	58,58,58,58	0
57	MG	1B	220	1/1	0.92	0.24	39,39,39,39	0
57	MG	1A	3514	1/1	0.92	0.23	68,68,68,68	0
57	MG	2A	3267	1/1	0.92	0.41	59,59,59,59	0
57	MG	2a	1642	1/1	0.92	0.21	57,57,57,57	0
57	MG	1A	3949	1/1	0.92	0.18	45,45,45,45	0
57	MG	1A	3802	1/1	0.92	0.10	41,41,41,41	0
57	MG	2A	3035	1/1	0.92	0.16	47,47,47,47	0
57	MG	1A	3050	1/1	0.92	0.11	24,24,24,24	0
57	MG	1A	3135	1/1	0.92	0.17	34,34,34,34	0
57	MG	1a	1670	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3600	1/1	0.92	0.19	58,58,58,58	0
57	MG	2A	3049	1/1	0.92	0.34	41,41,41,41	0
57	MG	1D	308	1/1	0.92	0.27	41,41,41,41	0
57	MG	1E	306	1/1	0.92	0.17	20,20,20,20	0
57	MG	2a	1662	1/1	0.92	0.06	64,64,64,64	0
57	MG	2A	3287	1/1	0.92	0.30	50,50,50,50	0
57	MG	1A	3657	1/1	0.92	0.19	17,17,17,17	0
57	MG	2A	3289	1/1	0.92	0.19	70,70,70,70	0
57	MG	2A	3290	1/1	0.92	0.19	43,43,43,43	0
57	MG	2A	3620	1/1	0.92	0.22	54,54,54,54	0
57	MG	2A	3626	1/1	0.92	0.19	48,48,48,48	0
57	MG	1A	3810	1/1	0.92	0.14	59,59,59,59	0
57	MG	2A	3293	1/1	0.92	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3968	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3811	1/1	0.92	0.17	65,65,65,65	0
57	MG	2A	3298	1/1	0.92	0.13	51,51,51,51	0
57	MG	1A	3458	1/1	0.92	0.22	53,53,53,53	0
57	MG	1A	3819	1/1	0.92	0.18	27,27,27,27	0
57	MG	2a	1700	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3076	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3046	1/1	0.92	0.20	16,16,16,16	0
57	MG	1A	3331	1/1	0.92	0.27	47,47,47,47	0
57	MG	2A	3649	1/1	0.92	0.26	78,78,78,78	0
57	MG	1A	3088	1/1	0.92	0.20	17,17,17,17	0
57	MG	1a	1691	1/1	0.92	0.25	52,52,52,52	0
57	MG	1A	3530	1/1	0.92	0.27	29,29,29,29	0
57	MG	2A	3314	1/1	0.92	0.18	56,56,56,56	0
57	MG	2a	1718	1/1	0.92	0.10	61,61,61,61	0
57	MG	2a	1719	1/1	0.92	0.23	57,57,57,57	0
57	MG	2A	3089	1/1	0.92	0.13	61,61,61,61	0
57	MG	2a	1722	1/1	0.92	0.11	66,66,66,66	0
57	MG	2A	3092	1/1	0.92	0.12	44,44,44,44	0
57	MG	1R	201	1/1	0.92	0.46	55,55,55,55	0
57	MG	2a	1732	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3147	1/1	0.92	0.17	25,25,25,25	0
57	MG	1A	3535	1/1	0.92	0.26	26,26,26,26	0
57	MG	2A	3675	1/1	0.92	0.12	58,58,58,58	0
57	MG	1A	3538	1/1	0.92	0.18	39,39,39,39	0
57	MG	1A	3271	1/1	0.92	0.29	48,48,48,48	0
57	MG	2A	3681	1/1	0.92	0.14	53,53,53,53	0
57	MG	2a	1751	1/1	0.92	0.23	69,69,69,69	0
57	MG	1T	202	1/1	0.92	0.21	57,57,57,57	0
57	MG	1a	1707	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3692	1/1	0.92	0.16	54,54,54,54	0
57	MG	1A	3205	1/1	0.92	0.19	29,29,29,29	0
57	MG	2A	3333	1/1	0.92	0.21	58,58,58,58	0
57	MG	1A	3246	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3398	1/1	0.92	0.12	44,44,44,44	0
57	MG	1a	1712	1/1	0.92	0.10	35,35,35,35	0
57	MG	1A	3281	1/1	0.92	0.73	32,32,32,32	0
57	MG	1a	1714	1/1	0.92	0.23	54,54,54,54	0
57	MG	2A	3709	1/1	0.92	0.23	53,53,53,53	0
57	MG	2a	1773	1/1	0.92	0.08	50,50,50,50	0
57	MG	1A	4010	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3346	1/1	0.92	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4011	1/1	0.92	0.15	55,55,55,55	0
57	MG	2A	3120	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3728	1/1	0.92	0.20	58,58,58,58	0
57	MG	1Z	305	1/1	0.92	0.13	30,30,30,30	0
57	MG	2a	1790	1/1	0.92	0.21	70,70,70,70	0
57	MG	2A	3733	1/1	0.92	0.14	50,50,50,50	0
57	MG	1a	1719	1/1	0.92	0.14	57,57,57,57	0
57	MG	2a	1795	1/1	0.92	0.21	66,66,66,66	0
57	MG	2a	1798	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	3868	1/1	0.92	0.63	45,45,45,45	0
57	MG	2A	3130	1/1	0.92	0.32	51,51,51,51	0
57	MG	2A	3357	1/1	0.92	0.63	68,68,68,68	0
57	MG	1A	3115	1/1	0.92	0.29	47,47,47,47	0
57	MG	1A	4020	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3752	1/1	0.92	0.27	57,57,57,57	0
57	MG	1A	3406	1/1	0.92	0.10	44,44,44,44	0
57	MG	1a	1730	1/1	0.92	0.09	60,60,60,60	0
57	MG	2a	1810	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3407	1/1	0.92	0.14	37,37,37,37	0
57	MG	1A	3577	1/1	0.92	0.17	43,43,43,43	0
57	MG	1l	102	1/1	0.92	0.42	43,43,43,43	0
57	MG	2a	1817	1/1	0.92	0.15	51,51,51,51	0
57	MG	2a	1820	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3882	1/1	0.92	0.17	25,25,25,25	0
57	MG	2a	1824	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3731	1/1	0.92	0.15	53,53,53,53	0
57	MG	2A	3767	1/1	0.92	0.10	51,51,51,51	0
57	MG	2d	301	1/1	0.92	0.26	45,45,45,45	0
57	MG	2A	3770	1/1	0.92	0.10	61,61,61,61	0
57	MG	1A	3581	1/1	0.92	0.28	42,42,42,42	0
57	MG	2l	201	1/1	0.92	0.33	68,68,68,68	0
57	MG	1a	1746	1/1	0.92	0.10	49,49,49,49	0
57	MG	1a	1747	1/1	0.92	0.13	52,52,52,52	0
57	MG	15	105	1/1	0.92	0.23	36,36,36,36	0
57	MG	2A	3781	1/1	0.92	0.28	73,73,73,73	0
57	MG	1a	1755	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3394	1/1	0.92	0.23	32,32,32,32	0
57	MG	2w	109	1/1	0.92	0.20	73,73,73,73	0
57	MG	1a	1759	1/1	0.92	0.11	45,45,45,45	0
57	MG	1A	4038	1/1	0.92	0.20	49,49,49,49	0
57	MG	1A	3410	1/1	0.92	0.18	45,45,45,45	0
57	MG	2x	105	1/1	0.92	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3405	1/1	0.92	0.22	53,53,53,53	0
57	MG	2A	3166	1/1	0.92	0.18	51,51,51,51	0
57	MG	2A	3409	1/1	0.92	0.23	44,44,44,44	0
57	MG	1A	3061	1/1	0.92	0.19	40,40,40,40	0
57	MG	1A	4050	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3798	1/1	0.92	0.13	58,58,58,58	0
57	MG	2A	3466	1/1	0.93	0.16	53,53,53,53	0
57	MG	2A	3467	1/1	0.93	0.18	51,51,51,51	0
57	MG	1A	3053	1/1	0.93	0.15	51,51,51,51	0
57	MG	1v	102	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3791	1/1	0.93	0.17	23,23,23,23	0
57	MG	1w	102	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3230	1/1	0.93	0.15	51,51,51,51	0
57	MG	2A	3478	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3794	1/1	0.93	0.13	22,22,22,22	0
57	MG	2A	3480	1/1	0.93	0.16	49,49,49,49	0
57	MG	1B	207	1/1	0.93	0.15	59,59,59,59	0
57	MG	1B	208	1/1	0.93	0.16	45,45,45,45	0
57	MG	1w	109	1/1	0.93	0.11	48,48,48,48	0
57	MG	2B	214	1/1	0.93	0.14	50,50,50,50	0
57	MG	1a	1643	1/1	0.93	0.16	63,63,63,63	0
57	MG	1A	3320	1/1	0.93	0.26	45,45,45,45	0
57	MG	2A	3497	1/1	0.93	0.21	46,46,46,46	0
57	MG	2D	304	1/1	0.93	0.28	40,40,40,40	0
57	MG	1A	3653	1/1	0.93	0.23	36,36,36,36	0
57	MG	1A	3153	1/1	0.93	0.19	35,35,35,35	0
57	MG	1A	3009	1/1	0.93	0.13	24,24,24,24	0
57	MG	1x	109	1/1	0.93	0.29	64,64,64,64	0
57	MG	2A	3503	1/1	0.93	0.17	54,54,54,54	0
57	MG	1A	3658	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3953	1/1	0.93	0.16	47,47,47,47	0
57	MG	1B	224	1/1	0.93	0.21	33,33,33,33	0
57	MG	1x	114	1/1	0.93	0.13	50,50,50,50	0
57	MG	1A	3086	1/1	0.93	0.20	30,30,30,30	0
57	MG	2A	3518	1/1	0.93	0.14	47,47,47,47	0
57	MG	2A	3004	1/1	0.93	0.33	56,56,56,56	0
57	MG	1A	3661	1/1	0.93	0.16	32,32,32,32	0
57	MG	1A	3038	1/1	0.93	0.13	26,26,26,26	0
57	MG	1B	232	1/1	0.93	0.14	64,64,64,64	0
57	MG	2A	3015	1/1	0.93	0.40	49,49,49,49	0
57	MG	2A	3017	1/1	0.93	0.16	48,48,48,48	0
57	MG	1a	1669	1/1	0.93	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3667	1/1	0.93	0.13	24,24,24,24	0
57	MG	1A	3967	1/1	0.93	0.21	60,60,60,60	0
57	MG	1A	3016	1/1	0.93	0.36	53,53,53,53	0
57	MG	1A	3969	1/1	0.93	0.11	48,48,48,48	0
57	MG	2A	3042	1/1	0.93	0.26	51,51,51,51	0
57	MG	1A	3547	1/1	0.93	0.20	34,34,34,34	0
57	MG	2A	3543	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3547	1/1	0.93	0.21	40,40,40,40	0
57	MG	28	101	1/1	0.93	0.41	59,59,59,59	0
57	MG	1F	307	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3471	1/1	0.93	0.23	45,45,45,45	0
57	MG	1A	3974	1/1	0.93	0.13	23,23,23,23	0
57	MG	2A	3555	1/1	0.93	0.13	67,67,67,67	0
57	MG	2A	3050	1/1	0.93	0.30	66,66,66,66	0
57	MG	2A	3052	1/1	0.93	0.19	45,45,45,45	0
57	MG	1a	1682	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3057	1/1	0.93	0.15	46,46,46,46	0
57	MG	1a	1684	1/1	0.93	0.13	60,60,60,60	0
57	MG	1G	202	1/1	0.93	0.23	64,64,64,64	0
57	MG	2a	1613	1/1	0.93	0.28	52,52,52,52	0
57	MG	2A	3065	1/1	0.93	0.18	46,46,46,46	0
57	MG	1A	3550	1/1	0.93	0.18	32,32,32,32	0
57	MG	2A	3069	1/1	0.93	0.29	54,54,54,54	0
57	MG	1A	3219	1/1	0.93	0.11	32,32,32,32	0
57	MG	2A	3296	1/1	0.93	0.23	50,50,50,50	0
57	MG	2a	1624	1/1	0.93	0.23	55,55,55,55	0
57	MG	2A	3595	1/1	0.93	0.22	63,63,63,63	0
57	MG	1a	1689	1/1	0.93	0.25	42,42,42,42	0
57	MG	1N	201	1/1	0.93	0.40	53,53,53,53	0
57	MG	1A	3835	1/1	0.93	0.14	46,46,46,46	0
57	MG	1A	3978	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3077	1/1	0.93	0.22	24,24,24,24	0
57	MG	1P	203	1/1	0.93	0.12	23,23,23,23	0
57	MG	1A	3840	1/1	0.93	0.18	56,56,56,56	0
57	MG	1A	3558	1/1	0.93	0.26	49,49,49,49	0
57	MG	2A	3616	1/1	0.93	0.12	49,49,49,49	0
57	MG	2A	3617	1/1	0.93	0.24	38,38,38,38	0
57	MG	1A	3561	1/1	0.93	0.20	31,31,31,31	0
57	MG	1A	3338	1/1	0.93	0.22	26,26,26,26	0
57	MG	1A	3847	1/1	0.93	0.11	41,41,41,41	0
57	MG	1A	3993	1/1	0.93	0.17	25,25,25,25	0
57	MG	1R	206	1/1	0.93	0.31	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3162	1/1	0.93	0.39	43,43,43,43	0
57	MG	2A	3322	1/1	0.93	0.10	64,64,64,64	0
57	MG	2A	3323	1/1	0.93	0.13	48,48,48,48	0
57	MG	2a	1656	1/1	0.93	0.12	67,67,67,67	0
57	MG	2A	3635	1/1	0.93	0.23	56,56,56,56	0
57	MG	2A	3324	1/1	0.93	0.10	60,60,60,60	0
57	MG	1S	203	1/1	0.93	0.09	56,56,56,56	0
57	MG	2a	1663	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3697	1/1	0.93	0.12	21,21,21,21	0
57	MG	2a	1671	1/1	0.93	0.28	49,49,49,49	0
57	MG	1A	3699	1/1	0.93	0.13	37,37,37,37	0
57	MG	2a	1675	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3708	1/1	0.93	0.09	57,57,57,57	0
57	MG	2a	1677	1/1	0.93	0.13	68,68,68,68	0
57	MG	1A	4005	1/1	0.93	0.17	33,33,33,33	0
57	MG	1A	3095	1/1	0.93	0.17	46,46,46,46	0
57	MG	1Y	202	1/1	0.93	0.23	61,61,61,61	0
57	MG	1A	3169	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	3031	1/1	0.93	0.16	21,21,21,21	0
57	MG	2A	3335	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3280	1/1	0.93	0.62	40,40,40,40	0
57	MG	2a	1693	1/1	0.93	0.21	58,58,58,58	0
57	MG	2A	3663	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3340	1/1	0.93	0.13	67,67,67,67	0
57	MG	1A	3725	1/1	0.93	0.35	56,56,56,56	0
57	MG	1A	4019	1/1	0.93	0.29	43,43,43,43	0
57	MG	2a	1702	1/1	0.93	0.13	56,56,56,56	0
57	MG	1a	1728	1/1	0.93	0.17	61,61,61,61	0
57	MG	1A	3878	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3345	1/1	0.93	0.25	49,49,49,49	0
57	MG	2a	1706	1/1	0.93	0.08	63,63,63,63	0
57	MG	2a	1708	1/1	0.93	0.15	66,66,66,66	0
57	MG	2a	1709	1/1	0.93	0.10	65,65,65,65	0
57	MG	2A	3683	1/1	0.93	0.08	55,55,55,55	0
57	MG	2A	3687	1/1	0.93	0.22	52,52,52,52	0
57	MG	1a	1732	1/1	0.93	0.07	45,45,45,45	0
57	MG	1A	3412	1/1	0.93	0.18	49,49,49,49	0
57	MG	2A	3690	1/1	0.93	0.12	28,28,28,28	0
57	MG	1A	3414	1/1	0.93	0.12	42,42,42,42	0
