



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2026 – 11:23 PM UTC

PDB ID : 8VTX / pdb_00008vtx
Title : Crystal structure of the A2058-N6-dimethylated *Thermus thermophilus* 70S ribosome in complex with macrolone MCX-128, mRNA, aminoacylated A-site Phe-tRNA_{phe}, aminoacylated P-site fMet-tRNA_{met}, and deacylated E-site tRNA_{phe} at 2.40Å resolution
Authors : Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2024-01-27
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

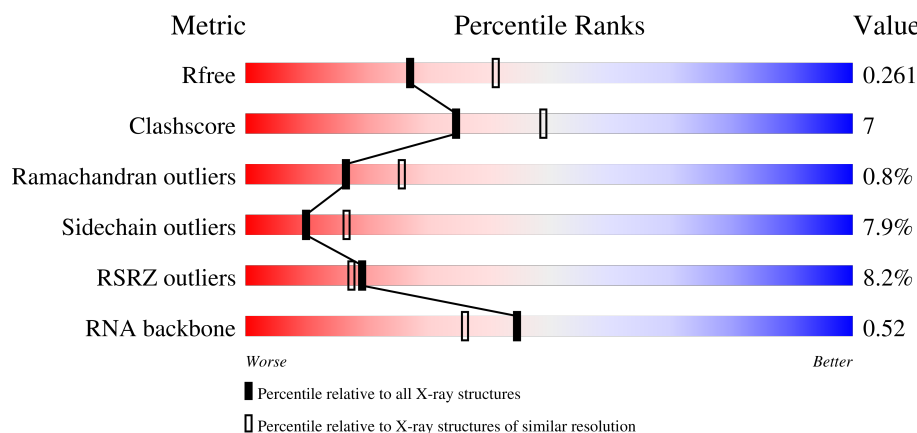
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)
RNA backbone	3690	1084 (2.70-2.10)

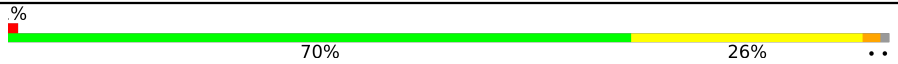
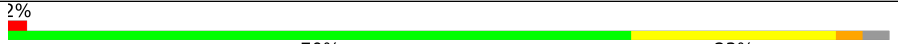
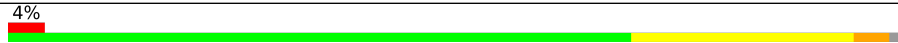
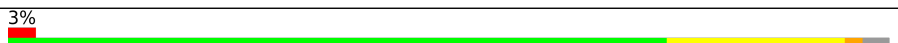
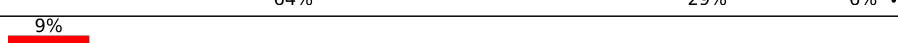
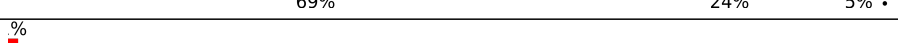
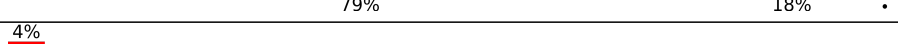
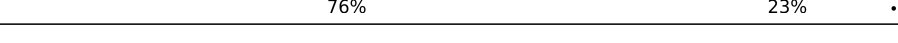
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	2A	2915	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

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

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Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
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	

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Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
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	10	108	-	-	-	X
57	MG	1A	3507	-	-	-	X
57	MG	1U	209	-	-	-	X
57	MG	2A	3149	-	-	-	X
57	MG	2A	3277	-	-	-	X
57	MG	2A	3364	-	-	-	X
57	MG	2A	3400	-	-	-	X
57	MG	2a	1761	-	-	-	X
61	SF4	2d	303	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 300319 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 MF-mRNA.

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

- Molecule 54 is a RNA chain called Aminoacylated Phe-tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	286	517	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	279	501	72	2			

- Molecule 55 is a RNA chain called Aminoacylated fMet-tRNA_{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a RNA chain called Deacylated tRNA_{phe}.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1093	Total	Mg	0	0
			1093	1093		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	14	Total	Mg	0	0
			14	14		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	14	Total	Mg	0	0
			14	14		

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	15	7	Total 7	Mg 7	0	0
57	16	1	Total 1	Mg 1	0	0
57	17	7	Total 7	Mg 7	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	214	Total 214	Mg 214	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	1	Total 1	Mg 1	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	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	1	Total 1	Mg 1	0	0
57	1w	8	Total 8	Mg 8	0	0
57	1x	14	Total 14	Mg 14	0	0
57	2A	854	Total 854	Mg 854	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2B	18	Total 18	Mg 18	0	0
57	2D	8	Total 8	Mg 8	0	0
57	2E	11	Total 11	Mg 11	0	0
57	2F	5	Total 5	Mg 5	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	2	Total 2	Mg 2	0	0
57	2Q	2	Total 2	Mg 2	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	4	Total 4	Mg 4	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	3	Total 3	Mg 3	0	0
57	25	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	26	1	Total Mg 1 1	0	0
57	27	3	Total Mg 3 3	0	0
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	210	Total Mg 210 210	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2l	5	Total Mg 5 5	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	3	Total Mg 3 3	0	0
57	2w	7	Total Mg 7 7	0	0
57	2x	7	Total Mg 7 7	0	0
57	2y	5	Total Mg 5 5	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

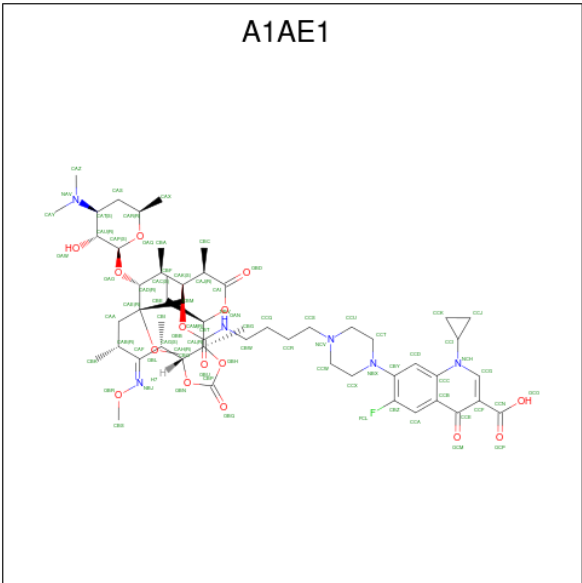
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0

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

- Molecule 59 is 1-cyclopropyl-7-(4-{4-[(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-14-(methoxyimino)-3a,7,9,11,13,15-hexamethyl-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl]oxy}carbonyl)amino]butyl}piperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AE1) (formula: C₅₄H₈₁FN₆O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total C F N O 76 54 1 6 15	0	0
59	2A	1	Total C F N O 76 54 1 6 15	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

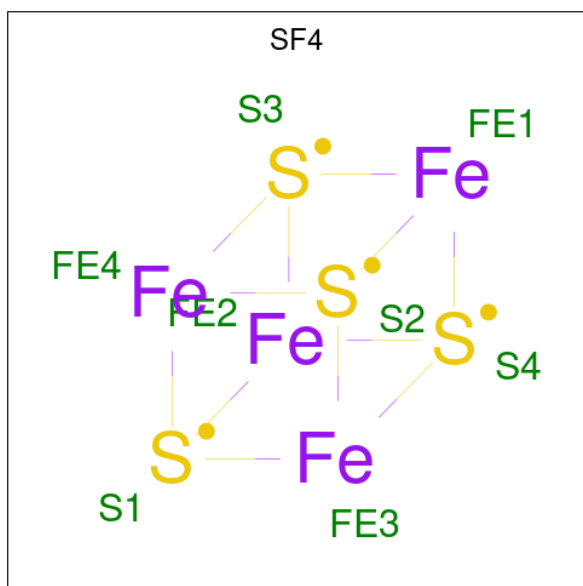
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0

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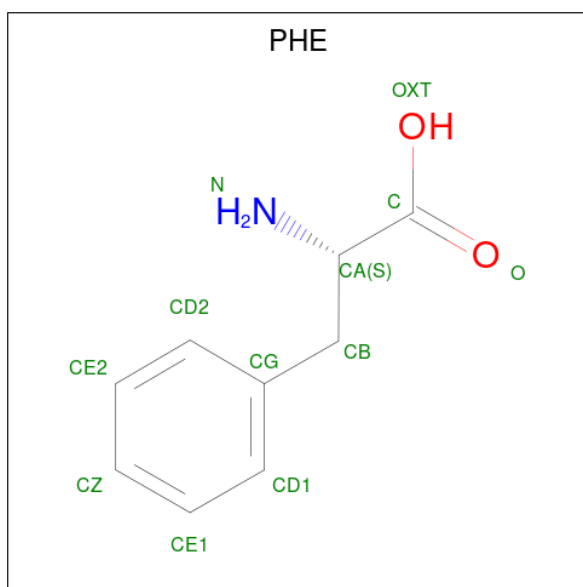
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