57	MG	1A	3033	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3242	1/1	0.93	0.47	38,38,38,38	0
57	MG	1A	3433	1/1	0.93	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3100	1/1	0.93	0.54	47,47,47,47	0
57	MG	13	107	1/1	0.93	0.20	53,53,53,53	0
57	MG	2a	1731	1/1	0.93	0.21	57,57,57,57	0
57	MG	1A	3182	1/1	0.93	0.17	34,34,34,34	0
57	MG	1A	4039	1/1	0.93	0.10	29,29,29,29	0
57	MG	2a	1734	1/1	0.93	0.18	57,57,57,57	0
57	MG	1a	1752	1/1	0.93	0.09	50,50,50,50	0
57	MG	2A	3711	1/1	0.93	0.16	51,51,51,51	0
57	MG	2a	1743	1/1	0.93	0.36	62,62,62,62	0
57	MG	15	108	1/1	0.93	0.17	37,37,37,37	0
57	MG	2A	3715	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	3295	1/1	0.93	0.30	34,34,34,34	0
57	MG	2a	1750	1/1	0.93	0.21	45,45,45,45	0
57	MG	2A	3153	1/1	0.93	0.27	55,55,55,55	0
57	MG	1A	3138	1/1	0.93	0.13	37,37,37,37	0
57	MG	17	106	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3139	1/1	0.93	0.17	50,50,50,50	0
57	MG	2A	3732	1/1	0.93	0.19	48,48,48,48	0
57	MG	18	101	1/1	0.93	0.36	48,48,48,48	0
57	MG	2A	3734	1/1	0.93	0.20	61,61,61,61	0
57	MG	1A	4053	1/1	0.93	0.19	39,39,39,39	0
57	MG	2A	3380	1/1	0.93	0.18	57,57,57,57	0
57	MG	2A	3382	1/1	0.93	0.11	51,51,51,51	0
57	MG	1A	4055	1/1	0.93	0.20	44,44,44,44	0
57	MG	2a	1771	1/1	0.93	0.19	56,56,56,56	0
57	MG	2A	3745	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3910	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3387	1/1	0.93	0.23	49,49,49,49	0
57	MG	2A	3749	1/1	0.93	0.10	64,64,64,64	0
57	MG	1a	1768	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3389	1/1	0.93	0.08	46,46,46,46	0
57	MG	1A	3746	1/1	0.93	0.13	49,49,49,49	0
57	MG	1a	1770	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	4066	1/1	0.93	0.22	54,54,54,54	0
57	MG	1a	1777	1/1	0.93	0.07	58,58,58,58	0
57	MG	1A	3912	1/1	0.93	0.18	33,33,33,33	0
57	MG	1a	1784	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3408	1/1	0.93	0.17	40,40,40,40	0
57	MG	1a	1785	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3771	1/1	0.93	0.15	71,71,71,71	0
57	MG	1A	3104	1/1	0.93	0.45	33,33,33,33	0
57	MG	1a	1788	1/1	0.93	0.21	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3775	1/1	0.93	0.18	74,74,74,74	0
57	MG	2A	3776	1/1	0.93	0.09	69,69,69,69	0
57	MG	1a	1609	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3448	1/1	0.93	0.07	55,55,55,55	0
57	MG	2A	3187	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3311	1/1	0.93	0.19	48,48,48,48	0
57	MG	1A	3608	1/1	0.93	0.19	34,34,34,34	0
57	MG	1A	4077	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3786	1/1	0.93	0.09	62,62,62,62	0
57	MG	2a	1819	1/1	0.93	0.16	73,73,73,73	0
57	MG	2A	3193	1/1	0.93	0.21	46,46,46,46	0
57	MG	1a	1798	1/1	0.93	0.24	61,61,61,61	0
57	MG	1a	1616	1/1	0.93	0.10	59,59,59,59	0
57	MG	2a	1825	1/1	0.93	0.20	61,61,61,61	0
57	MG	2a	1826	1/1	0.93	0.19	49,49,49,49	0
57	MG	1A	3374	1/1	0.93	0.18	42,42,42,42	0
57	MG	2A	3202	1/1	0.93	0.14	45,45,45,45	0
57	MG	2a	1830	1/1	0.93	0.14	67,67,67,67	0
57	MG	1a	1809	1/1	0.93	0.21	70,70,70,70	0
57	MG	1A	3621	1/1	0.93	0.32	53,53,53,53	0
57	MG	2A	3206	1/1	0.93	0.09	52,52,52,52	0
57	MG	2k	201	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3624	1/1	0.93	0.13	35,35,35,35	0
57	MG	2A	3436	1/1	0.93	0.30	41,41,41,41	0
57	MG	2A	3802	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3051	1/1	0.93	0.16	34,34,34,34	0
57	MG	2A	3439	1/1	0.93	0.17	59,59,59,59	0
57	MG	2A	3440	1/1	0.93	0.18	34,34,34,34	0
57	MG	1A	3052	1/1	0.93	0.19	32,32,32,32	0
57	MG	2w	108	1/1	0.93	0.06	69,69,69,69	0
57	MG	2A	3213	1/1	0.93	0.21	34,34,34,34	0
57	MG	1h	201	1/1	0.93	0.26	63,63,63,63	0
57	MG	1A	3456	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3457	1/1	0.93	0.19	41,41,41,41	0
57	MG	2A	3457	1/1	0.93	0.17	55,55,55,55	0
57	MG	2y	102	1/1	0.93	0.14	51,51,51,51	0
57	MG	1A	3638	1/1	0.93	0.17	42,42,42,42	0
57	MG	2y	105	1/1	0.93	0.23	63,63,63,63	0
57	MG	1A	3941	1/1	0.93	0.12	48,48,48,48	0
58	K	1A	3560	1/1	0.93	0.22	73,73,73,73	0
59	6IF	2A	3857	32/32	0.93	0.36	39,47,56,59	0
57	MG	2A	3463	1/1	0.93	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3835	1/1	0.93	0.19	46,46,46,46	0
57	MG	2A	3464	1/1	0.93	0.16	53,53,53,53	0
57	MG	2A	3841	1/1	0.93	0.15	60,60,60,60	0
57	MG	1A	3521	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3763	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3764	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3347	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3348	1/1	0.94	0.39	54,54,54,54	0
57	MG	1a	1621	1/1	0.94	0.30	54,54,54,54	0
57	MG	2A	3769	1/1	0.94	0.15	59,59,59,59	0
57	MG	2A	3051	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3857	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3444	1/1	0.94	0.14	26,26,26,26	0
57	MG	1A	3529	1/1	0.94	0.28	44,44,44,44	0
57	MG	1a	1625	1/1	0.94	0.28	50,50,50,50	0
57	MG	2A	3063	1/1	0.94	0.11	48,48,48,48	0
57	MG	1A	3861	1/1	0.94	0.20	46,46,46,46	0
57	MG	1a	1628	1/1	0.94	0.17	48,48,48,48	0
57	MG	2A	3362	1/1	0.94	0.41	65,65,65,65	0
57	MG	1A	3862	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	4059	1/1	0.94	0.21	42,42,42,42	0
57	MG	1A	4062	1/1	0.94	0.17	52,52,52,52	0
57	MG	1A	3864	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3286	1/1	0.94	0.17	33,33,33,33	0
57	MG	2A	3789	1/1	0.94	0.11	56,56,56,56	0
57	MG	2A	3371	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	4068	1/1	0.94	0.18	61,61,61,61	0
57	MG	1a	1639	1/1	0.94	0.16	50,50,50,50	0
57	MG	1A	3287	1/1	0.94	0.18	50,50,50,50	0
57	MG	1a	1642	1/1	0.94	0.18	52,52,52,52	0
57	MG	1A	4070	1/1	0.94	0.23	54,54,54,54	0
57	MG	2A	3083	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3532	1/1	0.94	0.23	41,41,41,41	0
57	MG	1A	4072	1/1	0.94	0.26	41,41,41,41	0
57	MG	2A	3386	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3087	1/1	0.94	0.20	62,62,62,62	0
57	MG	1a	1648	1/1	0.94	0.10	43,43,43,43	0
57	MG	2A	3806	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3674	1/1	0.94	0.18	37,37,37,37	0
57	MG	2A	3391	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3811	1/1	0.94	0.24	50,50,50,50	0
57	MG	1A	3534	1/1	0.94	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3813	1/1	0.94	0.18	52,52,52,52	0
57	MG	2A	3817	1/1	0.94	0.16	42,42,42,42	0
57	MG	2A	3819	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3397	1/1	0.94	0.18	41,41,41,41	0
57	MG	2A	3398	1/1	0.94	0.21	46,46,46,46	0
57	MG	1A	3129	1/1	0.94	0.10	31,31,31,31	0
57	MG	1A	3537	1/1	0.94	0.13	48,48,48,48	0
57	MG	1A	3685	1/1	0.94	0.18	12,12,12,12	0
57	MG	1A	3881	1/1	0.94	0.15	23,23,23,23	0
57	MG	2A	3828	1/1	0.94	0.26	49,49,49,49	0
57	MG	1a	1661	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3833	1/1	0.94	0.15	51,51,51,51	0
57	MG	1A	4080	1/1	0.94	0.21	40,40,40,40	0
57	MG	2A	3836	1/1	0.94	0.27	59,59,59,59	0
57	MG	1A	3083	1/1	0.94	0.23	24,24,24,24	0
57	MG	2A	3839	1/1	0.94	0.39	59,59,59,59	0
57	MG	1A	3085	1/1	0.94	0.33	32,32,32,32	0
57	MG	1a	1666	1/1	0.94	0.09	52,52,52,52	0
57	MG	1a	1668	1/1	0.94	0.14	55,55,55,55	0
57	MG	1A	4084	1/1	0.94	0.25	43,43,43,43	0
57	MG	1A	3884	1/1	0.94	0.18	33,33,33,33	0
57	MG	2A	3415	1/1	0.94	0.23	55,55,55,55	0
57	MG	1A	3888	1/1	0.94	0.14	33,33,33,33	0
57	MG	2A	3115	1/1	0.94	0.18	61,61,61,61	0
57	MG	2A	3420	1/1	0.94	0.33	61,61,61,61	0
57	MG	1A	3542	1/1	0.94	0.14	33,33,33,33	0
57	MG	2A	3423	1/1	0.94	0.23	58,58,58,58	0
57	MG	1A	3543	1/1	0.94	0.21	43,43,43,43	0
57	MG	1a	1674	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3698	1/1	0.94	0.12	17,17,17,17	0
57	MG	2A	3122	1/1	0.94	0.07	53,53,53,53	0
57	MG	2B	215	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3124	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	3368	1/1	0.94	0.16	44,44,44,44	0
57	MG	2A	3430	1/1	0.94	0.20	39,39,39,39	0
57	MG	2D	302	1/1	0.94	0.23	52,52,52,52	0
57	MG	2A	3126	1/1	0.94	0.14	41,41,41,41	0
57	MG	1A	3298	1/1	0.94	0.23	37,37,37,37	0
57	MG	1A	3067	1/1	0.94	0.16	18,18,18,18	0
57	MG	2A	3434	1/1	0.94	0.37	48,48,48,48	0
57	MG	1A	3907	1/1	0.94	0.17	22,22,22,22	0
57	MG	2A	3437	1/1	0.94	0.31	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1683	1/1	0.94	0.27	61,61,61,61	0
57	MG	1A	3303	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3215	1/1	0.94	0.19	27,27,27,27	0
57	MG	1B	210	1/1	0.94	0.32	49,49,49,49	0
57	MG	1A	3556	1/1	0.94	0.30	25,25,25,25	0
57	MG	2N	201	1/1	0.94	0.21	58,58,58,58	0
57	MG	2O	201	1/1	0.94	0.17	67,67,67,67	0
57	MG	1A	3109	1/1	0.94	0.31	32,32,32,32	0
57	MG	1B	217	1/1	0.94	0.25	25,25,25,25	0
57	MG	2A	3150	1/1	0.94	0.20	52,52,52,52	0
57	MG	1A	3110	1/1	0.94	0.20	33,33,33,33	0
57	MG	1A	3562	1/1	0.94	0.13	34,34,34,34	0
57	MG	2A	3460	1/1	0.94	0.19	42,42,42,42	0
57	MG	1B	221	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3918	1/1	0.94	0.17	35,35,35,35	0
57	MG	2X	102	1/1	0.94	0.15	69,69,69,69	0
57	MG	1A	3313	1/1	0.94	0.23	40,40,40,40	0
57	MG	2A	3465	1/1	0.94	0.13	36,36,36,36	0
57	MG	1A	3068	1/1	0.94	0.18	20,20,20,20	0
57	MG	23	101	1/1	0.94	0.10	51,51,51,51	0
57	MG	25	102	1/1	0.94	0.35	49,49,49,49	0
57	MG	1A	3570	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3468	1/1	0.94	0.12	60,60,60,60	0
57	MG	1B	229	1/1	0.94	0.14	39,39,39,39	0
57	MG	2A	3470	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3925	1/1	0.94	0.18	24,24,24,24	0
57	MG	1A	3926	1/1	0.94	0.13	21,21,21,21	0
57	MG	2A	3164	1/1	0.94	0.10	65,65,65,65	0
57	MG	28	103	1/1	0.94	0.21	53,53,53,53	0
57	MG	1B	233	1/1	0.94	0.15	29,29,29,29	0
57	MG	1D	306	1/1	0.94	0.14	24,24,24,24	0
57	MG	2A	3169	1/1	0.94	0.19	44,44,44,44	0
57	MG	1A	3383	1/1	0.94	0.36	31,31,31,31	0
57	MG	2A	3482	1/1	0.94	0.21	34,34,34,34	0
57	MG	1A	3254	1/1	0.94	0.22	47,47,47,47	0
57	MG	2A	3489	1/1	0.94	0.21	57,57,57,57	0
57	MG	1D	310	1/1	0.94	0.38	21,21,21,21	0
57	MG	1D	311	1/1	0.94	0.21	41,41,41,41	0
57	MG	1E	301	1/1	0.94	0.17	25,25,25,25	0
57	MG	1A	3469	1/1	0.94	0.24	36,36,36,36	0
57	MG	2a	1615	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3180	1/1	0.94	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1E	311	1/1	0.94	0.24	65,65,65,65	0
57	MG	1A	3578	1/1	0.94	0.14	40,40,40,40	0
57	MG	2A	3185	1/1	0.94	0.18	54,54,54,54	0
57	MG	1F	301	1/1	0.94	0.15	27,27,27,27	0
57	MG	2a	1625	1/1	0.94	0.21	62,62,62,62	0
57	MG	1F	304	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3015	1/1	0.94	0.22	48,48,48,48	0
57	MG	1A	3220	1/1	0.94	0.12	28,28,28,28	0
57	MG	1F	308	1/1	0.94	0.31	31,31,31,31	0
57	MG	1A	3585	1/1	0.94	0.15	30,30,30,30	0
57	MG	1F	314	1/1	0.94	0.11	37,37,37,37	0
57	MG	2A	3195	1/1	0.94	0.18	59,59,59,59	0
57	MG	1a	1735	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3748	1/1	0.94	0.22	41,41,41,41	0
57	MG	2A	3198	1/1	0.94	0.15	37,37,37,37	0
57	MG	2A	3201	1/1	0.94	0.23	55,55,55,55	0
57	MG	1A	3750	1/1	0.94	0.11	31,31,31,31	0
57	MG	1A	3754	1/1	0.94	0.18	18,18,18,18	0
57	MG	2a	1648	1/1	0.94	0.12	43,43,43,43	0
57	MG	1G	204	1/1	0.94	0.11	63,63,63,63	0
57	MG	1A	3321	1/1	0.94	0.19	32,32,32,32	0
57	MG	1A	3221	1/1	0.94	0.21	29,29,29,29	0
57	MG	1A	3396	1/1	0.94	0.69	49,49,49,49	0
57	MG	2A	3539	1/1	0.94	0.18	40,40,40,40	0
57	MG	2A	3209	1/1	0.94	0.29	60,60,60,60	0
57	MG	1a	1750	1/1	0.94	0.16	48,48,48,48	0
57	MG	1N	205	1/1	0.94	0.12	51,51,51,51	0
57	MG	1N	206	1/1	0.94	0.24	39,39,39,39	0
57	MG	2a	1660	1/1	0.94	0.18	59,59,59,59	0
57	MG	1O	202	1/1	0.94	0.28	64,64,64,64	0
57	MG	1O	203	1/1	0.94	0.15	43,43,43,43	0
57	MG	2a	1664	1/1	0.94	0.14	53,53,53,53	0
57	MG	2a	1667	1/1	0.94	0.20	43,43,43,43	0
57	MG	1a	1760	1/1	0.94	0.13	65,65,65,65	0
57	MG	2A	3551	1/1	0.94	0.25	44,44,44,44	0
57	MG	2A	3552	1/1	0.94	0.18	60,60,60,60	0
57	MG	1A	3479	1/1	0.94	0.23	42,42,42,42	0
57	MG	2A	3225	1/1	0.94	0.29	40,40,40,40	0
57	MG	2A	3556	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3181	1/1	0.94	0.17	63,63,63,63	0
57	MG	1Q	202	1/1	0.94	0.11	40,40,40,40	0
57	MG	2A	3566	1/1	0.94	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3076	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	3483	1/1	0.94	0.37	54,54,54,54	0
57	MG	2A	3574	1/1	0.94	0.25	55,55,55,55	0
57	MG	2a	1689	1/1	0.94	0.25	72,72,72,72	0
57	MG	2a	1690	1/1	0.94	0.14	70,70,70,70	0
57	MG	1A	3956	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3767	1/1	0.94	0.12	21,21,21,21	0
57	MG	1A	3772	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3962	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3585	1/1	0.94	0.11	40,40,40,40	0
57	MG	2a	1697	1/1	0.94	0.26	68,68,68,68	0
57	MG	1A	3330	1/1	0.94	0.24	36,36,36,36	0
57	MG	2a	1701	1/1	0.94	0.17	51,51,51,51	0
57	MG	1a	1771	1/1	0.94	0.13	60,60,60,60	0
57	MG	1a	1773	1/1	0.94	0.07	50,50,50,50	0
57	MG	1S	201	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3964	1/1	0.94	0.16	33,33,33,33	0
57	MG	1A	3775	1/1	0.94	0.14	34,34,34,34	0
57	MG	2a	1707	1/1	0.94	0.30	65,65,65,65	0
57	MG	2A	3602	1/1	0.94	0.15	42,42,42,42	0
57	MG	1A	3485	1/1	0.94	0.17	32,32,32,32	0
57	MG	1T	203	1/1	0.94	0.14	32,32,32,32	0
57	MG	2A	3244	1/1	0.94	0.23	41,41,41,41	0
57	MG	1T	205	1/1	0.94	0.11	46,46,46,46	0
57	MG	1A	3120	1/1	0.94	0.33	30,30,30,30	0
57	MG	2A	3612	1/1	0.94	0.11	44,44,44,44	0
57	MG	2A	3249	1/1	0.94	0.11	36,36,36,36	0
57	MG	1V	204	1/1	0.94	0.26	32,32,32,32	0
57	MG	1A	3270	1/1	0.94	0.16	30,30,30,30	0
57	MG	2A	3619	1/1	0.94	0.21	63,63,63,63	0
57	MG	1A	3971	1/1	0.94	0.26	22,22,22,22	0
57	MG	2a	1724	1/1	0.94	0.13	54,54,54,54	0
57	MG	2a	1726	1/1	0.94	0.12	60,60,60,60	0
57	MG	2a	1728	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3622	1/1	0.94	0.25	39,39,39,39	0
57	MG	1A	3783	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3627	1/1	0.94	0.24	61,61,61,61	0
57	MG	1W	207	1/1	0.94	0.19	44,44,44,44	0
57	MG	1W	208	1/1	0.94	0.16	36,36,36,36	0
57	MG	2a	1735	1/1	0.94	0.30	51,51,51,51	0
57	MG	1W	210	1/1	0.94	0.18	30,30,30,30	0
57	MG	1X	103	1/1	0.94	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1740	1/1	0.94	0.24	50,50,50,50	0
57	MG	1a	1804	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3784	1/1	0.94	0.09	50,50,50,50	0
57	MG	1a	1810	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3639	1/1	0.94	0.27	55,55,55,55	0
57	MG	2A	3265	1/1	0.94	0.22	54,54,54,54	0
57	MG	1Z	302	1/1	0.94	0.17	37,37,37,37	0
57	MG	2A	3268	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3646	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3006	1/1	0.94	0.22	45,45,45,45	0
57	MG	2a	1756	1/1	0.94	0.22	48,48,48,48	0
57	MG	1A	3786	1/1	0.94	0.19	22,22,22,22	0
57	MG	1A	3606	1/1	0.94	0.20	44,44,44,44	0
57	MG	2a	1759	1/1	0.94	0.04	57,57,57,57	0
57	MG	1A	3793	1/1	0.94	0.14	18,18,18,18	0
57	MG	1l	201	1/1	0.94	0.19	52,52,52,52	0
57	MG	1A	3337	1/1	0.94	0.23	46,46,46,46	0
57	MG	1A	3609	1/1	0.94	0.19	37,37,37,37	0
57	MG	1A	3236	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3988	1/1	0.94	0.11	55,55,55,55	0
57	MG	10	106	1/1	0.94	0.18	56,56,56,56	0
57	MG	2A	3664	1/1	0.94	0.08	54,54,54,54	0
57	MG	2a	1776	1/1	0.94	0.22	60,60,60,60	0
57	MG	1A	3615	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3240	1/1	0.94	0.30	30,30,30,30	0
57	MG	1l	103	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3677	1/1	0.94	0.24	58,58,58,58	0
57	MG	1A	3416	1/1	0.94	0.10	54,54,54,54	0
57	MG	13	101	1/1	0.94	0.19	41,41,41,41	0
57	MG	2A	3294	1/1	0.94	0.30	61,61,61,61	0
57	MG	2A	3682	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3277	1/1	0.94	0.26	29,29,29,29	0
57	MG	2A	3684	1/1	0.94	0.10	72,72,72,72	0
57	MG	1A	3629	1/1	0.94	0.14	67,67,67,67	0
57	MG	1A	3420	1/1	0.94	0.18	31,31,31,31	0
57	MG	15	103	1/1	0.94	0.17	33,33,33,33	0
57	MG	1A	3348	1/1	0.94	0.23	55,55,55,55	0
57	MG	2A	3691	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3816	1/1	0.94	0.20	39,39,39,39	0
57	MG	2a	1805	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3693	1/1	0.94	0.16	66,66,66,66	0
57	MG	1A	3432	1/1	0.94	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3279	1/1	0.94	0.24	38,38,38,38	0
57	MG	2A	3698	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	4008	1/1	0.94	0.14	50,50,50,50	0
57	MG	2a	1813	1/1	0.94	0.29	60,60,60,60	0
57	MG	1A	4009	1/1	0.94	0.11	33,33,33,33	0
57	MG	2A	3702	1/1	0.94	0.14	53,53,53,53	0
57	MG	17	108	1/1	0.94	0.21	37,37,37,37	0
57	MG	1A	3641	1/1	0.94	0.15	22,22,22,22	0
57	MG	2A	3706	1/1	0.94	0.09	63,63,63,63	0
57	MG	2a	1821	1/1	0.94	0.13	66,66,66,66	0
57	MG	2A	3311	1/1	0.94	0.25	52,52,52,52	0
57	MG	2a	1823	1/1	0.94	0.26	55,55,55,55	0
57	MG	1A	3512	1/1	0.94	0.19	22,22,22,22	0
57	MG	2A	3002	1/1	0.94	0.34	54,54,54,54	0
57	MG	2A	3003	1/1	0.94	0.35	49,49,49,49	0
57	MG	1A	3829	1/1	0.94	0.20	47,47,47,47	0
57	MG	2A	3716	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	4016	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3648	1/1	0.94	0.18	35,35,35,35	0
57	MG	2A	3722	1/1	0.94	0.16	38,38,38,38	0
57	MG	2A	3723	1/1	0.94	0.17	56,56,56,56	0
57	MG	2A	3010	1/1	0.94	0.20	53,53,53,53	0
57	MG	2A	3011	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3729	1/1	0.94	0.14	31,31,31,31	0
57	MG	1A	3350	1/1	0.94	0.17	50,50,50,50	0
57	MG	2r	101	1/1	0.94	0.31	68,68,68,68	0
57	MG	2v	101	1/1	0.94	0.30	65,65,65,65	0
57	MG	2A	3731	1/1	0.94	0.23	37,37,37,37	0
57	MG	1A	3436	1/1	0.94	0.17	36,36,36,36	0
57	MG	1A	3842	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	3189	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3060	1/1	0.94	0.23	37,37,37,37	0
57	MG	1A	3441	1/1	0.94	0.26	35,35,35,35	0
57	MG	2A	3737	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3030	1/1	0.94	0.21	55,55,55,55	0
57	MG	1A	3011	1/1	0.94	0.14	40,40,40,40	0
57	MG	2A	3744	1/1	0.94	0.19	57,57,57,57	0
57	MG	1A	3849	1/1	0.94	0.16	42,42,42,42	0
57	MG	2A	3038	1/1	0.94	0.14	28,28,28,28	0
57	MG	2A	3338	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3041	1/1	0.94	0.23	47,47,47,47	0
57	MG	1A	3850	1/1	0.94	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1617	1/1	0.94	0.10	44,44,44,44	0
57	MG	2A	3756	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3854	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	4042	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3048	1/1	0.94	0.17	24,24,24,24	0
57	MG	1A	3256	1/1	0.95	0.21	40,40,40,40	0
57	MG	2A	3403	1/1	0.95	0.32	45,45,45,45	0
57	MG	1E	307	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3322	1/1	0.95	0.16	37,37,37,37	0
57	MG	2A	3406	1/1	0.95	0.16	31,31,31,31	0
57	MG	1A	3214	1/1	0.95	0.16	32,32,32,32	0
57	MG	1A	3401	1/1	0.95	0.24	45,45,45,45	0
57	MG	1A	3403	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3124	1/1	0.95	0.23	44,44,44,44	0
57	MG	1A	3952	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	3091	1/1	0.95	0.33	26,26,26,26	0
57	MG	1A	3768	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3123	1/1	0.95	0.16	54,54,54,54	0
57	MG	1F	313	1/1	0.95	0.58	55,55,55,55	0
57	MG	1a	1696	1/1	0.95	0.23	43,43,43,43	0
57	MG	2A	3417	1/1	0.95	0.21	55,55,55,55	0
57	MG	2A	3807	1/1	0.95	0.14	53,53,53,53	0
57	MG	1a	1697	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3771	1/1	0.95	0.10	31,31,31,31	0
57	MG	2A	3421	1/1	0.95	0.14	35,35,35,35	0
57	MG	1A	3262	1/1	0.95	0.16	50,50,50,50	0
57	MG	1a	1701	1/1	0.95	0.16	50,50,50,50	0
57	MG	2A	3815	1/1	0.95	0.17	24,24,24,24	0
57	MG	2A	3816	1/1	0.95	0.09	76,76,76,76	0
57	MG	2A	3132	1/1	0.95	0.29	41,41,41,41	0
57	MG	2A	3818	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3133	1/1	0.95	0.24	47,47,47,47	0
57	MG	2A	3134	1/1	0.95	0.23	39,39,39,39	0
57	MG	1a	1702	1/1	0.95	0.21	55,55,55,55	0
57	MG	1G	201	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3773	1/1	0.95	0.13	31,31,31,31	0
57	MG	2A	3141	1/1	0.95	0.22	58,58,58,58	0
57	MG	1A	3408	1/1	0.95	0.24	31,31,31,31	0
57	MG	1a	1706	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3019	1/1	0.95	0.13	29,29,29,29	0
57	MG	2A	3831	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3147	1/1	0.95	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3435	1/1	0.95	0.08	59,59,59,59	0
57	MG	1G	205	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3012	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3601	1/1	0.95	0.15	19,19,19,19	0
57	MG	1N	202	1/1	0.95	0.24	26,26,26,26	0
57	MG	1A	3165	1/1	0.95	0.18	48,48,48,48	0
57	MG	1A	3413	1/1	0.95	0.12	44,44,44,44	0
57	MG	2A	3850	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	3970	1/1	0.95	0.22	43,43,43,43	0
57	MG	1O	201	1/1	0.95	0.62	68,68,68,68	0
57	MG	2A	3448	1/1	0.95	0.17	41,41,41,41	0
57	MG	2A	3449	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3062	1/1	0.95	0.20	48,48,48,48	0
57	MG	2A	3452	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3454	1/1	0.95	0.17	50,50,50,50	0
57	MG	1A	3607	1/1	0.95	0.24	36,36,36,36	0
57	MG	2B	206	1/1	0.95	0.21	65,65,65,65	0
57	MG	1A	3080	1/1	0.95	0.16	31,31,31,31	0
57	MG	1A	3788	1/1	0.95	0.21	46,46,46,46	0
57	MG	2B	211	1/1	0.95	0.23	43,43,43,43	0
57	MG	1A	3790	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3461	1/1	0.95	0.14	47,47,47,47	0
57	MG	1a	1724	1/1	0.95	0.18	67,67,67,67	0
57	MG	1A	3417	1/1	0.95	0.12	45,45,45,45	0
57	MG	1a	1726	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3610	1/1	0.95	0.14	21,21,21,21	0
57	MG	1Q	206	1/1	0.95	0.25	35,35,35,35	0
57	MG	1A	3339	1/1	0.95	0.34	39,39,39,39	0