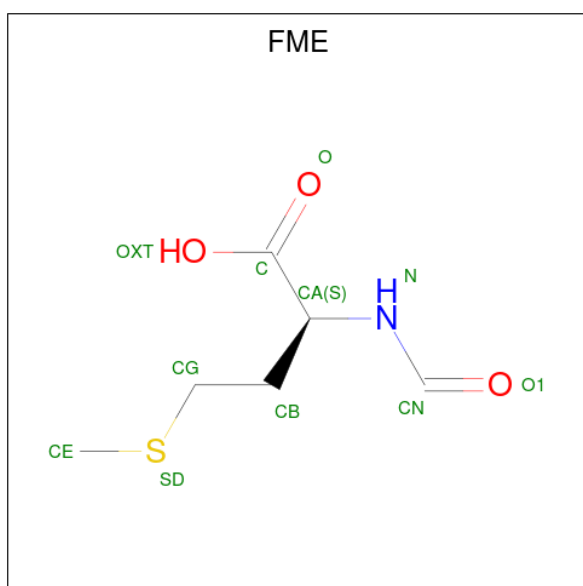
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $\text{C}_9\text{H}_{11}\text{NO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
62	1w	1	Total	C	N	O	0	0
			11	9	1	1		
62	2w	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
63	1x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
63	2x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1A	2061	Total O 2061 2061	0	0
64	1B	60	Total O 60 60	0	0
64	1D	29	Total O 29 29	0	0
64	1E	27	Total O 27 27	0	0
64	1F	16	Total O 16 16	0	0
64	1G	1	Total O 1 1	0	0
64	1H	1	Total O 1 1	0	0
64	1N	5	Total O 5 5	0	0
64	1O	6	Total O 6 6	0	0
64	1P	22	Total O 22 22	0	0
64	1Q	9	Total O 9 9	0	0
64	1R	10	Total O 10 10	0	0
64	1S	4	Total O 4 4	0	0
64	1T	8	Total O 8 8	0	0
64	1U	10	Total O 10 10	0	0
64	1V	8	Total O 8 8	0	0
64	1W	9	Total O 9 9	0	0
64	1X	6	Total O 6 6	0	0
64	1Y	3	Total O 3 3	0	0
64	1Z	1	Total O 1 1	0	0
64	10	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	11	11	Total 11	O 11	0	0
64	12	3	Total 3	O 3	0	0
64	13	5	Total 5	O 5	0	0
64	14	1	Total 1	O 1	0	0
64	15	9	Total 9	O 9	0	0
64	16	1	Total 1	O 1	0	0
64	17	11	Total 11	O 11	0	0
64	18	11	Total 11	O 11	0	0
64	1a	388	Total 388	O 388	0	0
64	1b	1	Total 1	O 1	0	0
64	1c	2	Total 2	O 2	0	0
64	1d	2	Total 2	O 2	0	0
64	1e	3	Total 3	O 3	0	0
64	1f	1	Total 1	O 1	0	0
64	1g	1	Total 1	O 1	0	0
64	1i	1	Total 1	O 1	0	0
64	1j	2	Total 2	O 2	0	0
64	1l	7	Total 7	O 7	0	0
64	1m	1	Total 1	O 1	0	0
64	1n	2	Total 2	O 2	0	0
64	1o	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	1p	1	Total 1	O 1	0	0
64	1q	2	Total 2	O 2	0	0
64	1u	1	Total 1	O 1	0	0
64	1v	5	Total 5	O 5	0	0
64	1w	14	Total 14	O 14	0	0
64	1x	15	Total 15	O 15	0	0
64	1y	1	Total 1	O 1	0	0
64	2A	1142	Total 1142	O 1142	0	0
64	2B	19	Total 19	O 19	0	0
64	2D	23	Total 23	O 23	0	0
64	2E	12	Total 12	O 12	0	0
64	2F	12	Total 12	O 12	0	0
64	2I	2	Total 2	O 2	0	0
64	2O	2	Total 2	O 2	0	0
64	2P	11	Total 11	O 11	0	0
64	2Q	2	Total 2	O 2	0	0
64	2R	3	Total 3	O 3	0	0
64	2T	5	Total 5	O 5	0	0
64	2U	3	Total 3	O 3	0	0
64	2V	1	Total 1	O 1	0	0
64	2X	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	2Y	1	Total	O	0	0
			1	1		
64	2Z	1	Total	O	0	0
			1	1		
64	20	3	Total	O	0	0
			3	3		
64	21	11	Total	O	0	0
			11	11		
64	23	2	Total	O	0	0
			2	2		
64	25	2	Total	O	0	0
			2	2		
64	27	5	Total	O	0	0
			5	5		
64	28	3	Total	O	0	0
			3	3		
64	29	1	Total	O	0	0
			1	1		
64	2a	221	Total	O	0	0
			221	221		
64	2c	1	Total	O	0	0
			1	1		
64	2d	2	Total	O	0	0
			2	2		
64	2g	1	Total	O	0	0
			1	1		
64	2j	3	Total	O	0	0
			3	3		
64	2l	4	Total	O	0	0
			4	4		
64	2p	2	Total	O	0	0
			2	2		
64	2q	1	Total	O	0	0
			1	1		
64	2r	1	Total	O	0	0
			1	1		
64	2t	1	Total	O	0	0
			1	1		
64	2v	2	Total	O	0	0
			2	2		
64	2w	3	Total	O	0	0
			3	3		

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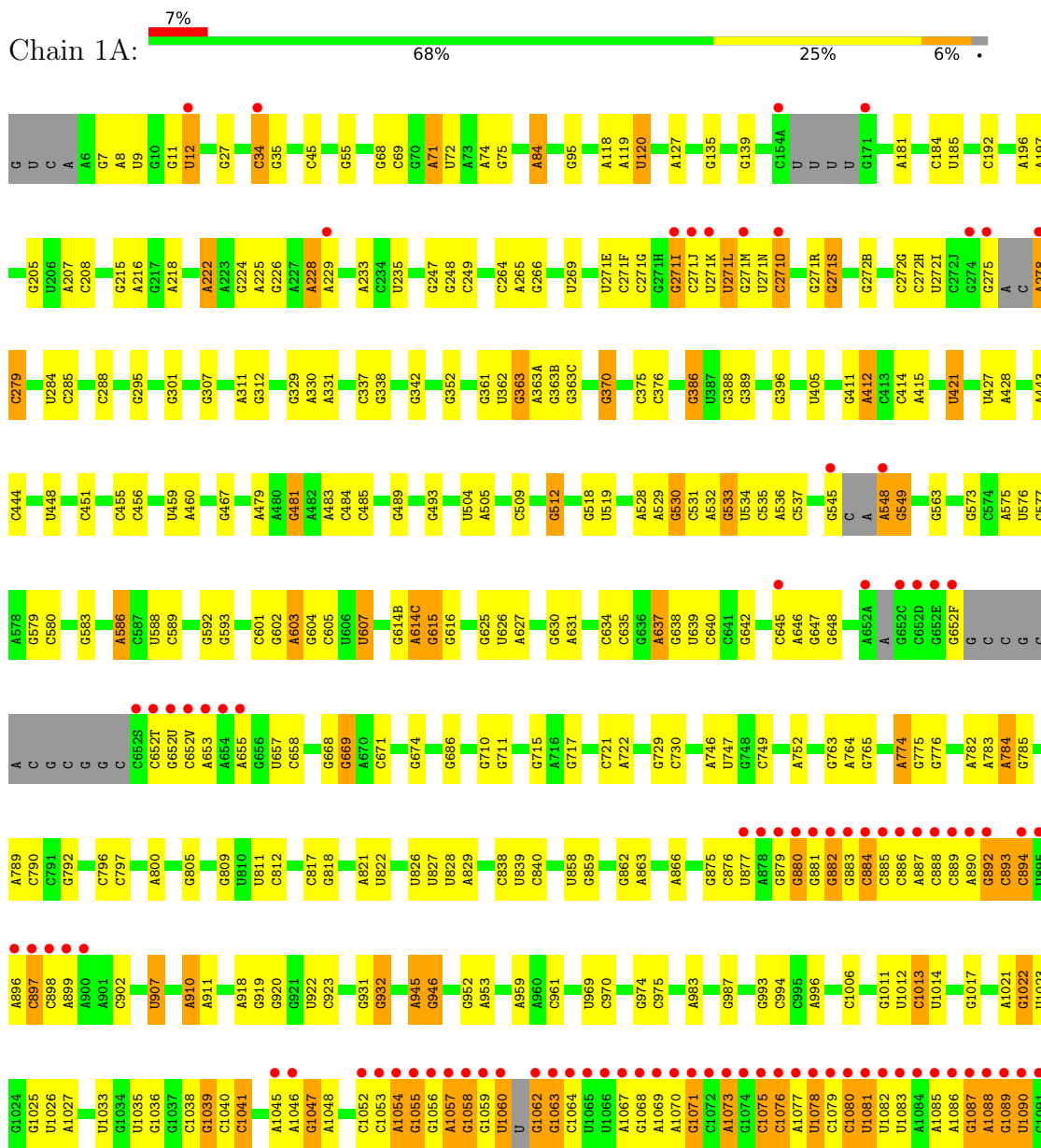
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	2x	7	Total	O	0	0
			7	7		
64	2y	2	Total	O	0	0
			2	2		