57	MG	2A	3175	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3498	1/1	0.95	0.28	48,48,48,48	0
57	MG	1a	1734	1/1	0.95	0.06	36,36,36,36	0
57	MG	2E	304	1/1	0.95	0.13	44,44,44,44	0
57	MG	2E	306	1/1	0.95	0.14	39,39,39,39	0
57	MG	2A	3471	1/1	0.95	0.13	54,54,54,54	0
57	MG	2A	3472	1/1	0.95	0.20	56,56,56,56	0
57	MG	2F	302	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3986	1/1	0.95	0.17	21,21,21,21	0
57	MG	2A	3474	1/1	0.95	0.18	39,39,39,39	0
57	MG	1A	3618	1/1	0.95	0.10	33,33,33,33	0
57	MG	2F	306	1/1	0.95	0.30	44,44,44,44	0
57	MG	1a	1737	1/1	0.95	0.10	51,51,51,51	0
57	MG	2A	3182	1/1	0.95	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1740	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3501	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3622	1/1	0.95	0.16	19,19,19,19	0
57	MG	2A	3481	1/1	0.95	0.28	46,46,46,46	0
57	MG	1A	3623	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3502	1/1	0.95	0.13	54,54,54,54	0
57	MG	2A	3488	1/1	0.95	0.11	45,45,45,45	0
57	MG	1T	201	1/1	0.95	0.15	49,49,49,49	0
57	MG	1A	3504	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3493	1/1	0.95	0.37	36,36,36,36	0
57	MG	1A	3419	1/1	0.95	0.23	37,37,37,37	0
57	MG	1A	3995	1/1	0.95	0.27	28,28,28,28	0
57	MG	1A	3998	1/1	0.95	0.15	24,24,24,24	0
57	MG	1U	203	1/1	0.95	0.17	33,33,33,33	0
57	MG	1a	1758	1/1	0.95	0.07	52,52,52,52	0
57	MG	1U	204	1/1	0.95	0.16	38,38,38,38	0
57	MG	2A	3200	1/1	0.95	0.25	39,39,39,39	0
57	MG	1V	202	1/1	0.95	0.26	30,30,30,30	0
57	MG	1V	203	1/1	0.95	0.23	16,16,16,16	0
57	MG	1A	3081	1/1	0.95	0.21	29,29,29,29	0
57	MG	2A	3505	1/1	0.95	0.24	56,56,56,56	0
57	MG	2A	3508	1/1	0.95	0.29	42,42,42,42	0
57	MG	1A	4002	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3424	1/1	0.95	0.18	35,35,35,35	0
57	MG	1A	3426	1/1	0.95	0.14	41,41,41,41	0
57	MG	1A	3224	1/1	0.95	0.22	40,40,40,40	0
57	MG	2a	1604	1/1	0.95	0.14	41,41,41,41	0
57	MG	2A	3516	1/1	0.95	0.20	41,41,41,41	0
57	MG	1A	3428	1/1	0.95	0.09	34,34,34,34	0
57	MG	2A	3210	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3430	1/1	0.95	0.18	38,38,38,38	0
57	MG	1X	102	1/1	0.95	0.21	27,27,27,27	0
57	MG	2A	3523	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3645	1/1	0.95	0.12	40,40,40,40	0
57	MG	2A	3525	1/1	0.95	0.16	55,55,55,55	0
57	MG	2A	3216	1/1	0.95	0.22	45,45,45,45	0
57	MG	1X	107	1/1	0.95	0.17	57,57,57,57	0
57	MG	2a	1617	1/1	0.95	0.12	65,65,65,65	0
57	MG	2a	1618	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3517	1/1	0.95	0.15	62,62,62,62	0
57	MG	2A	3532	1/1	0.95	0.17	52,52,52,52	0
57	MG	1a	1774	1/1	0.95	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3534	1/1	0.95	0.12	45,45,45,45	0
57	MG	1Y	203	1/1	0.95	0.23	48,48,48,48	0
57	MG	2A	3223	1/1	0.95	0.19	39,39,39,39	0
57	MG	2A	3224	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3833	1/1	0.95	0.11	30,30,30,30	0
57	MG	1a	1778	1/1	0.95	0.12	49,49,49,49	0
57	MG	1A	4012	1/1	0.95	0.14	23,23,23,23	0
57	MG	1A	3343	1/1	0.95	0.51	35,35,35,35	0
57	MG	1A	4015	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1786	1/1	0.95	0.11	61,61,61,61	0
57	MG	2a	1635	1/1	0.95	0.11	72,72,72,72	0
57	MG	1A	3839	1/1	0.95	0.17	36,36,36,36	0
57	MG	2a	1637	1/1	0.95	0.17	58,58,58,58	0
57	MG	1A	3652	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3063	1/1	0.95	0.17	29,29,29,29	0
57	MG	1A	3180	1/1	0.95	0.26	54,54,54,54	0
57	MG	2a	1643	1/1	0.95	0.21	62,62,62,62	0
57	MG	1A	3232	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3522	1/1	0.95	0.12	50,50,50,50	0
57	MG	2a	1646	1/1	0.95	0.09	66,66,66,66	0
57	MG	2A	3559	1/1	0.95	0.12	44,44,44,44	0
57	MG	2A	3560	1/1	0.95	0.16	49,49,49,49	0
57	MG	1A	4024	1/1	0.95	0.15	49,49,49,49	0
57	MG	1l	101	1/1	0.95	0.33	35,35,35,35	0
57	MG	2A	3240	1/1	0.95	0.19	62,62,62,62	0
57	MG	1a	1799	1/1	0.95	0.17	59,59,59,59	0
57	MG	1A	4025	1/1	0.95	0.19	30,30,30,30	0
57	MG	2A	3571	1/1	0.95	0.28	65,65,65,65	0
57	MG	2A	3572	1/1	0.95	0.14	28,28,28,28	0
57	MG	1A	3523	1/1	0.95	0.17	26,26,26,26	0
57	MG	1A	3848	1/1	0.95	0.14	16,16,16,16	0
57	MG	1a	1805	1/1	0.95	0.20	72,72,72,72	0
57	MG	2A	3246	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3247	1/1	0.95	0.28	52,52,52,52	0
57	MG	2a	1666	1/1	0.95	0.14	48,48,48,48	0
57	MG	1a	1807	1/1	0.95	0.20	38,38,38,38	0
57	MG	1l	105	1/1	0.95	0.12	41,41,41,41	0
57	MG	2A	3588	1/1	0.95	0.12	41,41,41,41	0
57	MG	1l	106	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3592	1/1	0.95	0.21	39,39,39,39	0
57	MG	1A	4033	1/1	0.95	0.07	39,39,39,39	0
57	MG	2A	3594	1/1	0.95	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3252	1/1	0.95	0.18	43,43,43,43	0
57	MG	2A	3596	1/1	0.95	0.06	50,50,50,50	0
57	MG	13	104	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3525	1/1	0.95	0.21	38,38,38,38	0
57	MG	1A	4035	1/1	0.95	0.14	25,25,25,25	0
57	MG	13	108	1/1	0.95	0.13	36,36,36,36	0
57	MG	2a	1688	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3282	1/1	0.95	0.11	25,25,25,25	0
57	MG	15	102	1/1	0.95	0.13	28,28,28,28	0
57	MG	2A	3608	1/1	0.95	0.38	45,45,45,45	0
57	MG	1A	3851	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3261	1/1	0.95	0.14	57,57,57,57	0
57	MG	2A	3262	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3528	1/1	0.95	0.23	32,32,32,32	0
57	MG	15	106	1/1	0.95	0.15	36,36,36,36	0
57	MG	2a	1699	1/1	0.95	0.08	66,66,66,66	0
57	MG	15	107	1/1	0.95	0.11	26,26,26,26	0
57	MG	1A	3668	1/1	0.95	0.23	16,16,16,16	0
57	MG	1A	4044	1/1	0.95	0.14	36,36,36,36	0
57	MG	17	102	1/1	0.95	0.19	33,33,33,33	0
57	MG	17	104	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3438	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3066	1/1	0.95	0.18	27,27,27,27	0
57	MG	2A	3279	1/1	0.95	0.26	42,42,42,42	0
57	MG	1A	3284	1/1	0.95	0.17	38,38,38,38	0
57	MG	1x	101	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3001	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3533	1/1	0.95	0.20	50,50,50,50	0
57	MG	2A	3285	1/1	0.95	0.19	56,56,56,56	0
57	MG	1x	104	1/1	0.95	0.13	42,42,42,42	0
57	MG	2a	1715	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3640	1/1	0.95	0.28	44,44,44,44	0
57	MG	2A	3641	1/1	0.95	0.23	54,54,54,54	0
57	MG	1A	4056	1/1	0.95	0.15	49,49,49,49	0
57	MG	2A	3643	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	4057	1/1	0.95	0.18	48,48,48,48	0
57	MG	1x	107	1/1	0.95	0.11	58,58,58,58	0
57	MG	19	101	1/1	0.95	0.17	32,32,32,32	0
57	MG	2A	3647	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3863	1/1	0.95	0.15	29,29,29,29	0
57	MG	1A	3238	1/1	0.95	0.12	21,21,21,21	0
57	MG	2a	1730	1/1	0.95	0.39	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4060	1/1	0.95	0.26	31,31,31,31	0
57	MG	1A	3026	1/1	0.95	0.19	63,63,63,63	0
57	MG	2A	3653	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3681	1/1	0.95	0.19	51,51,51,51	0
57	MG	1A	3446	1/1	0.95	0.22	37,37,37,37	0
57	MG	2a	1736	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3291	1/1	0.95	0.18	56,56,56,56	0
57	MG	2a	1738	1/1	0.95	0.38	49,49,49,49	0
57	MG	1a	1611	1/1	0.95	0.17	27,27,27,27	0
57	MG	1A	3364	1/1	0.95	0.34	37,37,37,37	0
57	MG	1A	3874	1/1	0.95	0.24	26,26,26,26	0
57	MG	1A	3875	1/1	0.95	0.19	37,37,37,37	0
57	MG	2A	3009	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3142	1/1	0.95	0.17	22,22,22,22	0
57	MG	1A	3187	1/1	0.95	0.26	31,31,31,31	0
57	MG	1A	3112	1/1	0.95	0.15	28,28,28,28	0
57	MG	2A	3308	1/1	0.95	0.24	44,44,44,44	0
57	MG	2A	3309	1/1	0.95	0.15	49,49,49,49	0
57	MG	1A	4075	1/1	0.95	0.30	35,35,35,35	0
57	MG	1A	3880	1/1	0.95	0.14	24,24,24,24	0
57	MG	2A	3317	1/1	0.95	0.18	43,43,43,43	0
57	MG	1A	3454	1/1	0.95	0.14	37,37,37,37	0
57	MG	2A	3685	1/1	0.95	0.15	61,61,61,61	0
57	MG	2a	1760	1/1	0.95	0.16	63,63,63,63	0
57	MG	2A	3319	1/1	0.95	0.18	57,57,57,57	0
57	MG	2A	3020	1/1	0.95	0.14	48,48,48,48	0
57	MG	2a	1763	1/1	0.95	0.12	67,67,67,67	0
57	MG	1A	3700	1/1	0.95	0.20	29,29,29,29	0
57	MG	1A	3702	1/1	0.95	0.20	35,35,35,35	0
57	MG	2a	1767	1/1	0.95	0.16	71,71,71,71	0
57	MG	2a	1768	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3027	1/1	0.95	0.54	52,52,52,52	0
57	MG	1A	3703	1/1	0.95	0.25	34,34,34,34	0
57	MG	1A	4081	1/1	0.95	0.10	33,33,33,33	0
57	MG	2A	3034	1/1	0.95	0.26	49,49,49,49	0
57	MG	1A	3706	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3707	1/1	0.95	0.15	51,51,51,51	0
57	MG	2A	3040	1/1	0.95	0.26	57,57,57,57	0
57	MG	1A	3548	1/1	0.95	0.16	29,29,29,29	0
57	MG	1a	1631	1/1	0.95	0.13	54,54,54,54	0
57	MG	2A	3703	1/1	0.95	0.09	58,58,58,58	0
57	MG	2A	3332	1/1	0.95	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3300	1/1	0.95	0.08	25,25,25,25	0
57	MG	1A	3898	1/1	0.95	0.19	38,38,38,38	0
57	MG	1A	3710	1/1	0.95	0.14	23,23,23,23	0
57	MG	2a	1794	1/1	0.95	0.21	50,50,50,50	0
57	MG	1A	3901	1/1	0.95	0.15	34,34,34,34	0
57	MG	2a	1796	1/1	0.95	0.12	48,48,48,48	0
57	MG	2a	1797	1/1	0.95	0.11	70,70,70,70	0
57	MG	1A	3087	1/1	0.95	0.12	35,35,35,35	0
57	MG	1A	3904	1/1	0.95	0.33	37,37,37,37	0
57	MG	1A	3716	1/1	0.95	0.21	37,37,37,37	0
57	MG	1A	3197	1/1	0.95	0.16	37,37,37,37	0
57	MG	2A	3717	1/1	0.95	0.11	61,61,61,61	0
57	MG	2A	3718	1/1	0.95	0.16	55,55,55,55	0
57	MG	1A	3305	1/1	0.95	0.26	44,44,44,44	0
57	MG	2A	3056	1/1	0.95	0.11	61,61,61,61	0
57	MG	1a	1644	1/1	0.95	0.16	61,61,61,61	0
57	MG	1A	3306	1/1	0.95	0.17	29,29,29,29	0
57	MG	2A	3725	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3559	1/1	0.95	0.21	36,36,36,36	0
57	MG	1A	3199	1/1	0.95	0.13	28,28,28,28	0
57	MG	2A	3349	1/1	0.95	0.22	51,51,51,51	0
57	MG	1A	3201	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3914	1/1	0.95	0.10	27,27,27,27	0
57	MG	1a	1652	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3381	1/1	0.95	0.34	48,48,48,48	0
57	MG	2A	3071	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3567	1/1	0.95	0.20	34,34,34,34	0
57	MG	1a	1655	1/1	0.95	0.08	46,46,46,46	0
57	MG	1a	1656	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3734	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3361	1/1	0.95	0.18	27,27,27,27	0
57	MG	2A	3742	1/1	0.95	0.19	51,51,51,51	0
57	MG	1A	3007	1/1	0.95	0.17	32,32,32,32	0
57	MG	1A	3089	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3365	1/1	0.95	0.21	40,40,40,40	0
57	MG	2e	201	1/1	0.95	0.14	57,57,57,57	0
57	MG	2f	201	1/1	0.95	0.19	48,48,48,48	0
57	MG	1a	1662	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3081	1/1	0.95	0.07	65,65,65,65	0
57	MG	2A	3082	1/1	0.95	0.16	42,42,42,42	0
57	MG	1A	3154	1/1	0.95	0.08	55,55,55,55	0
57	MG	2l	203	1/1	0.95	0.31	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3575	1/1	0.95	0.14	35,35,35,35	0
57	MG	2m	201	1/1	0.95	0.14	73,73,73,73	0
57	MG	1A	3470	1/1	0.95	0.28	32,32,32,32	0
57	MG	1B	228	1/1	0.95	0.16	65,65,65,65	0
57	MG	2t	201	1/1	0.95	0.09	49,49,49,49	0
57	MG	2A	3759	1/1	0.95	0.17	52,52,52,52	0
57	MG	2v	102	1/1	0.95	0.19	57,57,57,57	0
57	MG	2w	102	1/1	0.95	0.14	62,62,62,62	0
57	MG	1a	1667	1/1	0.95	0.26	45,45,45,45	0
57	MG	1A	3744	1/1	0.95	0.16	23,23,23,23	0
57	MG	1A	3117	1/1	0.95	0.23	33,33,33,33	0
57	MG	2A	3381	1/1	0.95	0.12	62,62,62,62	0
57	MG	1A	3473	1/1	0.95	0.18	31,31,31,31	0
57	MG	1A	3935	1/1	0.95	0.18	63,63,63,63	0
57	MG	2A	3384	1/1	0.95	0.18	53,53,53,53	0
57	MG	1A	3580	1/1	0.95	0.49	40,40,40,40	0
57	MG	2A	3097	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3211	1/1	0.95	0.13	42,42,42,42	0
57	MG	2y	101	1/1	0.95	0.18	65,65,65,65	0
57	MG	1A	3752	1/1	0.95	0.27	40,40,40,40	0
57	MG	1A	3582	1/1	0.95	0.21	33,33,33,33	0
57	MG	2A	3390	1/1	0.95	0.20	55,55,55,55	0
57	MG	2A	3101	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3393	1/1	0.95	0.15	36,36,36,36	0
59	6IF	1A	4089	32/32	0.95	0.27	24,31,39,45	0
57	MG	1A	3072	1/1	0.95	0.20	31,31,31,31	0
57	MG	2A	3395	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3756	1/1	0.95	0.23	35,35,35,35	0
57	MG	2A	3106	1/1	0.95	0.11	43,43,43,43	0
57	MG	1E	304	1/1	0.95	0.59	40,40,40,40	0
57	MG	1A	3176	1/1	0.96	0.18	29,29,29,29	0
57	MG	1A	3265	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3751	1/1	0.96	0.27	58,58,58,58	0
57	MG	1A	3266	1/1	0.96	0.25	36,36,36,36	0
57	MG	2B	217	1/1	0.96	0.18	68,68,68,68	0
57	MG	1A	3327	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3014	1/1	0.96	0.67	52,52,52,52	0
57	MG	2A	3266	1/1	0.96	0.13	52,52,52,52	0
57	MG	1A	3930	1/1	0.96	0.21	33,33,33,33	0
57	MG	1A	3931	1/1	0.96	0.11	39,39,39,39	0
57	MG	2A	3269	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3409	1/1	0.96	0.36	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3019	1/1	0.96	0.14	35,35,35,35	0
57	MG	1A	3933	1/1	0.96	0.24	33,33,33,33	0
57	MG	2A	3277	1/1	0.96	0.32	55,55,55,55	0
57	MG	1B	231	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3544	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3024	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3329	1/1	0.96	0.11	54,54,54,54	0
57	MG	1a	1647	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3136	1/1	0.96	0.18	48,48,48,48	0
57	MG	2F	307	1/1	0.96	0.22	47,47,47,47	0
57	MG	2A	3283	1/1	0.96	0.24	46,46,46,46	0
57	MG	1D	304	1/1	0.96	0.11	25,25,25,25	0
57	MG	1A	3937	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3758	1/1	0.96	0.18	28,28,28,28	0
57	MG	2A	3558	1/1	0.96	0.11	34,34,34,34	0
57	MG	2P	202	1/1	0.96	0.08	49,49,49,49	0
57	MG	2A	3036	1/1	0.96	0.15	47,47,47,47	0
57	MG	1A	3269	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3039	1/1	0.96	0.07	50,50,50,50	0
57	MG	2R	202	1/1	0.96	0.14	47,47,47,47	0
57	MG	2A	3562	1/1	0.96	0.24	69,69,69,69	0
57	MG	1A	3332	1/1	0.96	0.40	62,62,62,62	0
57	MG	2T	205	1/1	0.96	0.11	44,44,44,44	0
57	MG	2U	202	1/1	0.96	0.32	50,50,50,50	0
57	MG	1A	3024	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3111	1/1	0.96	0.13	33,33,33,33	0
57	MG	2A	3044	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3272	1/1	0.96	0.13	27,27,27,27	0
57	MG	1A	3507	1/1	0.96	0.27	48,48,48,48	0
57	MG	1A	3509	1/1	0.96	0.17	30,30,30,30	0
57	MG	2A	3575	1/1	0.96	0.16	53,53,53,53	0
57	MG	23	102	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3770	1/1	0.96	0.14	19,19,19,19	0
57	MG	2A	3578	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3073	1/1	0.96	0.19	42,42,42,42	0
57	MG	1A	3948	1/1	0.96	0.06	49,49,49,49	0
57	MG	1F	303	1/1	0.96	0.16	22,22,22,22	0
57	MG	1A	3613	1/1	0.96	0.17	30,30,30,30	0
57	MG	1F	305	1/1	0.96	0.14	25,25,25,25	0
57	MG	2A	3587	1/1	0.96	0.18	43,43,43,43	0
57	MG	2A	3054	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	3032	1/1	0.96	0.22	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3616	1/1	0.96	0.23	29,29,29,29	0
57	MG	2A	3307	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	3275	1/1	0.96	0.24	43,43,43,43	0
57	MG	2A	3062	1/1	0.96	0.22	47,47,47,47	0
57	MG	2A	3310	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3599	1/1	0.96	0.10	70,70,70,70	0
57	MG	1F	309	1/1	0.96	0.15	34,34,34,34	0
57	MG	2A	3312	1/1	0.96	0.11	57,57,57,57	0
57	MG	2a	1611	1/1	0.96	0.13	63,63,63,63	0
57	MG	1F	310	1/1	0.96	0.18	29,29,29,29	0
57	MG	1A	3776	1/1	0.96	0.12	41,41,41,41	0
57	MG	1F	312	1/1	0.96	0.15	27,27,27,27	0
57	MG	1A	3620	1/1	0.96	0.14	40,40,40,40	0
57	MG	2a	1616	1/1	0.96	0.11	54,54,54,54	0
57	MG	1A	3421	1/1	0.96	0.23	39,39,39,39	0
57	MG	1A	3961	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3422	1/1	0.96	0.16	40,40,40,40	0
57	MG	1A	3276	1/1	0.96	0.21	20,20,20,20	0
57	MG	1A	3227	1/1	0.96	0.17	22,22,22,22	0
57	MG	1A	3346	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3229	1/1	0.96	0.11	26,26,26,26	0
57	MG	2A	3618	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3787	1/1	0.96	0.27	74,74,74,74	0
57	MG	1A	3630	1/1	0.96	0.15	29,29,29,29	0
57	MG	1A	3789	1/1	0.96	0.19	38,38,38,38	0
57	MG	2A	3625	1/1	0.96	0.10	47,47,47,47	0
57	MG	2a	1630	1/1	0.96	0.13	82,82,82,82	0
57	MG	1A	3429	1/1	0.96	0.17	30,30,30,30	0
57	MG	1A	3018	1/1	0.96	0.19	42,42,42,42	0
57	MG	2A	3084	1/1	0.96	0.23	47,47,47,47	0
57	MG	1A	3635	1/1	0.96	0.15	16,16,16,16	0
57	MG	1a	1693	1/1	0.96	0.13	43,43,43,43	0
57	MG	1a	1694	1/1	0.96	0.09	42,42,42,42	0
57	MG	2a	1638	1/1	0.96	0.20	62,62,62,62	0
57	MG	1A	3636	1/1	0.96	0.14	11,11,11,11	0
57	MG	1A	3795	1/1	0.96	0.18	46,46,46,46	0
57	MG	2A	3634	1/1	0.96	0.13	37,37,37,37	0
57	MG	2A	3339	1/1	0.96	0.11	53,53,53,53	0
57	MG	2A	3638	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3431	1/1	0.96	0.19	32,32,32,32	0
57	MG	1A	3231	1/1	0.96	0.12	32,32,32,32	0
57	MG	2a	1647	1/1	0.96	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1699	1/1	0.96	0.11	61,61,61,61	0
57	MG	2A	3095	1/1	0.96	0.06	63,63,63,63	0
57	MG	1P	202	1/1	0.96	0.24	33,33,33,33	0
57	MG	1A	3799	1/1	0.96	0.10	43,43,43,43	0
57	MG	1P	205	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3800	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3640	1/1	0.96	0.20	24,24,24,24	0
57	MG	1A	3803	1/1	0.96	0.11	26,26,26,26	0
57	MG	2A	3102	1/1	0.96	0.20	46,46,46,46	0
57	MG	2A	3103	1/1	0.96	0.18	62,62,62,62	0
57	MG	2a	1659	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3351	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3643	1/1	0.96	0.18	28,28,28,28	0
57	MG	1a	1708	1/1	0.96	0.16	66,66,66,66	0
57	MG	2A	3655	1/1	0.96	0.14	66,66,66,66	0
57	MG	2a	1665	1/1	0.96	0.06	57,57,57,57	0
57	MG	2A	3355	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3036	1/1	0.96	0.39	26,26,26,26	0
57	MG	2a	1668	1/1	0.96	0.11	54,54,54,54	0
57	MG	1A	3527	1/1	0.96	0.21	28,28,28,28	0
57	MG	2a	1670	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3109	1/1	0.96	0.15	59,59,59,59	0
57	MG	1A	3353	1/1	0.96	0.14	31,31,31,31	0
57	MG	2a	1673	1/1	0.96	0.26	57,57,57,57	0
57	MG	2a	1674	1/1	0.96	0.12	44,44,44,44	0
57	MG	2A	3360	1/1	0.96	0.08	41,41,41,41	0
57	MG	1R	205	1/1	0.96	0.24	23,23,23,23	0
57	MG	2A	3112	1/1	0.96	0.22	45,45,45,45	0
57	MG	2A	3672	1/1	0.96	0.15	45,45,45,45	0
57	MG	2A	3674	1/1	0.96	0.19	51,51,51,51	0
57	MG	1A	3812	1/1	0.96	0.13	21,21,21,21	0
57	MG	1A	3186	1/1	0.96	0.13	40,40,40,40	0
57	MG	2A	3366	1/1	0.96	0.27	52,52,52,52	0
57	MG	2a	1685	1/1	0.96	0.19	63,63,63,63	0
57	MG	2A	3116	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3996	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3815	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3355	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3005	1/1	0.96	0.24	46,46,46,46	0
57	MG	1a	1720	1/1	0.96	0.12	59,59,59,59	0
57	MG	2A	3686	1/1	0.96	0.07	64,64,64,64	0
57	MG	1A	3821	1/1	0.96	0.13	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3374	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3375	1/1	0.96	0.41	59,59,59,59	0
57	MG	2a	1698	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3151	1/1	0.96	0.20	30,30,30,30	0
57	MG	1A	3825	1/1	0.96	0.19	34,34,34,34	0
57	MG	1A	3152	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3195	1/1	0.96	0.17	31,31,31,31	0
57	MG	2A	3129	1/1	0.96	0.19	38,38,38,38	0
57	MG	1U	205	1/1	0.96	0.16	24,24,24,24	0
57	MG	2A	3697	1/1	0.96	0.17	34,34,34,34	0
57	MG	1U	207	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	3289	1/1	0.96	0.27	21,21,21,21	0
57	MG	1a	1731	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3363	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3119	1/1	0.96	0.28	35,35,35,35	0
57	MG	2A	3137	1/1	0.96	0.15	63,63,63,63	0
57	MG	1A	3834	1/1	0.96	0.12	46,46,46,46	0
57	MG	1W	201	1/1	0.96	0.19	33,33,33,33	0
57	MG	1A	3665	1/1	0.96	0.12	28,28,28,28	0
57	MG	2a	1716	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3539	1/1	0.96	0.22	42,42,42,42	0
57	MG	1a	1738	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3396	1/1	0.96	0.22	29,29,29,29	0
57	MG	1W	205	1/1	0.96	0.22	47,47,47,47	0
57	MG	1A	3540	1/1	0.96	0.14	42,42,42,42	0
57	MG	1A	3198	1/1	0.96	0.16	18,18,18,18	0
57	MG	2A	3149	1/1	0.96	0.14	52,52,52,52	0
57	MG	1A	3294	1/1	0.96	0.16	36,36,36,36	0
57	MG	2a	1727	1/1	0.96	0.15	61,61,61,61	0
57	MG	2A	3720	1/1	0.96	0.27	50,50,50,50	0
57	MG	1X	101	1/1	0.96	0.24	33,33,33,33	0
57	MG	1A	3065	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3544	1/1	0.96	0.26	53,53,53,53	0
57	MG	2A	3155	1/1	0.96	0.17	36,36,36,36	0
57	MG	2A	3156	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3099	1/1	0.96	0.26	34,34,34,34	0
57	MG	1A	3371	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3372	1/1	0.96	0.15	27,27,27,27	0
57	MG	1A	4026	1/1	0.96	0.22	25,25,25,25	0
57	MG	1a	1757	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3202	1/1	0.96	0.11	28,28,28,28	0
57	MG	1A	3684	1/1	0.96	0.16	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1741	1/1	0.96	0.16	66,66,66,66	0
57	MG	1A	4031	1/1	0.96	0.10	32,32,32,32	0
57	MG	2A	3165	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3054	1/1	0.96	0.21	28,28,28,28	0
57	MG	2a	1747	1/1	0.96	0.25	56,56,56,56	0
57	MG	2A	3419	1/1	0.96	0.18	45,45,45,45	0
57	MG	2a	1749	1/1	0.96	0.13	65,65,65,65	0
57	MG	1A	3552	1/1	0.96	0.16	25,25,25,25	0
57	MG	1A	3553	1/1	0.96	0.09	29,29,29,29	0
57	MG	2A	3743	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3170	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3690	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3102	1/1	0.96	0.14	23,23,23,23	0
57	MG	1A	3695	1/1	0.96	0.23	41,41,41,41	0
57	MG	1A	4040	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3751	1/1	0.96	0.14	41,41,41,41	0