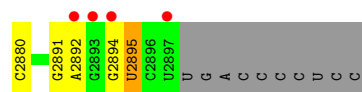
3 Residue-property plots

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

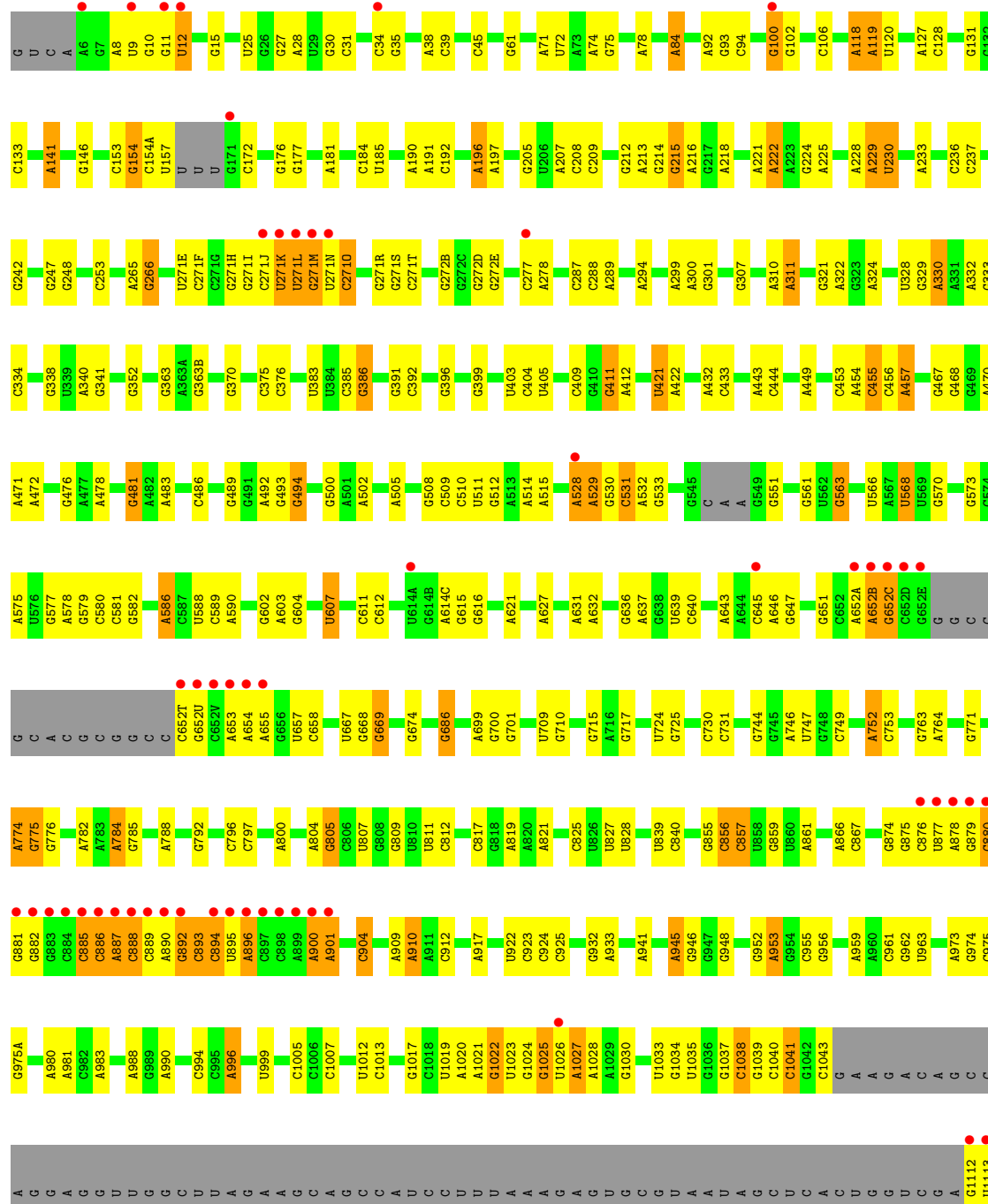
• Molecule 1: 23S Ribosomal RNA



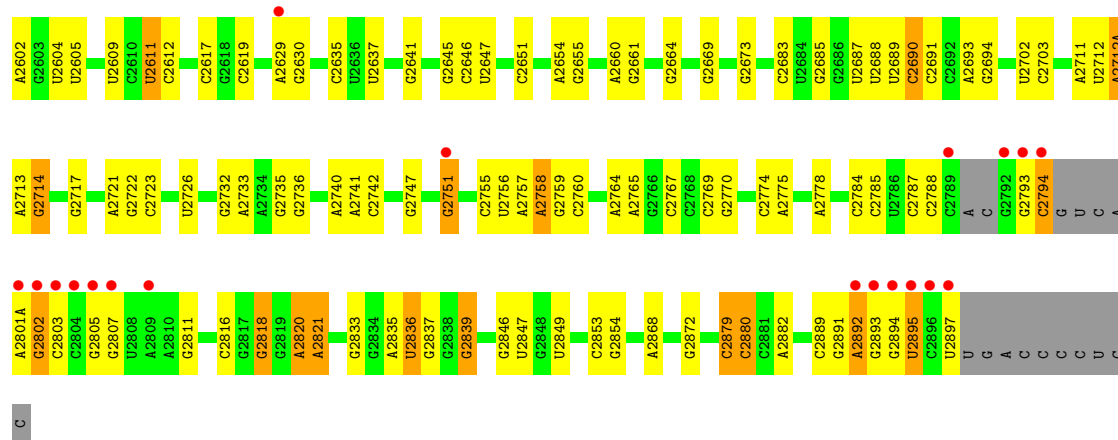
C2752	A2629	A2478	A2336	G2207	C2139	C2055	G1906		U1639		A1773		G1494	G1364	G1191	C1092
A2753	G2630	U2491	U2344	U2218	C2141	C2056	U1911		G1645		U1778		A1495	A1365	G1192	G1093
C2755					C2142	A2057	A1912		G1646		U1779		U1497	G1370	C1201	U1094
A2758	C2646	G2502	C2347	A2225	C2143	A2058	U1915		G1647		U1780			G1371		A1095
	U2647	A2503	U2348		U2144	A2059	U1916		C1648		A1780		U1503	U1372	G1225	A1096
A2765	G2648	U2504	G2349	G2235	C2145	A2060	A1917				C1781		C1504			
	U2649	G2505	G2350	C2236	C2146	G2061	U1917				A1782		U1505	U1379	G1229	A1098
	U2650			G2237	G2147	G2069	U1919				A1783		C1506	G1380	G1230	C1100
C2771		C2512	G2354	G2238	G2148		G1929				A1785		A1507	A1384	G1231	U1101
C2772	A2654	G2513		G2239	G2149		G1930				A1786		C1508	G1385		C1102
		U2514			U2150		U1931						C1509			
A2778	G2663	C2515	C2359	U2243	G2151	U2074	U1932				A1788		C1505	A1379	G1229	A1103
U2779		G2516	A2360	U2244	G2152	U2075	G1933				A1668		C1782	G1380	G1230	C1104
G2780	G2674	C2517	G2362		G2153	U2079	G1933				A1669		U1518	A1394	G1244	U1105
A2781		A2518		C2248	G2154	G2080	U1791				C1670		G1519	A1395		G1106
			A2377		G2155		A1936				U1671			U1396	A1253	G1107
C2787		G2529	A2378	G2251	G2156	G2094	A1937				U1794		G1532			U1108
C2788	C2683		G2379		C2157		A1938				C1795		G	C1399	G1256	C1109
G2789	U2684	G2535		A2288	A2158	U2098	U1939				U1796		U			
C2791	G2685		G2383	A2289	G2159	U2099	C1942				C1675		A	U1405	G1266	A1111
G2792	G2686	G2550	G2384		G2160	G2100	U1798				A1676		C	U1406	U1267	G1112
C2793	U2687	C2551	C2385	A2273	G2161	G2101	A1952				G1799			C1407	A1268	U1113
C2794	U2688	U2552		A2274	C2162	U2102	A1953				C1800		G1537		A1269	G1114
G	C2690	G2553	A2393	G2277	G2163	C2103	G1954				A1801			G1416	G1270	G1115
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C	G2692	U2562	G2407	C2283	G2165	C2105	C1962				A1803			G1418	U1272	
A	A2693	U2563	G2407	U2167	G2166	G2106	U1963				A1810		A1554	A1419	U1273	G1131
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G2805			U2424	C2292	C2111	C2110	A1700				G1699			G1424		G1137
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		C2575	C2427	G2299	C2175	G2115	G1984				A1829					
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G2819	U2712	G2578	G2429	C2306	C2178	U2118	G1992				G1710			A1301	G1154	
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	C2723	G2592			G2184	G2124	G2012				U1739			G1450	U1167	
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	U2726	A2602	G2446	A2320	G2186	A2126	C2020				G1750				G1171	
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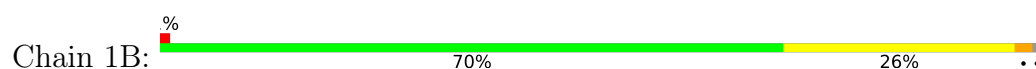
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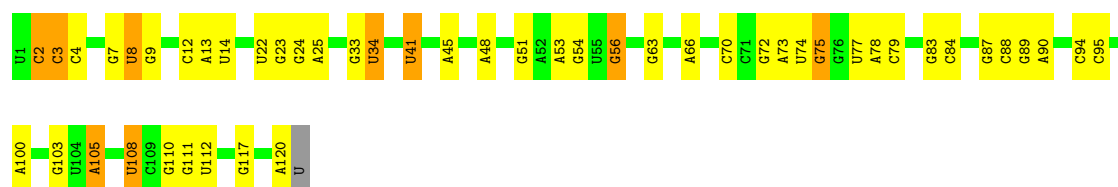




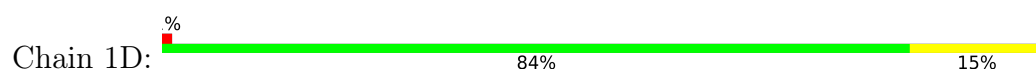
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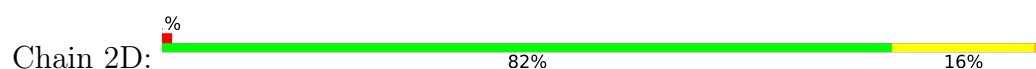
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

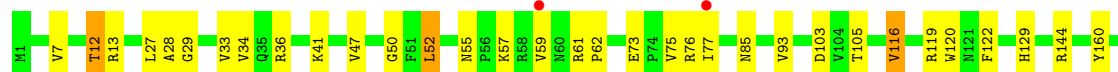
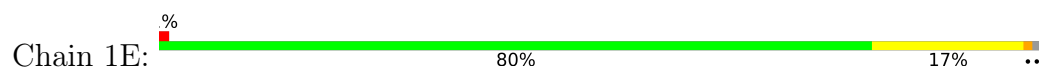


• Molecule 3: 50S ribosomal protein L2

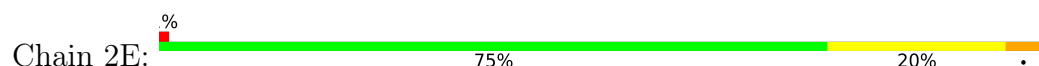




• Molecule 4: 50S ribosomal protein L3



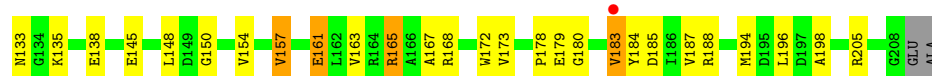
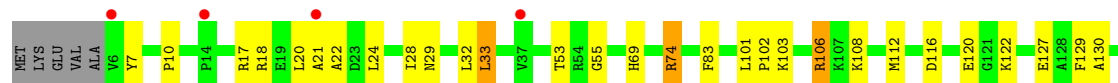
• Molecule 4: 50S ribosomal protein L3