57	MG	10	108	1/1	0.96	0.17	46,46,46,46	0
57	MG	10	109	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3696	1/1	0.96	0.25	18,18,18,18	0
57	MG	1A	3376	1/1	0.96	0.15	19,19,19,19	0
57	MG	2a	1764	1/1	0.96	0.17	50,50,50,50	0
57	MG	1A	3557	1/1	0.96	0.17	60,60,60,60	0
57	MG	1A	3865	1/1	0.96	0.11	27,27,27,27	0
57	MG	1A	3377	1/1	0.96	0.34	38,38,38,38	0
57	MG	1A	4051	1/1	0.96	0.14	22,22,22,22	0
57	MG	12	101	1/1	0.96	0.26	29,29,29,29	0
57	MG	1A	4052	1/1	0.96	0.09	40,40,40,40	0
57	MG	1a	1782	1/1	0.96	0.06	39,39,39,39	0
57	MG	13	102	1/1	0.96	0.33	39,39,39,39	0
57	MG	1A	3462	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3701	1/1	0.96	0.19	25,25,25,25	0
57	MG	13	106	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3304	1/1	0.96	0.26	29,29,29,29	0
57	MG	2a	1785	1/1	0.96	0.14	58,58,58,58	0
57	MG	1A	3103	1/1	0.96	0.17	25,25,25,25	0
57	MG	2A	3446	1/1	0.96	0.19	25,25,25,25	0
57	MG	2A	3774	1/1	0.96	0.20	67,67,67,67	0
57	MG	2A	3447	1/1	0.96	0.15	44,44,44,44	0
57	MG	2a	1791	1/1	0.96	0.20	57,57,57,57	0
57	MG	1A	3704	1/1	0.96	0.08	44,44,44,44	0
57	MG	1a	1791	1/1	0.96	0.08	59,59,59,59	0
57	MG	2A	3778	1/1	0.96	0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1792	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3705	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3453	1/1	0.96	0.45	49,49,49,49	0
57	MG	1A	3563	1/1	0.96	0.16	23,23,23,23	0
57	MG	2A	3784	1/1	0.96	0.13	79,79,79,79	0
57	MG	15	104	1/1	0.96	0.23	25,25,25,25	0
57	MG	2A	3204	1/1	0.96	0.18	41,41,41,41	0
57	MG	1A	3564	1/1	0.96	0.20	24,24,24,24	0
57	MG	1A	3021	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	4064	1/1	0.96	0.24	38,38,38,38	0
57	MG	1a	1801	1/1	0.96	0.10	63,63,63,63	0
57	MG	1A	3209	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	4067	1/1	0.96	0.24	47,47,47,47	0
57	MG	16	101	1/1	0.96	0.23	44,44,44,44	0
57	MG	1a	1806	1/1	0.96	0.10	49,49,49,49	0
57	MG	2A	3214	1/1	0.96	0.23	40,40,40,40	0
57	MG	1A	3382	1/1	0.96	0.42	45,45,45,45	0
57	MG	1A	3711	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3130	1/1	0.96	0.22	43,43,43,43	0
57	MG	1A	3384	1/1	0.96	0.23	39,39,39,39	0
57	MG	2A	3220	1/1	0.96	0.16	57,57,57,57	0
57	MG	1A	3885	1/1	0.96	0.14	42,42,42,42	0
57	MG	1e	201	1/1	0.96	0.22	61,61,61,61	0
57	MG	1A	3887	1/1	0.96	0.17	21,21,21,21	0
57	MG	1A	3718	1/1	0.96	0.12	43,43,43,43	0
57	MG	1A	3572	1/1	0.96	0.23	41,41,41,41	0
57	MG	1A	3893	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3573	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3895	1/1	0.96	0.15	41,41,41,41	0
57	MG	1A	3042	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3897	1/1	0.96	0.15	35,35,35,35	0
57	MG	2A	3485	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3726	1/1	0.96	0.17	26,26,26,26	0
57	MG	2A	3820	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3487	1/1	0.96	0.13	50,50,50,50	0
57	MG	1a	1605	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3727	1/1	0.96	0.13	22,22,22,22	0
57	MG	2A	3491	1/1	0.96	0.19	54,54,54,54	0
57	MG	1A	3386	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3826	1/1	0.96	0.16	28,28,28,28	0
57	MG	1A	3167	1/1	0.96	0.26	39,39,39,39	0
57	MG	1A	3257	1/1	0.96	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3579	1/1	0.96	0.31	36,36,36,36	0
57	MG	2A	3830	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3069	1/1	0.96	0.17	22,22,22,22	0
57	MG	1A	3259	1/1	0.96	0.20	39,39,39,39	0
57	MG	1A	3394	1/1	0.96	0.20	30,30,30,30	0
57	MG	2w	104	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3583	1/1	0.96	0.18	33,33,33,33	0
57	MG	2A	3837	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3319	1/1	0.96	0.23	34,34,34,34	0
57	MG	1B	205	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3738	1/1	0.96	0.13	28,28,28,28	0
57	MG	2x	101	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3170	1/1	0.96	0.25	28,28,28,28	0
57	MG	1A	3915	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	3013	1/1	0.96	0.24	24,24,24,24	0
57	MG	1A	3917	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3400	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3175	1/1	0.96	0.25	16,16,16,16	0
57	MG	2y	103	1/1	0.96	0.09	43,43,43,43	0
57	MG	1B	216	1/1	0.96	0.22	30,30,30,30	0
57	MG	2A	3515	1/1	0.96	0.14	52,52,52,52	0
57	MG	1y	101	1/1	0.96	0.12	64,64,64,64	0
57	MG	1A	3323	1/1	0.96	0.22	37,37,37,37	0
57	MG	1a	1630	1/1	0.96	0.20	58,58,58,58	0
57	MG	1B	218	1/1	0.96	0.24	43,43,43,43	0
57	MG	2A	3521	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3923	1/1	0.96	0.18	10,10,10,10	0
57	MG	1a	1633	1/1	0.96	0.23	35,35,35,35	0
57	MG	2B	212	1/1	0.96	0.20	41,41,41,41	0
57	MG	2A	3652	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3028	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3958	1/1	0.97	0.18	62,62,62,62	0
57	MG	2A	3032	1/1	0.97	0.16	52,52,52,52	0
57	MG	1A	3632	1/1	0.97	0.15	27,27,27,27	0
57	MG	2A	3657	1/1	0.97	0.15	42,42,42,42	0
57	MG	2A	3658	1/1	0.97	0.23	49,49,49,49	0
57	MG	1A	3555	1/1	0.97	0.77	45,45,45,45	0
57	MG	1A	3493	1/1	0.97	0.16	35,35,35,35	0
57	MG	2A	3661	1/1	0.97	0.28	51,51,51,51	0
57	MG	1A	3391	1/1	0.97	0.20	34,34,34,34	0
57	MG	1A	3041	1/1	0.97	0.17	34,34,34,34	0
57	MG	1A	3442	1/1	0.97	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3966	1/1	0.97	0.07	58,58,58,58	0
57	MG	1A	3308	1/1	0.97	0.22	46,46,46,46	0
57	MG	2A	3669	1/1	0.97	0.22	43,43,43,43	0
57	MG	2A	3670	1/1	0.97	0.16	41,41,41,41	0
57	MG	2A	3671	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3499	1/1	0.97	0.12	34,34,34,34	0
57	MG	2A	3673	1/1	0.97	0.19	50,50,50,50	0
57	MG	1B	211	1/1	0.97	0.21	46,46,46,46	0
57	MG	1B	212	1/1	0.97	0.10	60,60,60,60	0
57	MG	1B	213	1/1	0.97	0.18	43,43,43,43	0
57	MG	1A	3852	1/1	0.97	0.16	20,20,20,20	0
57	MG	1A	3853	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3500	1/1	0.97	0.23	36,36,36,36	0
57	MG	1a	1716	1/1	0.97	0.20	53,53,53,53	0
57	MG	2a	1623	1/1	0.97	0.22	58,58,58,58	0
57	MG	1A	3642	1/1	0.97	0.14	31,31,31,31	0
57	MG	1A	3740	1/1	0.97	0.20	10,10,10,10	0
57	MG	1A	3741	1/1	0.97	0.29	39,39,39,39	0
57	MG	1A	3395	1/1	0.97	0.12	36,36,36,36	0
57	MG	2A	3055	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3237	1/1	0.97	0.23	37,37,37,37	0
57	MG	13	103	1/1	0.97	0.22	30,30,30,30	0
57	MG	1A	3397	1/1	0.97	0.18	37,37,37,37	0
57	MG	2A	3059	1/1	0.97	0.17	55,55,55,55	0
57	MG	1A	3647	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3505	1/1	0.97	0.16	36,36,36,36	0
57	MG	1B	226	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3983	1/1	0.97	0.19	32,32,32,32	0
57	MG	1a	1729	1/1	0.97	0.09	54,54,54,54	0
57	MG	2a	1639	1/1	0.97	0.18	46,46,46,46	0
57	MG	2A	3068	1/1	0.97	0.12	40,40,40,40	0
57	MG	2A	3458	1/1	0.97	0.24	49,49,49,49	0
57	MG	1A	3649	1/1	0.97	0.23	31,31,31,31	0
57	MG	15	101	1/1	0.97	0.21	29,29,29,29	0
57	MG	1A	3650	1/1	0.97	0.18	34,34,34,34	0
57	MG	1A	3310	1/1	0.97	0.35	38,38,38,38	0
57	MG	1A	3753	1/1	0.97	0.20	47,47,47,47	0
57	MG	1A	3990	1/1	0.97	0.09	61,61,61,61	0
57	MG	2A	3075	1/1	0.97	0.22	37,37,37,37	0
57	MG	2A	3708	1/1	0.97	0.18	43,43,43,43	0
57	MG	1A	3059	1/1	0.97	0.21	33,33,33,33	0
57	MG	2A	3710	1/1	0.97	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1D	302	1/1	0.97	0.38	43,43,43,43	0
57	MG	2A	3712	1/1	0.97	0.12	58,58,58,58	0
57	MG	1D	303	1/1	0.97	0.09	36,36,36,36	0
57	MG	2a	1655	1/1	0.97	0.09	50,50,50,50	0
57	MG	2A	3714	1/1	0.97	0.16	51,51,51,51	0
57	MG	1A	3508	1/1	0.97	0.18	23,23,23,23	0
57	MG	2A	3080	1/1	0.97	0.11	34,34,34,34	0
57	MG	2A	3272	1/1	0.97	0.09	32,32,32,32	0
57	MG	1A	3873	1/1	0.97	0.28	28,28,28,28	0
57	MG	2a	1661	1/1	0.97	0.24	44,44,44,44	0
57	MG	17	101	1/1	0.97	0.21	31,31,31,31	0
57	MG	1A	3137	1/1	0.97	0.18	16,16,16,16	0
57	MG	1A	3450	1/1	0.97	0.22	37,37,37,37	0
57	MG	1D	309	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3876	1/1	0.97	0.09	52,52,52,52	0
57	MG	1a	1748	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3726	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3166	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	4000	1/1	0.97	0.14	28,28,28,28	0
57	MG	1E	302	1/1	0.97	0.22	34,34,34,34	0
57	MG	1a	1753	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3483	1/1	0.97	0.27	57,57,57,57	0
57	MG	1a	1754	1/1	0.97	0.11	49,49,49,49	0
57	MG	18	102	1/1	0.97	0.15	29,29,29,29	0
57	MG	1E	303	1/1	0.97	0.25	36,36,36,36	0
57	MG	18	104	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3452	1/1	0.97	0.27	49,49,49,49	0
57	MG	1A	3760	1/1	0.97	0.22	35,35,35,35	0
57	MG	2A	3738	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3660	1/1	0.97	0.14	34,34,34,34	0
57	MG	2a	1682	1/1	0.97	0.07	72,72,72,72	0
57	MG	1E	309	1/1	0.97	0.10	51,51,51,51	0
57	MG	2A	3741	1/1	0.97	0.09	48,48,48,48	0
57	MG	2a	1686	1/1	0.97	0.09	65,65,65,65	0
57	MG	1A	3402	1/1	0.97	0.24	24,24,24,24	0
57	MG	1A	3316	1/1	0.97	0.21	24,24,24,24	0
57	MG	1A	3017	1/1	0.97	0.15	30,30,30,30	0
57	MG	1A	4007	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3666	1/1	0.97	0.15	25,25,25,25	0
57	MG	1A	3359	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3769	1/1	0.97	0.15	21,21,21,21	0
57	MG	1A	3168	1/1	0.97	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3502	1/1	0.97	0.18	52,52,52,52	0
57	MG	1A	3891	1/1	0.97	0.16	20,20,20,20	0
57	MG	1a	1614	1/1	0.97	0.15	48,48,48,48	0
57	MG	1A	4013	1/1	0.97	0.17	17,17,17,17	0
57	MG	2A	3506	1/1	0.97	0.13	58,58,58,58	0
57	MG	2A	3113	1/1	0.97	0.10	43,43,43,43	0
57	MG	2A	3509	1/1	0.97	0.10	26,26,26,26	0
57	MG	1A	3098	1/1	0.97	0.19	28,28,28,28	0
57	MG	1A	3044	1/1	0.97	0.12	25,25,25,25	0
57	MG	1A	3671	1/1	0.97	0.11	26,26,26,26	0
57	MG	2A	3513	1/1	0.97	0.07	54,54,54,54	0
57	MG	1a	1780	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3172	1/1	0.97	0.20	32,32,32,32	0
57	MG	2A	3768	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3461	1/1	0.97	0.28	43,43,43,43	0
57	MG	2A	3517	1/1	0.97	0.12	46,46,46,46	0
57	MG	2A	3315	1/1	0.97	0.16	53,53,53,53	0
57	MG	2A	3316	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3365	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3173	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3678	1/1	0.97	0.17	23,23,23,23	0
57	MG	1A	3141	1/1	0.97	0.24	30,30,30,30	0
57	MG	1A	3680	1/1	0.97	0.17	25,25,25,25	0
57	MG	1A	3465	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3682	1/1	0.97	0.13	17,17,17,17	0
57	MG	2A	3780	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	4028	1/1	0.97	0.16	28,28,28,28	0
57	MG	2a	1725	1/1	0.97	0.17	60,60,60,60	0
57	MG	1A	3008	1/1	0.97	0.15	23,23,23,23	0