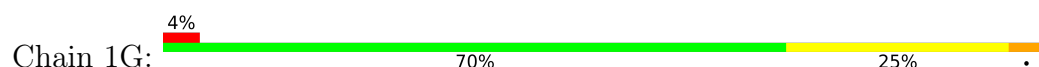
• Molecule 5: 50S ribosomal protein L4

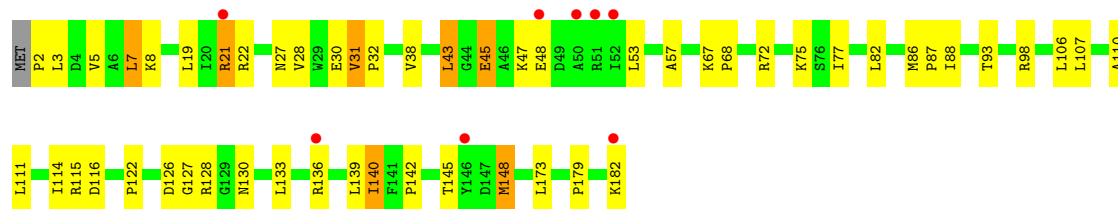


• Molecule 5: 50S ribosomal protein L4

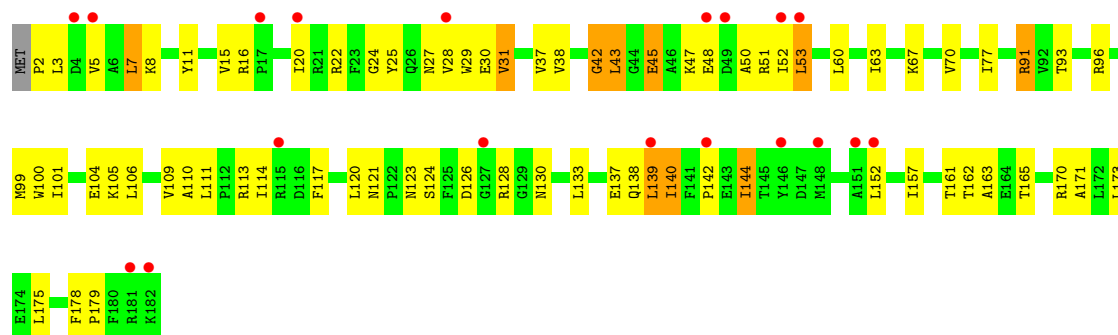


• Molecule 6: 50S ribosomal protein L5

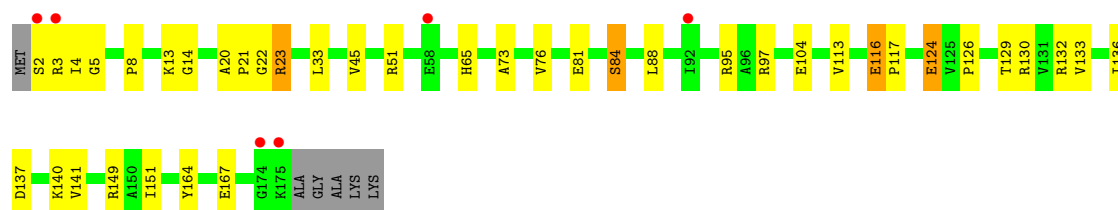
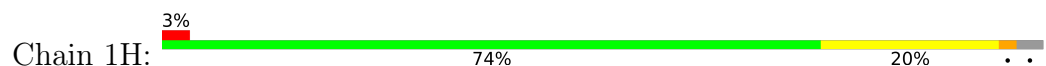




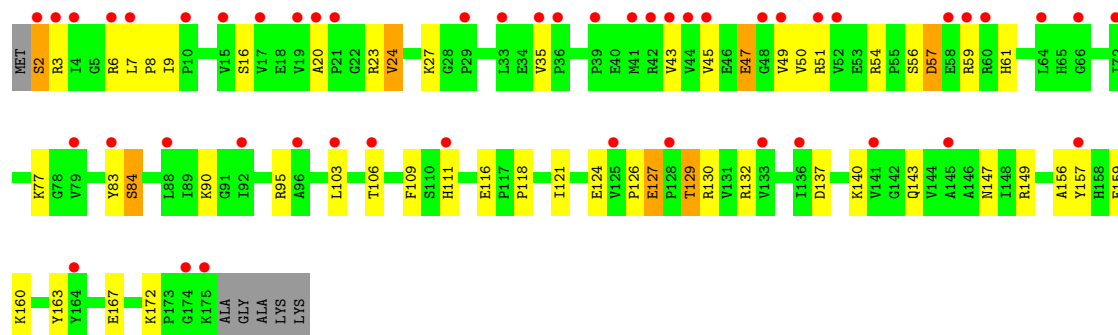
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

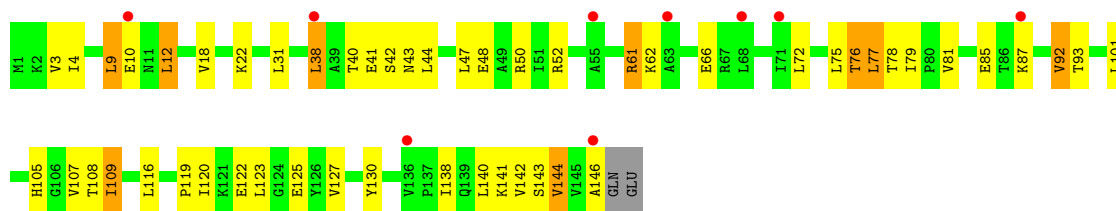


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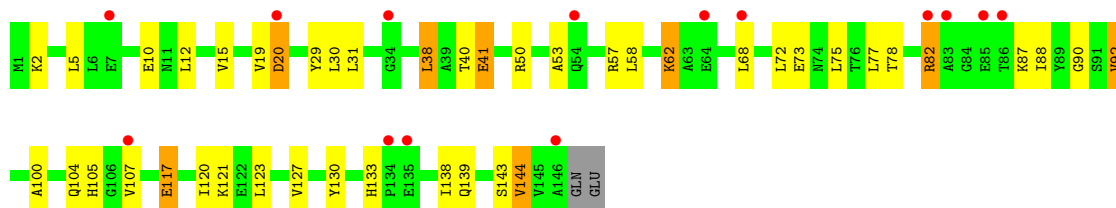


• Molecule 8: 50S ribosomal protein L9

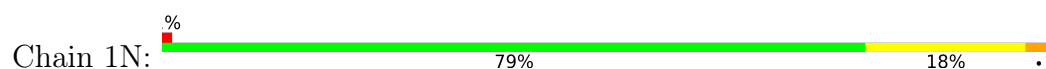




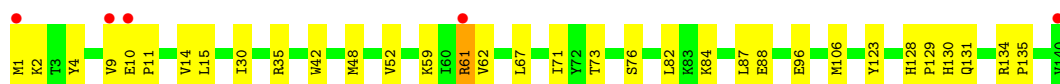
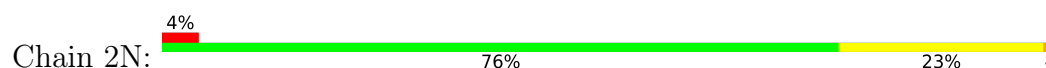
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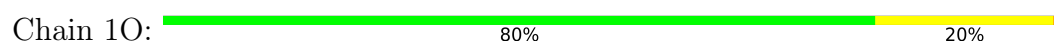
• Molecule 9: 50S ribosomal protein L13



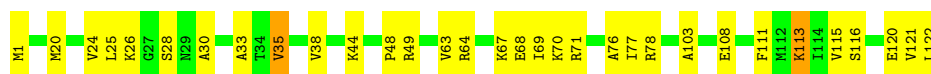
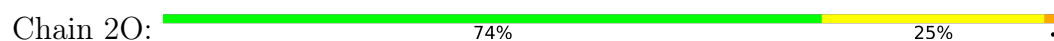
• Molecule 9: 50S ribosomal protein L13



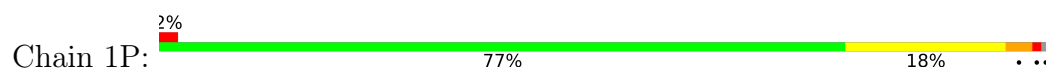
• Molecule 10: 50S ribosomal protein L14

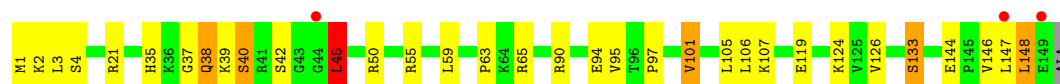


• Molecule 10: 50S ribosomal protein L14

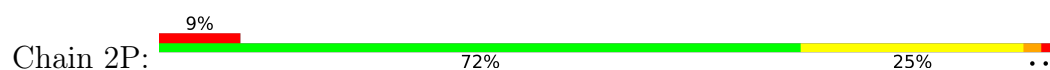


• Molecule 11: 50S ribosomal protein L15

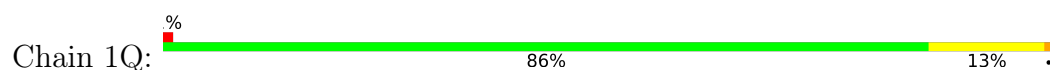




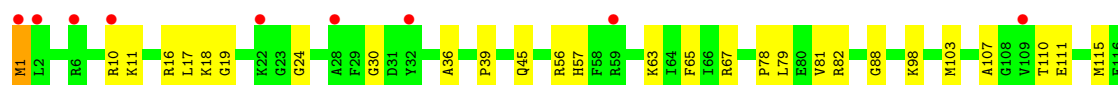
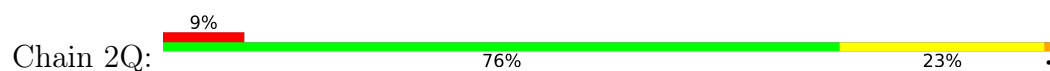
- Molecule 11: 50S ribosomal protein L15



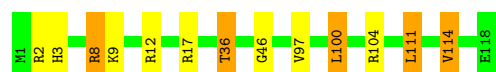
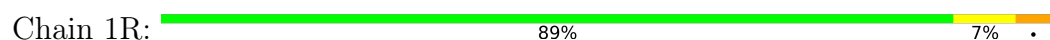
- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



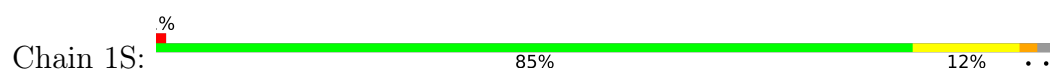
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

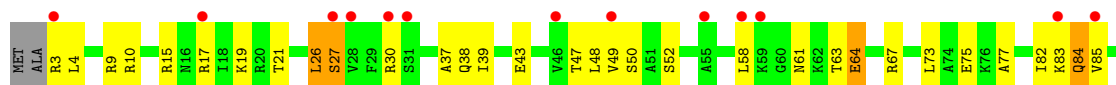


- Molecule 14: 50S ribosomal protein L18

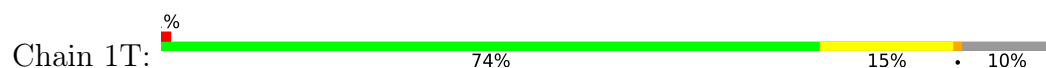




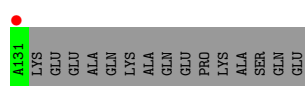
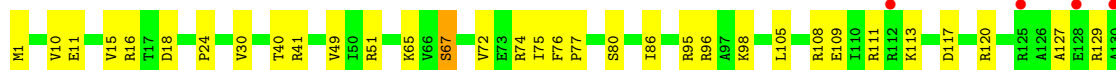
- Molecule 14: 50S ribosomal protein L18



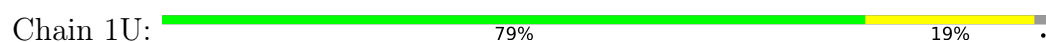
- Molecule 15: 50S ribosomal protein L19



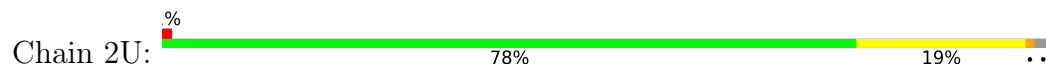
- Molecule 15: 50S ribosomal protein L19



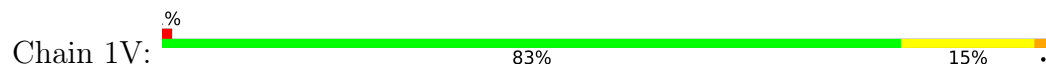
- Molecule 16: 50S ribosomal protein L20

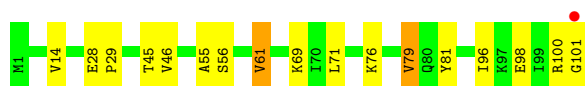


- Molecule 16: 50S ribosomal protein L20

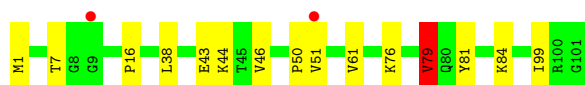
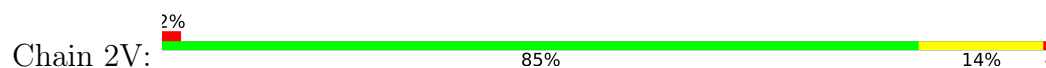


- Molecule 17: 50S ribosomal protein L21





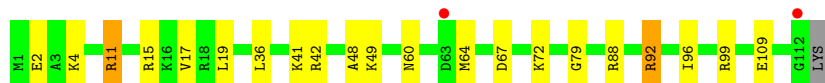
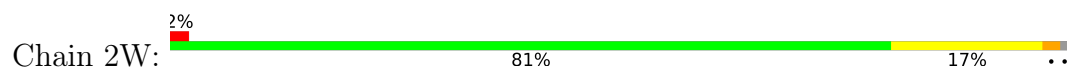
- Molecule 17: 50S ribosomal protein L21



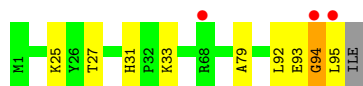
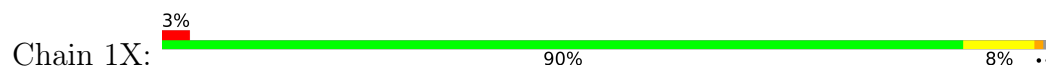
- Molecule 18: 50S ribosomal protein L22



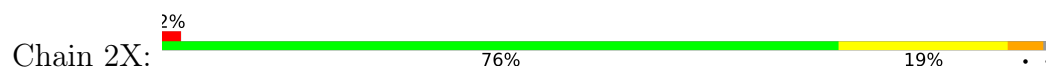
- Molecule 18: 50S ribosomal protein L22



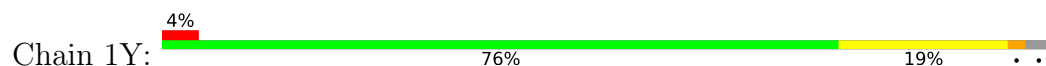
- Molecule 19: 50S ribosomal protein L23



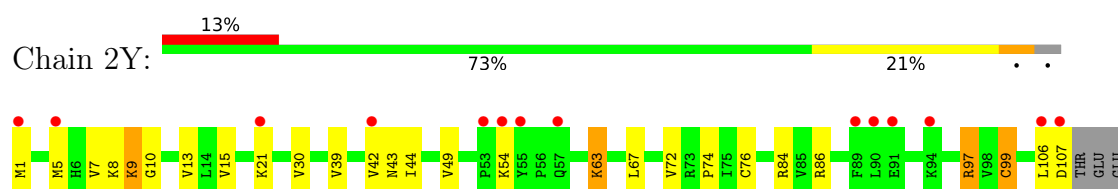
- Molecule 19: 50S ribosomal protein L23



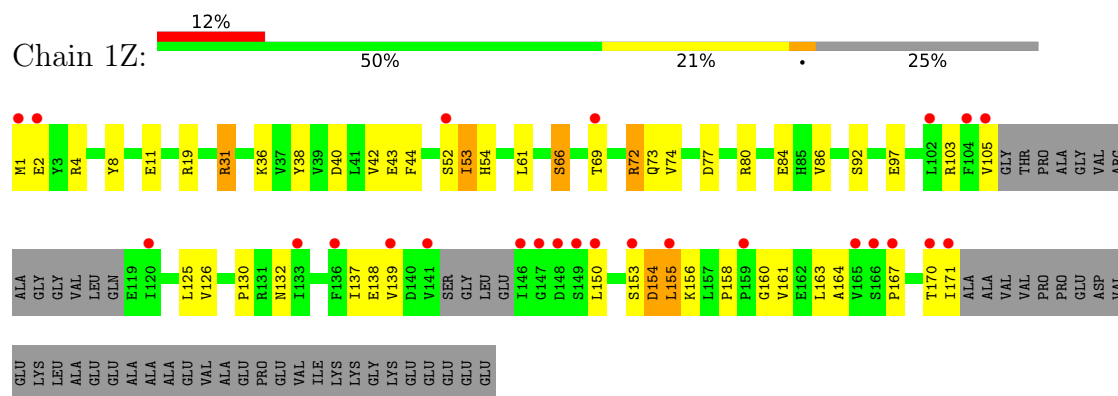
- Molecule 20: 50S ribosomal protein L24



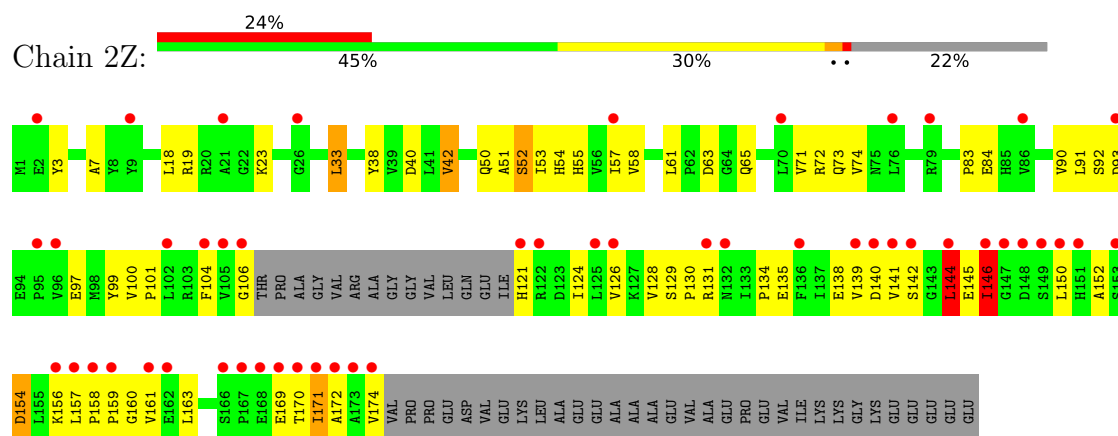
- Molecule 20: 50S ribosomal protein L24



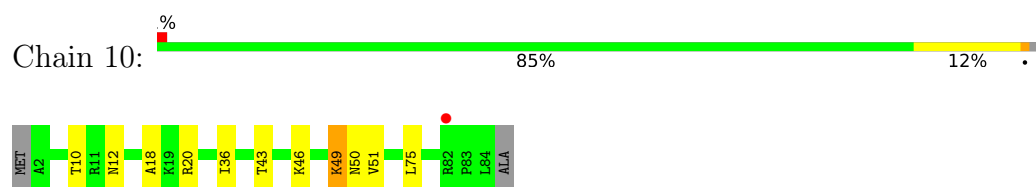
- Molecule 21: 50S ribosomal protein L25



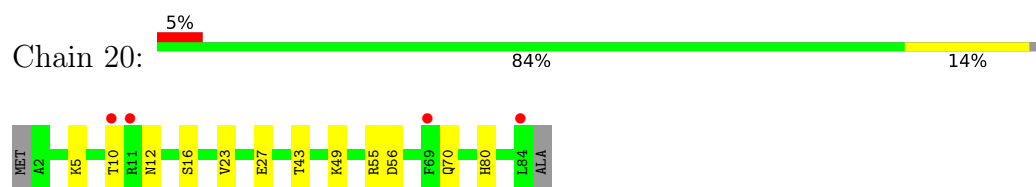
- Molecule 21: 50S ribosomal protein L25



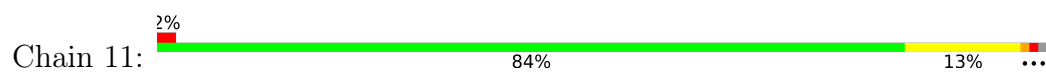
- Molecule 22: 50S ribosomal protein L27



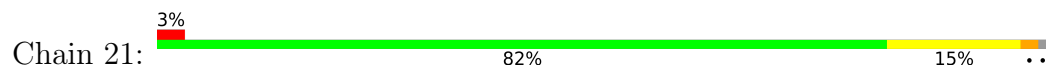
- Molecule 22: 50S ribosomal protein L27



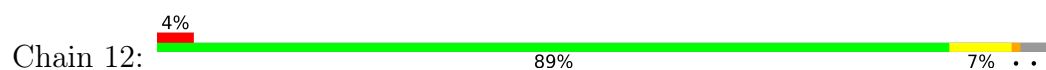
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



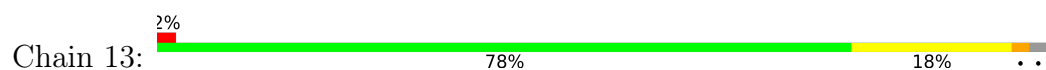
- Molecule 24: 50S ribosomal protein L29



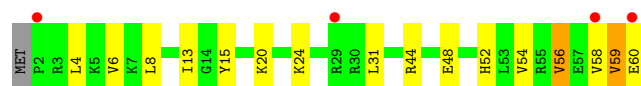
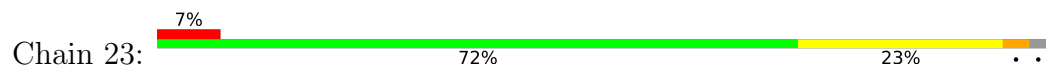
- Molecule 24: 50S ribosomal protein L29



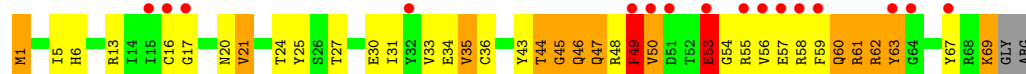
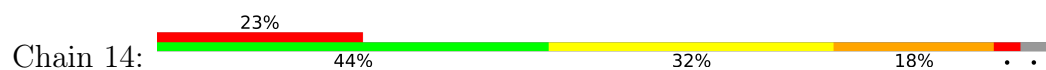
- Molecule 25: 50S ribosomal protein L30