57	MG	2A	3531	1/1	0.97	0.22	34,34,34,34	0
57	MG	1A	3415	1/1	0.97	0.11	47,47,47,47	0
57	MG	1A	3594	1/1	0.97	0.36	34,34,34,34	0
57	MG	1a	1795	1/1	0.97	0.09	53,53,53,53	0
57	MG	2A	3535	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3101	1/1	0.97	0.38	38,38,38,38	0
57	MG	1a	1797	1/1	0.97	0.14	42,42,42,42	0
57	MG	2A	3538	1/1	0.97	0.15	41,41,41,41	0
57	MG	2A	3136	1/1	0.97	0.14	29,29,29,29	0
57	MG	1a	1634	1/1	0.97	0.16	23,23,23,23	0
57	MG	2A	3794	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3144	1/1	0.97	0.09	40,40,40,40	0
57	MG	2A	3139	1/1	0.97	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3598	1/1	0.97	0.12	20,20,20,20	0
57	MG	1A	3792	1/1	0.97	0.19	23,23,23,23	0
57	MG	2a	1742	1/1	0.97	0.22	43,43,43,43	0
57	MG	2A	3545	1/1	0.97	0.23	30,30,30,30	0
57	MG	2A	3801	1/1	0.97	0.18	46,46,46,46	0
57	MG	2a	1745	1/1	0.97	0.16	65,65,65,65	0
57	MG	1A	3146	1/1	0.97	0.19	28,28,28,28	0
57	MG	2A	3143	1/1	0.97	0.24	44,44,44,44	0
57	MG	2A	3144	1/1	0.97	0.17	47,47,47,47	0
57	MG	1a	1803	1/1	0.97	0.12	47,47,47,47	0
57	MG	1P	201	1/1	0.97	0.23	28,28,28,28	0
57	MG	2A	3553	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	3022	1/1	0.97	0.12	16,16,16,16	0
57	MG	2a	1753	1/1	0.97	0.18	69,69,69,69	0
57	MG	1a	1641	1/1	0.97	0.16	66,66,66,66	0
57	MG	1A	4041	1/1	0.97	0.12	22,22,22,22	0
57	MG	2A	3557	1/1	0.97	0.13	47,47,47,47	0
57	MG	2A	3814	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3075	1/1	0.97	0.20	24,24,24,24	0
57	MG	1Q	201	1/1	0.97	0.27	28,28,28,28	0
57	MG	1A	4043	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3150	1/1	0.97	0.33	31,31,31,31	0
57	MG	1A	3919	1/1	0.97	0.10	42,42,42,42	0
57	MG	1Q	205	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3564	1/1	0.97	0.23	59,59,59,59	0
57	MG	2A	3565	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3536	1/1	0.97	0.33	40,40,40,40	0
57	MG	1A	4048	1/1	0.97	0.19	16,16,16,16	0
57	MG	1k	201	1/1	0.97	0.13	57,57,57,57	0
57	MG	1A	3921	1/1	0.97	0.15	32,32,32,32	0
57	MG	2a	1770	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3290	1/1	0.97	0.17	33,33,33,33	0
57	MG	2A	3573	1/1	0.97	0.24	48,48,48,48	0
57	MG	1A	3126	1/1	0.97	0.36	22,22,22,22	0
57	MG	2a	1774	1/1	0.97	0.08	68,68,68,68	0
57	MG	2a	1775	1/1	0.97	0.18	46,46,46,46	0
57	MG	1A	3478	1/1	0.97	0.16	34,34,34,34	0
57	MG	2a	1777	1/1	0.97	0.14	55,55,55,55	0
57	MG	2A	3576	1/1	0.97	0.23	48,48,48,48	0
57	MG	2a	1779	1/1	0.97	0.14	65,65,65,65	0
57	MG	1p	101	1/1	0.97	0.11	51,51,51,51	0
57	MG	2a	1781	1/1	0.97	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1782	1/1	0.97	0.15	50,50,50,50	0
57	MG	1A	3064	1/1	0.97	0.11	28,28,28,28	0
57	MG	2A	3579	1/1	0.97	0.15	54,54,54,54	0
57	MG	1a	1657	1/1	0.97	0.18	57,57,57,57	0
57	MG	1A	3336	1/1	0.97	0.08	60,60,60,60	0
57	MG	2A	3168	1/1	0.97	0.20	46,46,46,46	0
57	MG	2A	3583	1/1	0.97	0.22	42,42,42,42	0
57	MG	2A	3584	1/1	0.97	0.16	26,26,26,26	0
57	MG	2A	3846	1/1	0.97	0.09	48,48,48,48	0
57	MG	1a	1659	1/1	0.97	0.37	66,66,66,66	0
57	MG	1A	3049	1/1	0.97	0.18	25,25,25,25	0
57	MG	2A	3851	1/1	0.97	0.18	47,47,47,47	0
57	MG	1A	3078	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3929	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3589	1/1	0.97	0.27	57,57,57,57	0
57	MG	2A	3590	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3809	1/1	0.97	0.13	54,54,54,54	0
57	MG	1w	107	1/1	0.97	0.14	49,49,49,49	0
57	MG	1w	108	1/1	0.97	0.20	66,66,66,66	0
57	MG	1A	3040	1/1	0.97	0.16	36,36,36,36	0
57	MG	2A	3178	1/1	0.97	0.11	39,39,39,39	0
57	MG	1T	204	1/1	0.97	0.16	53,53,53,53	0
57	MG	2B	208	1/1	0.97	0.09	60,60,60,60	0
57	MG	2A	3597	1/1	0.97	0.15	63,63,63,63	0
57	MG	2B	210	1/1	0.97	0.17	66,66,66,66	0
57	MG	1A	3545	1/1	0.97	0.12	53,53,53,53	0
57	MG	2a	1812	1/1	0.97	0.14	46,46,46,46	0
57	MG	2A	3377	1/1	0.97	0.27	35,35,35,35	0
57	MG	1A	3619	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3157	1/1	0.97	0.21	33,33,33,33	0
57	MG	2a	1816	1/1	0.97	0.18	56,56,56,56	0
57	MG	1A	3486	1/1	0.97	0.17	38,38,38,38	0
57	MG	2a	1818	1/1	0.97	0.25	63,63,63,63	0
57	MG	1A	3936	1/1	0.97	0.09	40,40,40,40	0
57	MG	2A	3605	1/1	0.97	0.12	43,43,43,43	0
57	MG	2B	218	1/1	0.97	0.20	58,58,58,58	0
57	MG	2A	3606	1/1	0.97	0.12	49,49,49,49	0
57	MG	1A	3264	1/1	0.97	0.18	48,48,48,48	0
57	MG	1U	209	1/1	0.97	0.10	38,38,38,38	0
57	MG	2D	303	1/1	0.97	0.19	28,28,28,28	0
57	MG	2A	3189	1/1	0.97	0.22	59,59,59,59	0
57	MG	1V	201	1/1	0.97	0.40	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1828	1/1	0.97	0.15	52,52,52,52	0
57	MG	1A	3714	1/1	0.97	0.23	30,30,30,30	0
57	MG	2A	3613	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3131	1/1	0.97	0.08	29,29,29,29	0
57	MG	2E	305	1/1	0.97	0.10	44,44,44,44	0
57	MG	2A	3615	1/1	0.97	0.22	49,49,49,49	0
57	MG	2f	202	1/1	0.97	0.15	67,67,67,67	0
57	MG	1a	1677	1/1	0.97	0.09	63,63,63,63	0
57	MG	2E	308	1/1	0.97	0.16	38,38,38,38	0
57	MG	1x	113	1/1	0.97	0.10	61,61,61,61	0
57	MG	1a	1678	1/1	0.97	0.14	51,51,51,51	0
57	MG	2l	202	1/1	0.97	0.14	51,51,51,51	0
57	MG	1x	115	1/1	0.97	0.19	54,54,54,54	0
57	MG	2A	3392	1/1	0.97	0.28	57,57,57,57	0
57	MG	1A	3344	1/1	0.97	0.18	36,36,36,36	0
57	MG	1A	3719	1/1	0.97	0.22	36,36,36,36	0
57	MG	2q	202	1/1	0.97	0.17	59,59,59,59	0
57	MG	1A	3625	1/1	0.97	0.16	33,33,33,33	0
57	MG	1A	3721	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	3722	1/1	0.97	0.13	66,66,66,66	0
57	MG	1W	204	1/1	0.97	0.13	31,31,31,31	0
57	MG	2w	101	1/1	0.97	0.15	53,53,53,53	0
57	MG	1A	3723	1/1	0.97	0.16	51,51,51,51	0
57	MG	2A	3401	1/1	0.97	0.22	41,41,41,41	0
57	MG	2A	3007	1/1	0.97	0.11	48,48,48,48	0
57	MG	2A	3008	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3831	1/1	0.97	0.11	29,29,29,29	0
57	MG	2Q	202	1/1	0.97	0.26	52,52,52,52	0
57	MG	1a	1687	1/1	0.97	0.16	42,42,42,42	0
57	MG	2A	3636	1/1	0.97	0.28	39,39,39,39	0
57	MG	2A	3637	1/1	0.97	0.21	35,35,35,35	0
57	MG	2T	202	1/1	0.97	0.13	42,42,42,42	0
57	MG	1A	3626	1/1	0.97	0.12	20,20,20,20	0
57	MG	1W	209	1/1	0.97	0.20	29,29,29,29	0
57	MG	2U	201	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3093	1/1	0.97	0.21	16,16,16,16	0
57	MG	1A	3267	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3016	1/1	0.97	0.18	54,54,54,54	0
57	MG	1A	3837	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	3838	1/1	0.97	0.21	56,56,56,56	0
57	MG	1X	105	1/1	0.97	0.17	48,48,48,48	0
57	MG	20	101	1/1	0.97	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	2A	3444	1/1	0.97	0.24	75,75,75,75	0
57	MG	1X	106	1/1	0.97	0.19	29,29,29,29	0
57	MG	2A	3219	1/1	0.97	0.15	39,39,39,39	0
60	ZN	1Y	204	1/1	0.97	0.15	70,70,70,70	0
57	MG	1A	3094	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3954	1/1	0.97	0.21	18,18,18,18	0
57	MG	1A	3728	1/1	0.97	0.14	57,57,57,57	0
57	MG	1A	3631	1/1	0.97	0.09	17,17,17,17	0
57	MG	17	103	1/1	0.98	0.16	27,27,27,27	0
57	MG	1E	310	1/1	0.98	0.18	17,17,17,17	0
57	MG	1A	3903	1/1	0.98	0.14	29,29,29,29	0
57	MG	1E	312	1/1	0.98	0.16	31,31,31,31	0
57	MG	2A	3043	1/1	0.98	0.17	50,50,50,50	0
57	MG	1A	3028	1/1	0.98	0.23	29,29,29,29	0
57	MG	1A	4018	1/1	0.98	0.12	30,30,30,30	0
57	MG	1F	302	1/1	0.98	0.27	35,35,35,35	0
57	MG	1A	3905	1/1	0.98	0.24	32,32,32,32	0
57	MG	1a	1739	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3798	1/1	0.98	0.26	27,27,27,27	0
57	MG	1A	4021	1/1	0.98	0.21	29,29,29,29	0
57	MG	1A	3035	1/1	0.98	0.18	34,34,34,34	0
57	MG	1a	1743	1/1	0.98	0.11	50,50,50,50	0
57	MG	1A	3908	1/1	0.98	0.17	22,22,22,22	0
57	MG	1A	3200	1/1	0.98	0.19	32,32,32,32	0
57	MG	1A	3801	1/1	0.98	0.14	24,24,24,24	0
57	MG	1A	3278	1/1	0.98	0.21	32,32,32,32	0
57	MG	1A	3712	1/1	0.98	0.14	21,21,21,21	0
57	MG	1A	3627	1/1	0.98	0.20	38,38,38,38	0
57	MG	1A	3010	1/1	0.98	0.07	44,44,44,44	0
57	MG	2A	3060	1/1	0.98	0.12	65,65,65,65	0
57	MG	2A	3061	1/1	0.98	0.14	42,42,42,42	0
57	MG	1a	1608	1/1	0.98	0.20	48,48,48,48	0
57	MG	1A	3149	1/1	0.98	0.12	36,36,36,36	0
57	MG	2A	3797	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	4032	1/1	0.98	0.19	26,26,26,26	0
57	MG	1A	3807	1/1	0.98	0.15	30,30,30,30	0
57	MG	2A	3598	1/1	0.98	0.08	43,43,43,43	0
57	MG	2a	1684	1/1	0.98	0.12	62,62,62,62	0
57	MG	1a	1756	1/1	0.98	0.16	42,42,42,42	0
57	MG	2A	3067	1/1	0.98	0.14	48,48,48,48	0
57	MG	2A	3803	1/1	0.98	0.14	38,38,38,38	0
57	MG	2A	3237	1/1	0.98	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3808	1/1	0.98	0.16	32,32,32,32	0
57	MG	1A	3203	1/1	0.98	0.14	26,26,26,26	0
57	MG	2a	1691	1/1	0.98	0.17	44,44,44,44	0
57	MG	1A	4036	1/1	0.98	0.12	38,38,38,38	0
57	MG	2A	3808	1/1	0.98	0.09	57,57,57,57	0
57	MG	1A	3328	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3435	1/1	0.98	0.26	28,28,28,28	0
57	MG	1A	3204	1/1	0.98	0.11	54,54,54,54	0
57	MG	1A	3245	1/1	0.98	0.17	47,47,47,47	0
57	MG	1N	203	1/1	0.98	0.24	26,26,26,26	0
57	MG	2A	3610	1/1	0.98	0.16	38,38,38,38	0
57	MG	1A	3497	1/1	0.98	0.25	61,61,61,61	0
57	MG	1A	3043	1/1	0.98	0.20	22,22,22,22	0
57	MG	1A	3817	1/1	0.98	0.13	21,21,21,21	0
57	MG	1A	3818	1/1	0.98	0.17	22,22,22,22	0
57	MG	1A	3439	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3285	1/1	0.98	0.16	39,39,39,39	0
57	MG	1a	1626	1/1	0.98	0.14	56,56,56,56	0
57	MG	1a	1772	1/1	0.98	0.07	48,48,48,48	0
57	MG	2A	3254	1/1	0.98	0.19	55,55,55,55	0
57	MG	1A	3020	1/1	0.98	0.14	21,21,21,21	0
57	MG	2a	1710	1/1	0.98	0.12	58,58,58,58	0
57	MG	2A	3621	1/1	0.98	0.08	41,41,41,41	0
57	MG	1A	3824	1/1	0.98	0.13	35,35,35,35	0
57	MG	2A	3623	1/1	0.98	0.11	32,32,32,32	0
57	MG	2A	3624	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3566	1/1	0.98	0.16	32,32,32,32	0
57	MG	1A	3334	1/1	0.98	0.34	33,33,33,33	0
57	MG	1A	3503	1/1	0.98	0.13	33,33,33,33	0
57	MG	2A	3832	1/1	0.98	0.24	44,44,44,44	0
57	MG	1a	1779	1/1	0.98	0.08	46,46,46,46	0
57	MG	2A	3834	1/1	0.98	0.24	53,53,53,53	0
57	MG	2a	1721	1/1	0.98	0.06	52,52,52,52	0
57	MG	2A	3090	1/1	0.98	0.13	47,47,47,47	0
57	MG	1A	4054	1/1	0.98	0.24	27,27,27,27	0
57	MG	1A	3828	1/1	0.98	0.20	27,27,27,27	0
57	MG	1A	3569	1/1	0.98	0.19	33,33,33,33	0
57	MG	1a	1783	1/1	0.98	0.08	47,47,47,47	0
57	MG	2A	3840	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3014	1/1	0.98	0.14	22,22,22,22	0
57	MG	2A	3445	1/1	0.98	0.22	54,54,54,54	0
57	MG	2A	3843	1/1	0.98	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3844	1/1	0.98	0.09	44,44,44,44	0
57	MG	2A	3845	1/1	0.98	0.18	32,32,32,32	0
57	MG	1A	3646	1/1	0.98	0.13	31,31,31,31	0
57	MG	2A	3847	1/1	0.98	0.10	37,37,37,37	0
57	MG	2A	3848	1/1	0.98	0.13	47,47,47,47	0
57	MG	1A	3832	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3039	1/1	0.98	0.31	24,24,24,24	0
57	MG	1A	4061	1/1	0.98	0.22	43,43,43,43	0
57	MG	2A	3450	1/1	0.98	0.48	42,42,42,42	0
57	MG	1A	3388	1/1	0.98	0.24	37,37,37,37	0
57	MG	2A	3854	1/1	0.98	0.22	47,47,47,47	0
57	MG	1A	3134	1/1	0.98	0.17	34,34,34,34	0
57	MG	2A	3274	1/1	0.98	0.16	38,38,38,38	0
57	MG	1A	3836	1/1	0.98	0.10	38,38,38,38	0
57	MG	2A	3455	1/1	0.98	0.31	60,60,60,60	0
57	MG	2B	203	1/1	0.98	0.17	54,54,54,54	0
57	MG	2A	3276	1/1	0.98	0.19	47,47,47,47	0
57	MG	1A	4065	1/1	0.98	0.18	30,30,30,30	0
57	MG	1A	3574	1/1	0.98	0.19	55,55,55,55	0
57	MG	1A	3178	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3212	1/1	0.98	0.18	38,38,38,38	0
57	MG	1A	3292	1/1	0.98	0.11	43,43,43,43	0
57	MG	1A	3841	1/1	0.98	0.12	44,44,44,44	0
57	MG	1A	3393	1/1	0.98	0.42	31,31,31,31	0
57	MG	1A	3742	1/1	0.98	0.18	37,37,37,37	0
57	MG	1a	1651	1/1	0.98	0.13	40,40,40,40	0
57	MG	1A	3950	1/1	0.98	0.06	10,10,10,10	0
57	MG	1U	201	1/1	0.98	0.17	23,23,23,23	0
57	MG	1A	3656	1/1	0.98	0.13	18,18,18,18	0
57	MG	1A	3092	1/1	0.98	0.10	25,25,25,25	0
57	MG	1A	3745	1/1	0.98	0.18	25,25,25,25	0
57	MG	2A	3291	1/1	0.98	0.13	48,48,48,48	0
57	MG	2A	3118	1/1	0.98	0.14	59,59,59,59	0
57	MG	1A	3513	1/1	0.98	0.20	40,40,40,40	0
57	MG	1U	206	1/1	0.98	0.28	36,36,36,36	0
57	MG	1A	3955	1/1	0.98	0.11	30,30,30,30	0
57	MG	1U	208	1/1	0.98	0.22	26,26,26,26	0
57	MG	2A	3668	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3342	1/1	0.98	0.19	42,42,42,42	0
57	MG	1A	3156	1/1	0.98	0.23	21,21,21,21	0
57	MG	1A	3749	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3959	1/1	0.98	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3118	1/1	0.98	0.15	20,20,20,20	0
57	MG	2A	3128	1/1	0.98	0.16	73,73,73,73	0
57	MG	1A	3663	1/1	0.98	0.14	17,17,17,17	0
57	MG	2A	3676	1/1	0.98	0.16	42,42,42,42	0
57	MG	1A	3296	1/1	0.98	0.23	39,39,39,39	0
57	MG	2A	3678	1/1	0.98	0.19	44,44,44,44	0
57	MG	1A	3347	1/1	0.98	0.25	47,47,47,47	0
57	MG	1A	3586	1/1	0.98	0.20	43,43,43,43	0
57	MG	1A	3297	1/1	0.98	0.45	62,62,62,62	0
57	MG	1A	3859	1/1	0.98	0.11	30,30,30,30	0
57	MG	2a	1783	1/1	0.98	0.20	50,50,50,50	0
57	MG	2A	3490	1/1	0.98	0.14	41,41,41,41	0
57	MG	1n	102	1/1	0.98	0.08	39,39,39,39	0
57	MG	2a	1786	1/1	0.98	0.14	60,60,60,60	0
57	MG	1W	206	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3048	1/1	0.98	0.24	29,29,29,29	0
57	MG	1A	3183	1/1	0.98	0.12	44,44,44,44	0
57	MG	1a	1675	1/1	0.98	0.11	45,45,45,45	0
57	MG	1A	3301	1/1	0.98	0.24	32,32,32,32	0
57	MG	1A	3074	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3524	1/1	0.98	0.20	29,29,29,29	0
57	MG	1w	104	1/1	0.98	0.12	55,55,55,55	0
57	MG	1A	3405	1/1	0.98	0.10	43,43,43,43	0
57	MG	1A	3675	1/1	0.98	0.12	40,40,40,40	0
57	MG	2A	3695	1/1	0.98	0.14	51,51,51,51	0
57	MG	1X	104	1/1	0.98	0.15	36,36,36,36	0
57	MG	1A	3121	1/1	0.98	0.24	31,31,31,31	0
57	MG	2a	1800	1/1	0.98	0.26	59,59,59,59	0
57	MG	1A	3595	1/1	0.98	0.26	33,33,33,33	0
57	MG	2V	201	1/1	0.98	0.20	43,43,43,43	0
57	MG	1A	3122	1/1	0.98	0.31	37,37,37,37	0
57	MG	1Y	201	1/1	0.98	0.21	33,33,33,33	0
57	MG	2A	3507	1/1	0.98	0.20	33,33,33,33	0
57	MG	1A	3123	1/1	0.98	0.30	38,38,38,38	0
57	MG	2A	3152	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3871	1/1	0.98	0.18	42,42,42,42	0
57	MG	2a	1809	1/1	0.98	0.12	65,65,65,65	0
57	MG	20	102	1/1	0.98	0.14	38,38,38,38	0
57	MG	21	101	1/1	0.98	0.27	40,40,40,40	0
57	MG	1A	3979	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3980	1/1	0.98	0.16	51,51,51,51	0
57	MG	1A	3872	1/1	0.98	0.23	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	25	101	1/1	0.98	0.20	38,38,38,38	0
57	MG	1A	3222	1/1	0.98	0.22	22,22,22,22	0
57	MG	1A	3985	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3164	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3600	1/1	0.98	0.23	38,38,38,38	0
57	MG	1A	3468	1/1	0.98	0.29	61,61,61,61	0
57	MG	2A	3337	1/1	0.98	0.11	42,42,42,42	0
57	MG	1B	223	1/1	0.98	0.13	61,61,61,61	0
57	MG	1A	3602	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	3190	1/1	0.98	0.20	23,23,23,23	0
57	MG	1A	3191	1/1	0.98	0.19	27,27,27,27	0
57	MG	2a	1602	1/1	0.98	0.13	43,43,43,43	0
57	MG	1A	3689	1/1	0.98	0.23	22,22,22,22	0
57	MG	1A	3605	1/1	0.98	0.17	23,23,23,23	0
57	MG	2A	3526	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3691	1/1	0.98	0.09	29,29,29,29	0
57	MG	1A	3192	1/1	0.98	0.29	26,26,26,26	0
57	MG	2A	3529	1/1	0.98	0.13	45,45,45,45	0
57	MG	1A	3781	1/1	0.98	0.22	47,47,47,47	0
57	MG	2A	3171	1/1	0.98	0.19	39,39,39,39	0
57	MG	1A	3694	1/1	0.98	0.23	26,26,26,26	0
57	MG	1A	3999	1/1	0.98	0.13	33,33,33,33	0
57	MG	1B	234	1/1	0.98	0.16	22,22,22,22	0
57	MG	12	102	1/1	0.98	0.22	38,38,38,38	0
57	MG	1D	301	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3228	1/1	0.98	0.21	22,22,22,22	0
57	MG	2A	3012	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3362	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3889	1/1	0.98	0.14	23,23,23,23	0
57	MG	1D	305	1/1	0.98	0.27	44,44,44,44	0
57	MG	1A	3890	1/1	0.98	0.20	21,21,21,21	0
57	MG	1A	3312	1/1	0.98	0.18	28,28,28,28	0
57	MG	2A	3184	1/1	0.98	0.19	44,44,44,44	0
57	MG	1A	3193	1/1	0.98	0.34	34,34,34,34	0
57	MG	1A	3106	1/1	0.98	0.15	25,25,25,25	0
57	MG	1A	3107	1/1	0.98	0.25	41,41,41,41	0
57	MG	2A	3188	1/1	0.98	0.14	52,52,52,52	0
57	MG	2A	3550	1/1	0.98	0.21	28,28,28,28	0
57	MG	2A	3021	1/1	0.98	0.11	33,33,33,33	0
57	MG	2A	3022	1/1	0.98	0.17	43,43,43,43	0
57	MG	2A	3748	1/1	0.98	0.14	45,45,45,45	0
57	MG	1A	3367	1/1	0.98	0.31	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3750	1/1	0.98	0.13	30,30,30,30	0
57	MG	1D	312	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3196	1/1	0.98	0.10	24,24,24,24	0
57	MG	2A	3753	1/1	0.98	0.17	48,48,48,48	0
57	MG	2A	3026	1/1	0.98	0.34	50,50,50,50	0
57	MG	2A	3755	1/1	0.98	0.11	66,66,66,66	0
57	MG	2x	106	1/1	0.98	0.19	58,58,58,58	0
57	MG	1A	3481	1/1	0.98	0.32	43,43,43,43	0
57	MG	1A	3233	1/1	0.98	0.18	50,50,50,50	0
57	MG	2A	3029	1/1	0.98	0.28	55,55,55,55	0
57	MG	1A	3899	1/1	0.98	0.17	54,54,54,54	0
57	MG	2A	3760	1/1	0.98	0.12	59,59,59,59	0
57	MG	2A	3376	1/1	0.98	0.12	53,53,53,53	0
57	MG	1E	305	1/1	0.98	0.24	29,29,29,29	0
57	MG	1A	3234	1/1	0.98	0.25	52,52,52,52	0
57	MG	1a	1727	1/1	0.98	0.18	48,48,48,48	0
57	MG	1A	3425	1/1	0.98	0.15	52,52,52,52	0
57	MG	1E	308	1/1	0.98	0.19	30,30,30,30	0
57	MG	2A	3037	1/1	0.98	0.17	38,38,38,38	0
57	MG	2A	3568	1/1	0.98	0.12	41,41,41,41	0
57	MG	2A	3569	1/1	0.98	0.16	44,44,44,44	0
60	ZN	29	501	1/1	0.98	0.06	64,64,64,64	0
57	MG	1A	3084	1/1	0.98	0.14	41,41,41,41	0
57	MG	1A	3617	1/1	0.99	0.14	27,27,27,27	0
57	MG	1A	3171	1/1	0.99	0.14	27,27,27,27	0
57	MG	2A	3199	1/1	0.99	0.08	39,39,39,39	0
57	MG	1A	4049	1/1	0.99	0.17	21,21,21,21	0
57	MG	1a	1606	1/1	0.99	0.20	66,66,66,66	0
57	MG	1A	3423	1/1	0.99	0.22	32,32,32,32	0
57	MG	2A	3787	1/1	0.99	0.23	62,62,62,62	0
57	MG	1A	3765	1/1	0.99	0.19	22,22,22,22	0
57	MG	1E	314	1/1	0.99	0.11	27,27,27,27	0
57	MG	2A	3031	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	3071	1/1	0.99	0.14	23,23,23,23	0
57	MG	1A	3034	1/1	0.99	0.16	16,16,16,16	0
57	MG	2A	3091	1/1	0.99	0.15	36,36,36,36	0
57	MG	2A	3724	1/1	0.99	0.14	56,56,56,56	0
57	MG	1A	3030	1/1	0.99	0.15	18,18,18,18	0
57	MG	1A	3673	1/1	0.99	0.18	31,31,31,31	0
57	MG	2A	3211	1/1	0.99	0.09	33,33,33,33	0
57	MG	1A	3226	1/1	0.99	0.20	26,26,26,26	0
57	MG	2A	3273	1/1	0.99	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1775	1/1	0.99	0.33	50,50,50,50	0
57	MG	2A	3400	1/1	0.99	0.15	54,54,54,54	0
57	MG	1A	3239	1/1	0.99	0.20	34,34,34,34	0
57	MG	1A	3845	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	3886	1/1	0.99	0.14	37,37,37,37	0
57	MG	2A	3666	1/1	0.99	0.16	40,40,40,40	0
57	MG	1A	3158	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3114	1/1	0.99	0.18	24,24,24,24	0
57	MG	1A	3345	1/1	0.99	0.15	25,25,25,25	0
57	MG	1A	3145	1/1	0.99	0.26	30,30,30,30	0
57	MG	1A	3299	1/1	0.99	0.23	22,22,22,22	0
57	MG	1A	3654	1/1	0.99	0.20	23,23,23,23	0
57	MG	2E	302	1/1	0.99	0.07	37,37,37,37	0
57	MG	1A	3315	1/1	0.99	0.26	25,25,25,25	0
57	MG	1A	3814	1/1	0.99	0.18	23,23,23,23	0
57	MG	1A	3779	1/1	0.99	0.19	21,21,21,21	0
57	MG	1A	3683	1/1	0.99	0.18	19,19,19,19	0
57	MG	1A	3856	1/1	0.99	0.22	26,26,26,26	0
57	MG	1V	205	1/1	0.99	0.13	31,31,31,31	0
57	MG	2A	3546	1/1	0.99	0.12	46,46,46,46	0
57	MG	1A	3243	1/1	0.99	0.20	39,39,39,39	0
57	MG	1A	3782	1/1	0.99	0.16	20,20,20,20	0
57	MG	1A	3982	1/1	0.99	0.20	26,26,26,26	0
57	MG	2A	3484	1/1	0.99	0.14	44,44,44,44	0
57	MG	1A	3715	1/1	0.99	0.16	38,38,38,38	0
57	MG	1A	3984	1/1	0.99	0.17	17,17,17,17	0
57	MG	2a	1633	1/1	0.99	0.25	54,54,54,54	0
57	MG	1A	4029	1/1	0.99	0.14	29,29,29,29	0
57	MG	1A	3820	1/1	0.99	0.13	17,17,17,17	0
57	MG	1A	3472	1/1	0.99	0.17	34,34,34,34	0
57	MG	1A	3717	1/1	0.99	0.17	23,23,23,23	0
57	MG	1A	3823	1/1	0.99	0.07	22,22,22,22	0
57	MG	1A	3686	1/1	0.99	0.18	16,16,16,16	0
57	MG	1A	3045	1/1	0.99	0.18	27,27,27,27	0
57	MG	2A	3364	1/1	0.99	0.06	42,42,42,42	0
57	MG	1A	3188	1/1	0.99	0.14	25,25,25,25	0
57	MG	1a	1749	1/1	0.99	0.09	60,60,60,60	0
57	MG	1A	3612	1/1	0.99	0.16	10,10,10,10	0
57	MG	1A	3551	1/1	0.99	0.16	23,23,23,23	0
57	MG	1P	204	1/1	0.99	0.39	23,23,23,23	0
57	MG	1a	1808	1/1	0.99	0.11	49,49,49,49	0
57	MG	2T	204	1/1	0.99	0.06	35,35,35,35	0

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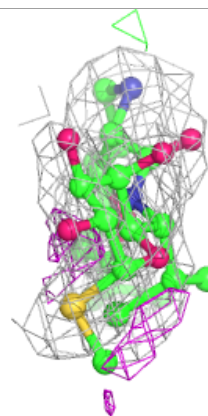
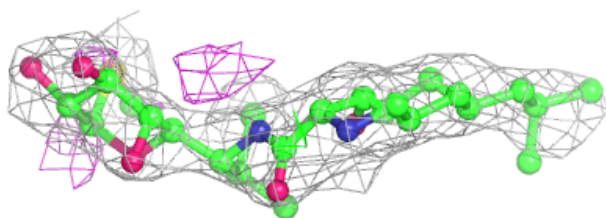
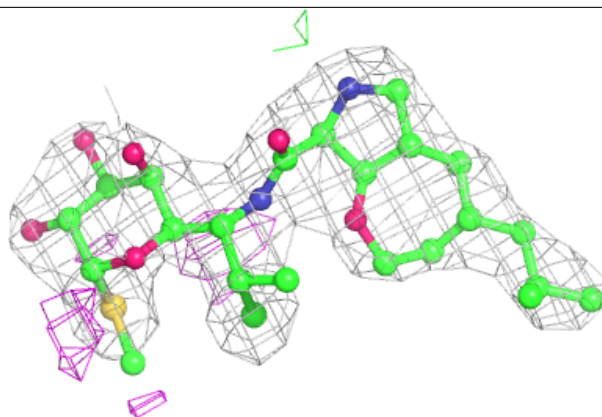
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3662	1/1	0.99	0.16	21,21,21,21	0
57	MG	2A	3701	1/1	0.99	0.15	27,27,27,27	0
57	MG	1A	3692	1/1	0.99	0.16	25,25,25,25	0
57	MG	1A	3614	1/1	0.99	0.18	17,17,17,17	0
57	MG	1B	201	1/1	0.99	0.20	40,40,40,40	0
57	MG	1A	3997	1/1	0.99	0.13	31,31,31,31	0
57	MG	2A	3313	1/1	0.99	0.17	55,55,55,55	0
57	MG	1Z	301	1/1	0.99	0.11	46,46,46,46	0
60	ZN	1n	103	1/1	0.99	0.07	59,59,59,59	0
57	MG	1A	3003	1/1	0.99	0.17	19,19,19,19	0
57	MG	1A	3639	1/1	0.99	0.21	24,24,24,24	0
60	ZN	25	105	1/1	0.99	0.15	58,58,58,58	0
60	ZN	26	102	1/1	0.99	0.17	50,50,50,50	0
57	MG	1A	3210	1/1	0.99	0.26	21,21,21,21	0
57	MG	1A	4046	1/1	0.99	0.15	35,35,35,35	0
61	SF4	1d	501	8/8	0.99	0.15	58,59,67,70	0
61	SF4	2d	302	8/8	0.99	0.13	65,77,84,86	0
60	ZN	15	110	1/1	1.00	0.20	44,44,44,44	0
60	ZN	16	102	1/1	1.00	0.16	43,43,43,43	0
60	ZN	19	102	1/1	1.00	0.18	39,39,39,39	0
57	MG	1A	3764	1/1	1.00	0.23	22,22,22,22	0

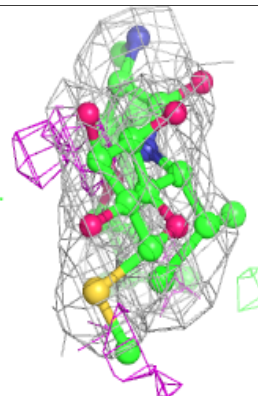
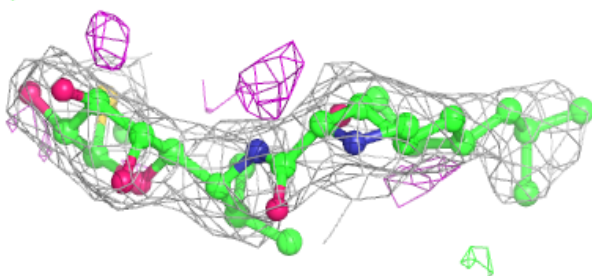
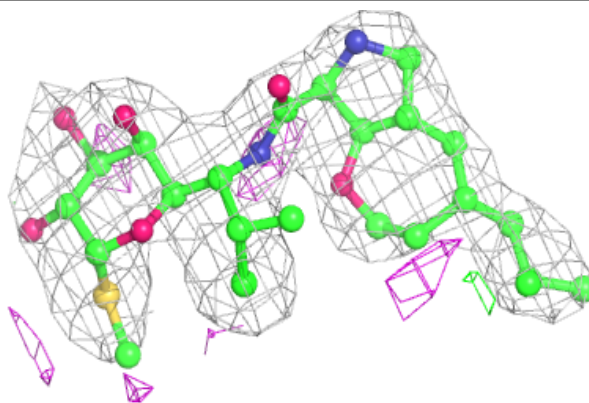
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6IF 2A 3857:

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

**Electron density around 6IF 1A 4089:**

$2mF_o-DF_c$ (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.