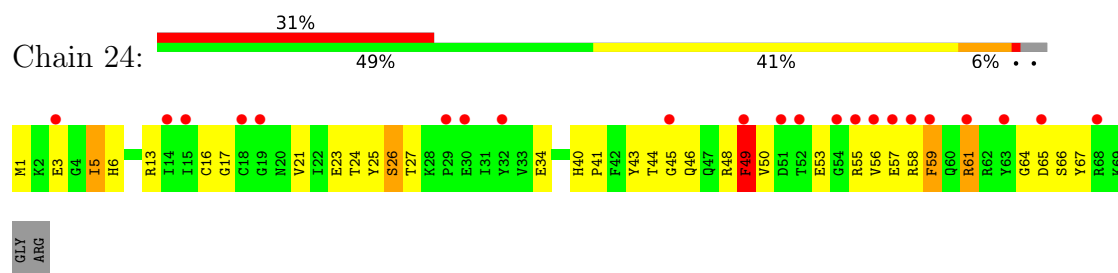
- Molecule 25: 50S ribosomal protein L30



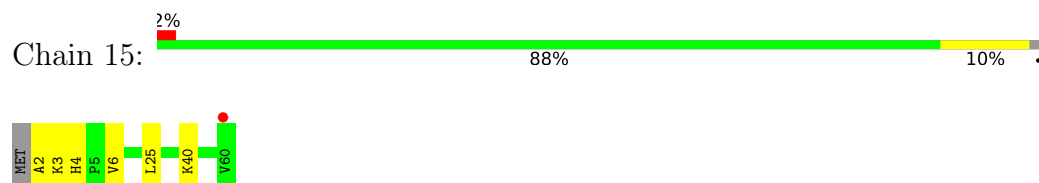
- Molecule 26: 50S ribosomal protein L31



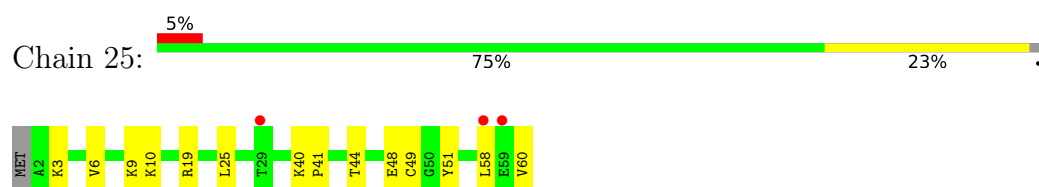
- Molecule 26: 50S ribosomal protein L31



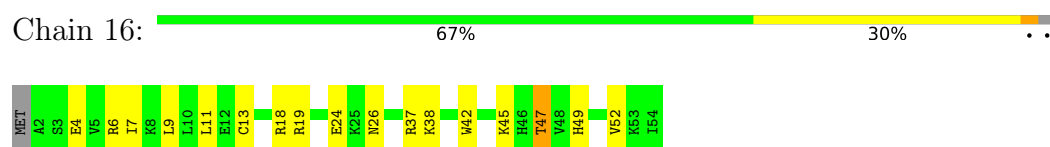
- Molecule 27: 50S ribosomal protein L32



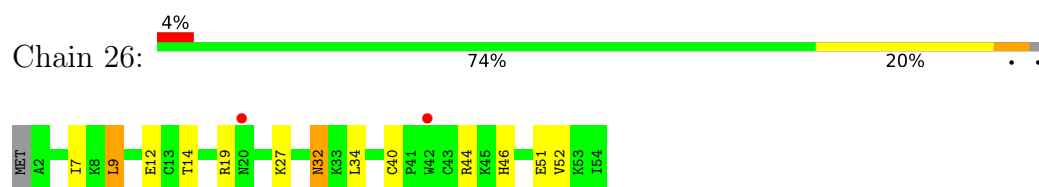
- Molecule 27: 50S ribosomal protein L32



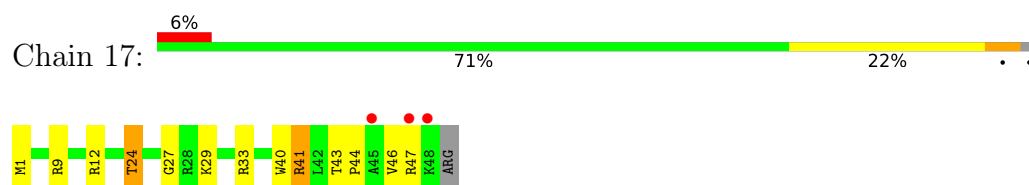
- Molecule 28: 50S ribosomal protein L33



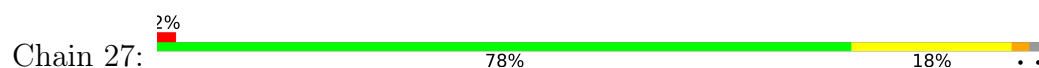
- Molecule 28: 50S ribosomal protein L33

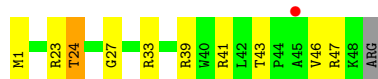


- Molecule 29: 50S ribosomal protein L34

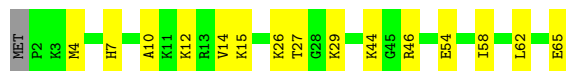


- Molecule 29: 50S ribosomal protein L34

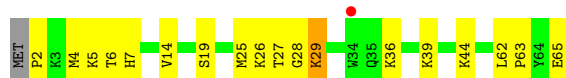




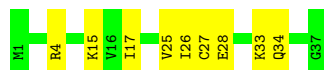
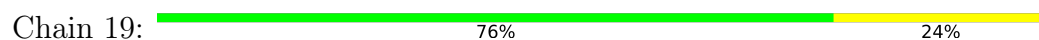
- Molecule 30: 50S ribosomal protein L35



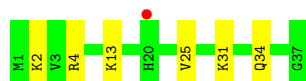
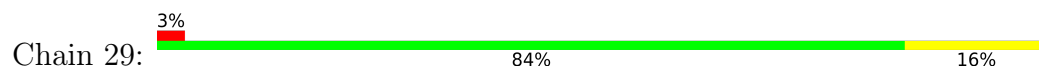
- Molecule 30: 50S ribosomal protein L35



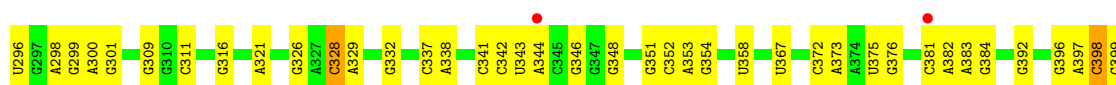
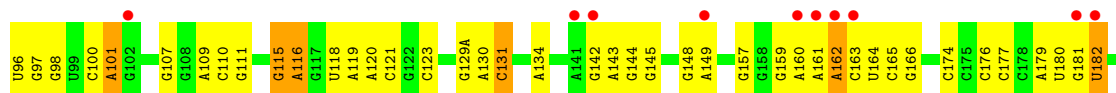
- Molecule 31: 50S ribosomal protein L36

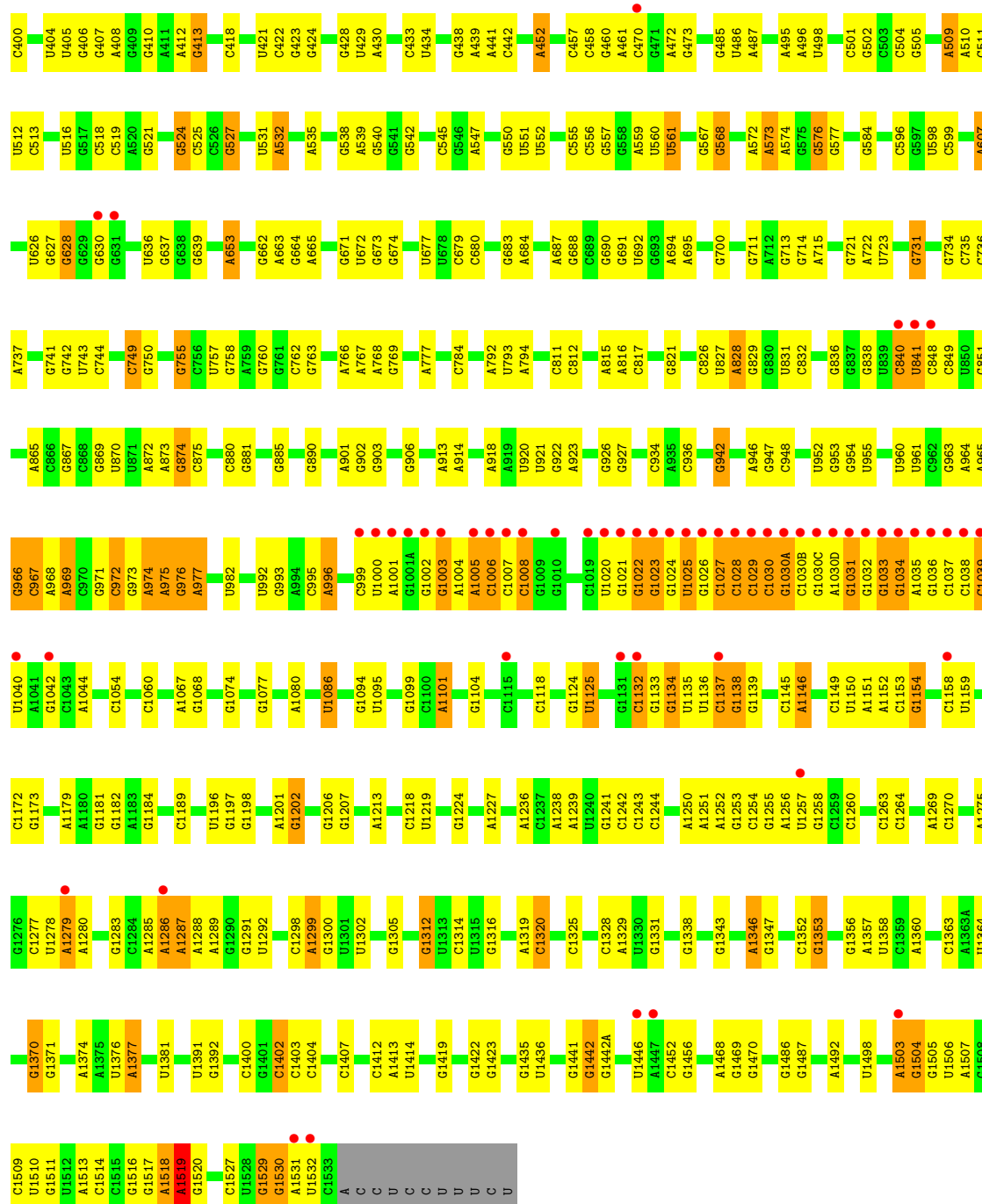


- Molecule 31: 50S ribosomal protein L36



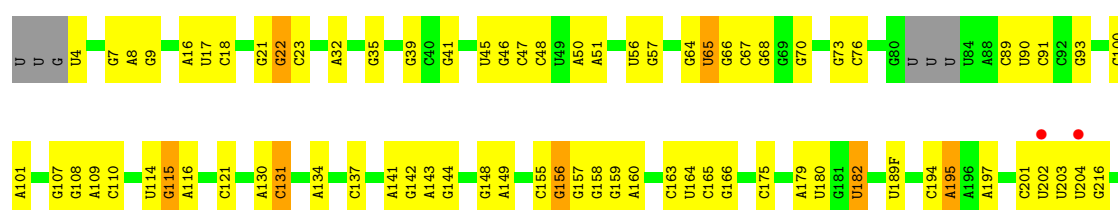
- Molecule 32: 16S Ribosomal RNA





• Molecule 32: 16S Ribosomal RNA

Chain 2a: 7% 56% 35% 7%



G1442A	G1356	U1278	U1205	G1134	C1063	G1003	C932	G776	A663	C556	A451	G350	U222
U1446	G1357	A1279	G1206	U1135	G1064	A1004	G933	C779	G664	C556	A451	G351	U223
A1447	U1358	A1280	G1207	U1136	U1065	C1006	C934	A780	A665	A559	A453	C352	G231
C1452	U1359	G1282	U1211	C1137	U1066	C1007	A935	C784	G666	U560	A453	A353	G232
G1456	A1360	G1283	U1212	G1138	A1067	C1008	C936	A787	G671	U561	C457	G354	C233
G1457	G1361	C1284	A1213	C1140	C1068	G1009	A937	A787	G672	C562	C458	C234	C234
G1464	C1362	A1285	G1216	C1141	C1069	G1010	A938	A792	G673	A563	C460	G357	
G1469	A1287	A1287	C1217	C1145	U1070	G1011	G939	A793	G674	C563	A461	U367	C245
G1470	A1288	G1218	C1218	U1146	U1072	U1012	G942	U793	G675	U565	C372	A246	A246
G1492	A1289	G1219	C1219	C1147	U1073	G1013	G946	A794	G676	U566	C471	G372	G247
G1497	G1290	G1220	G1220	U1148	U1074	U1014	A946	A816	G677	C567	A472	A373	
G1498	G1291	U1292	G1224	C1149	G1076	A1015	G947	C817	G678	C568	G473	G376	G251
A1502	U1297	U1297	A1225	U1150	U1077	A1016	G947	U820	G679	U570	G474	U252	U252
G1503	G1298	C1227	A1226	U1151	A1080	C1017	G952	U821	G685	U571	G475	U253	U253
G1504	A1299	A1227	C1227	A1152	G1081	C1018	G953	G826	G686	A572	G476	A381	G254
G1505	G1300	U1228	C1228	A1157	U1085	U1020	U955	U827	G688	A573	G477	A383	U256
U1506	U1301	C1234	A1229	C1158	U1086	G1021	A958	U828	A702	A573	G478	G384	G257
U1540	U1302	U1235	C1235	U1159	U1091	U1022	A959	A829	G707	G576	C489	G388	A262
G1511	C1303	A1236	G1237	G1160	A1092	U1025	U960	C838	C708	U580	A496	A389	A263
G1512	G1304	C1237	C1238	C1161	U1093	G1026	U961	U839	C709	C581	A498	G391	G266
G1513	G1305	A1239	A1238	G1163	G1094	C1027	A964	C840	U723	U582	A499	G392	G267
C1514	G1306	G1241	A1239	G1164	U1095	C1028	A965	U841	G730	C596	G500	A393	C267
G1517	G1307	U1242	A1240	C1165	C1096	C1029	G966	C848	G731	U588	C501	G396	C268
A1518	G1310	C1246	C1247	G1174	C1097	G1030	G967	U849	G732	G588	G505	A397	C269
A1519	G1311	A1248	A1249	U1175	U1098	U1030A	A968	C851	G733	G589	G505	A270	A270
G1520	C1312	C1249	C1249	G1176	C1099	G1030C	A969	G852	A733	C596	A509	G398	G289
G1521	U1313	A1250	A1250	U1177	A1101	A1030D	G971	G853	A737	U598	A510	U404	G289
G1525	A1318	A1251	A1251	G1178	C1102	G1031	C972	A859	C738	C599	C511	U405	G297
G1529	A1319	A1252	A1252	U1179	C1103	G1032	G973	G868	G741	C600	U512	A406	A298
G1530	C1320	G1253	G1253	A1180	A1104	G1033	A974	C869	G742	C601	C513	G407	G299
A1531	C1321	C1254	C1254	G1181	U1105	A1034	A975	G874	G743	U603	U516	A412	G301
U1532	G1322	A1256	A1256	U1182	G1106	A1035	G976	C874	G744	G604	C517	G413	G302
C	A1324	U1257	U1257	G1184	C1107	G1036	A977	U874	C744	C620	C518	A414	
A	C1325	C1260	C1260	G1187	C1114	C1037	A978	C748	C749	A621	G524	A415	G316
C	U1330	C1263	C1263	A1188	C1115	U1038	C979	C895	G749	G625	G525	G416	
C	G1331	C1264	C1264	C1189	C1116	U1040	U981	C895	G750	U626	C526	A321	A321
C	A1332	G1265	G1265	G1190	C1117	A1041	U982	A901	G753	U626	C527	C419	G326
C	G1333	A1268	A1268	U1193	C1118	C1043	A986	G902	A753	U630	U531	G424	A327
U	G1334	A1269	A1269	G1194	C1119	C1044	G987	C903	C754	A642	A532	G425	A327
U	G1338	C1270	C1270	C1195	U1122	C1045	U991	A909	C755	G646	G537	G426	A328
U	A1433	G1271	G1271	U1196	U1123	G1050	U992	A914	G756	C647	G538	U427	A329
C	G1434	G1272	G1272	U1197	G1124	C1051	G993	A918	A766	C651	A539	U428	G332
U	U1436	G1273	G1273	G1197	U1125	U1052	A994	A919	A767	G651	G541	A430	G333
U	G1437	G1274	G1274	C1200	U1126	C1054	A996	U920	G769	U652	G544	A439	C334
G1438	A1346	G1275	G1275	A1201	C1127	A1055	U997	U921	G773	A653	G545	U340	C335
C1439	G1347	A1276	A1276	G1202	U1128	G1057	G998	G922	U772	G656	G546	A441	G341
G1442	C1352	C1277	C1277	A1204	U1130	C1060	U1000	G926	G774	G661	G547	A442	C341
	G1353				C1132	G1061	U1001	G927	G775	G662	A553	G445	A344
					U1133	U1062	G1002	G927	A777			G446	G345
												G447	G346

Chain 1b:

20% 52% 32% 5% 10%

MET PRO VAL ILE THR V7 K8 E9 L10 L11 E12 A13 G14 V15 H16 F17 G18 H19 E20 R21 K22 R23 W24 Y33 A34 E35 R36 N37 G38 L39 H40 L41 I42 D43 L44 T47 F48 E49 E50 T54 F55 E59 A62 M63 R64 V71 G72 T73 K74 K75 Q76 A77 I80 V81 R82 M83 E84 R87 A88 G89 M90 G91 Y92 Y93 N94 Q95 R96 W97 M101 L102 T103 T107 I108 S109 Q110 R111 V112 A120 L121 F122 A123 S124 P125 E126 I127 E128 E129 R130 P131 K132 A133 E134 Q135 V136 R137 L138 K139 L142 E143 L149 S150 G151 F152 R153 L154 L155 R156 K157 L158 M159 D160 A161 I162 F163 G164 A165 V165 D166 K169 E170 L180 P183 V184 I185 A186 L187 A188 S192 D196 Y199 I200 L201 P202 G203 N204 D205 D206 A207 R208 S210 T211 Q212 L213 I214 A218 V219 D220 L221 I222 I223 R226 G227 G228 V229 V230 E231 P232 S233 P234 S235 Y236 A237 LEU VAL GLN GLU ALA GLU ALA THR THR PRO GLU GLY GLU SER GLU VAL GLU ALA

Chain 2b:

25% 49% 35% 6% 10%

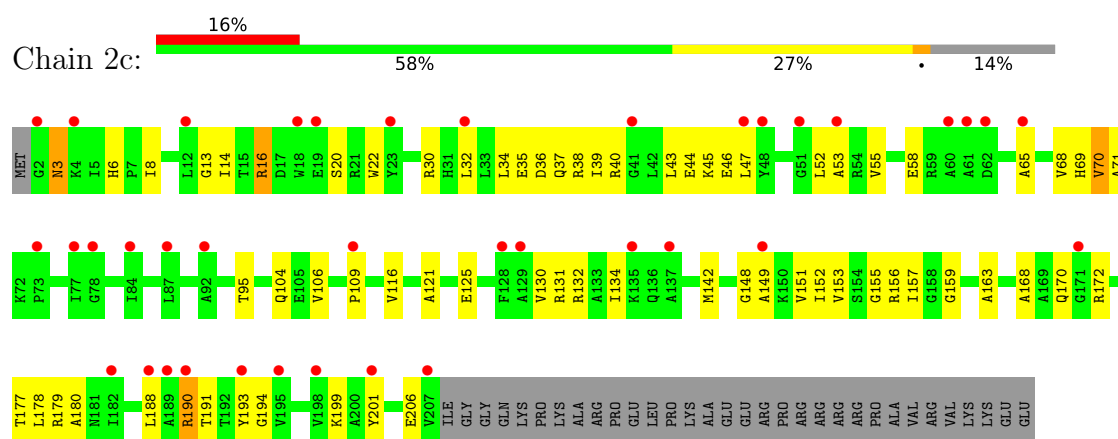
MET PRO VAL ILE THR V7 K8 E9 L10 L11 E12 A13 G14 V15 H16 F17 G18 H19 E20 R21 R22 R23 W24 R25 P26 A29 R30 Y31 I32 Y33 A34 E35 G38 I39 H40 I41 I42 I43 I44 T47 M48 E49 F50 L51 E52 F55 R56 F57 I58 L61 A62 M63 T67 I68 L69 F70 V71 K74 K75 K76 A77 K78 D79 I80 I81 R82 M83 H86 R87 A88 F91 Y92 Y93 I94 Q95 R96 W97 L102 I111 I112 I113 R114 E117 L118 I119 A120 I121 I122 I123 A124 I125 I126 I127 I128 I129 R130 I131 I132 K133 I134 I135 V136 R137 L138 K139 H140 R144 L149 S150 G151 F152 R153 L154 A161 I162 F163 V164 I165 D166 P167 T168 K169 E170 A173 V174 R175 R178 K179 P180 L185 A186 I187 A188 D189 T190 D191 S192 D195 L196 V197 I198 Y199 I200 I201 P202 G203 N204 D205 D206 A207 I208 R209 S210 I211 Q212 L215 S216 R217 V219 D220 L221 I222 I223 Q224 A225 R226 V230 F234 S235 Y236 A237 LEU VAL GLN GLU ALA GLU THR GLU THR PRO GLU GLY GLU SER GLU VAL GLU ALA

Chain 1c:

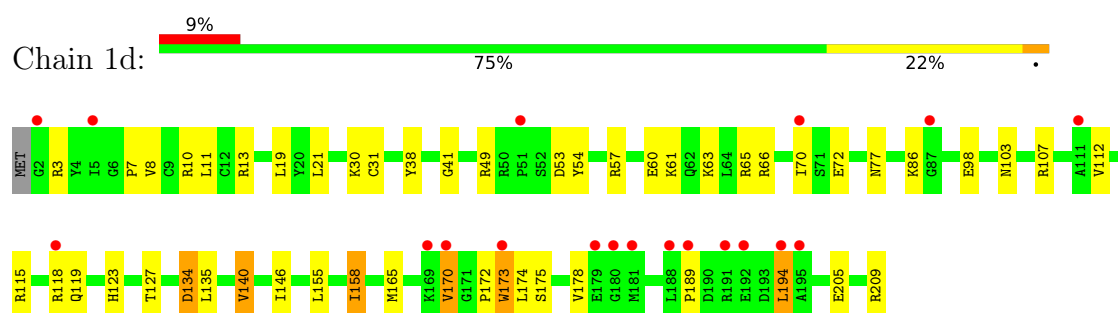
7% 66% 19% 14%

Sequence logo for Chain 1c. The y-axis represents information content in bits (0.0 to 1.0). The x-axis shows positions 1 to 200. The logo displays the conservation of amino acids at each position. A bar chart at the top indicates the percentage of positions with conservation greater than 0.5 bits: 7% (red), 66% (green), 19% (yellow), and 14% (grey).

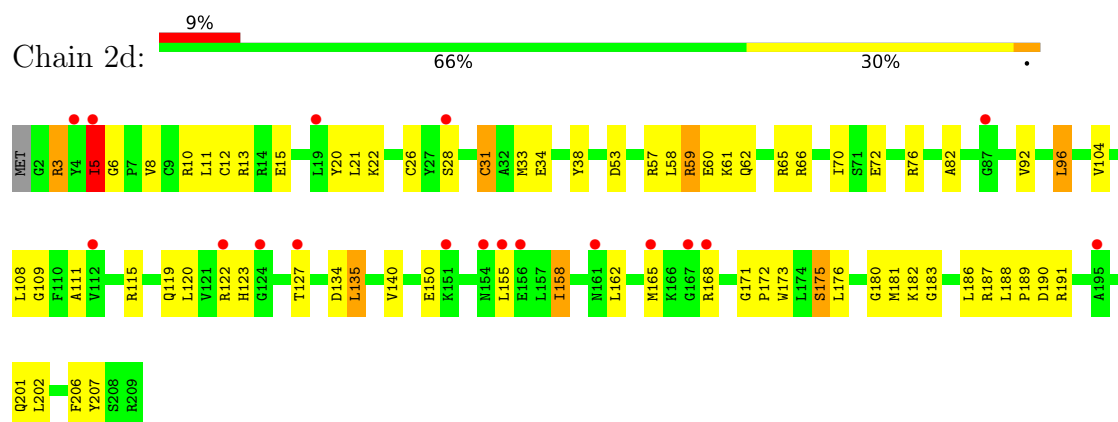
WORLDWIDE
PDB
PROTEIN DATA BANK



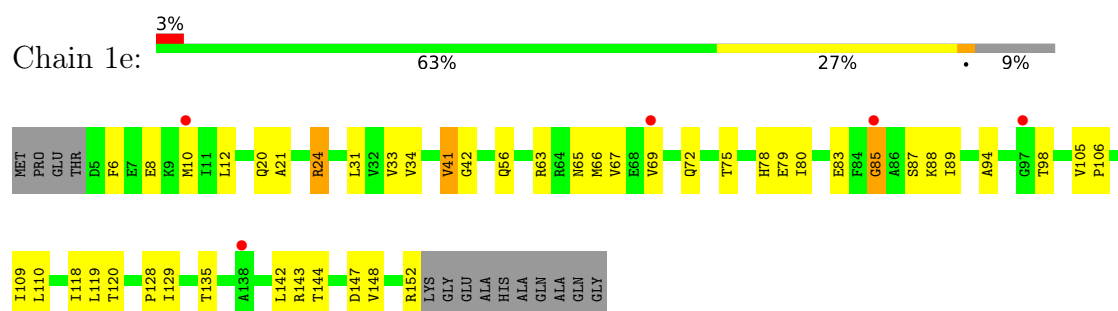
• Molecule 35: 30S ribosomal protein S4



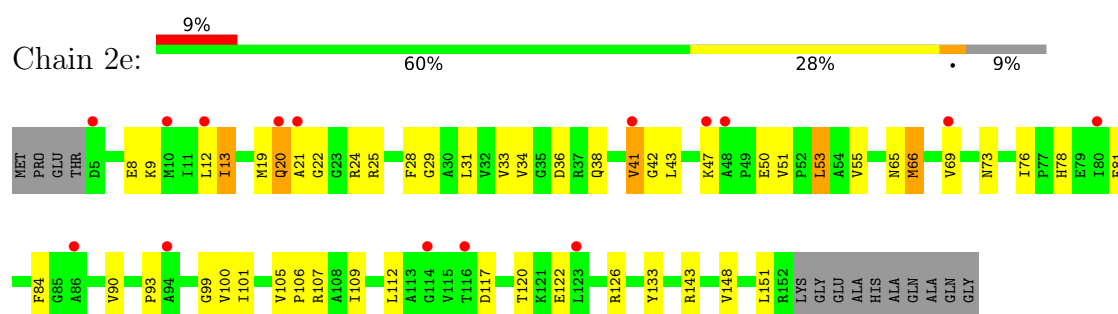
• Molecule 35: 30S ribosomal protein S4



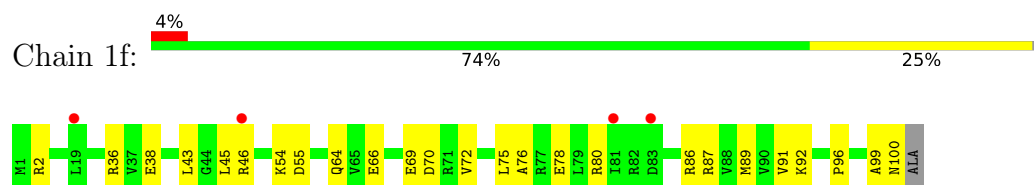
• Molecule 36: 30S ribosomal protein S5



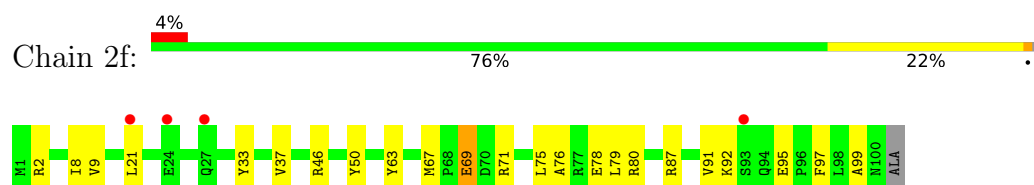
• Molecule 36: 30S ribosomal protein S5



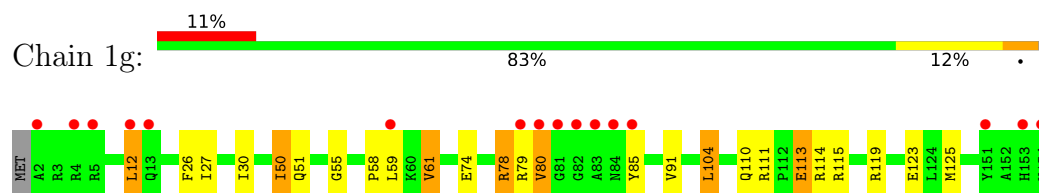
- Molecule 37: 30S ribosomal protein S6



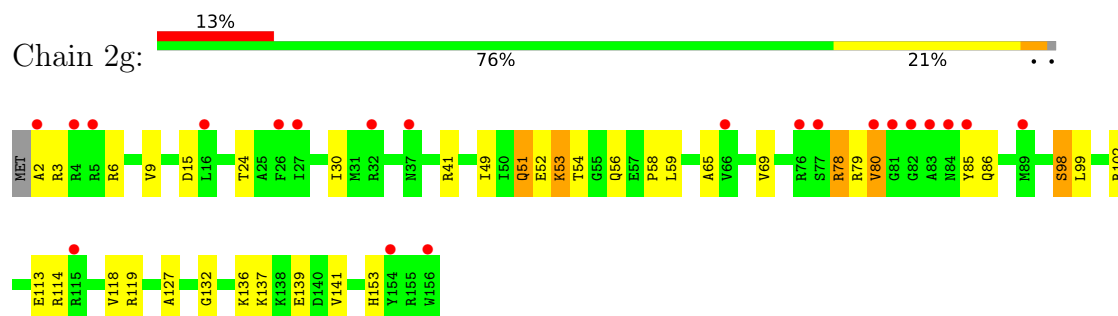
- Molecule 37: 30S ribosomal protein S6



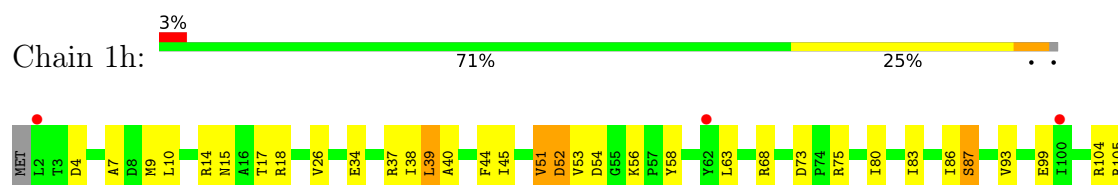
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

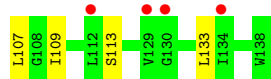
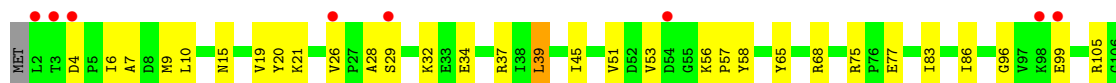
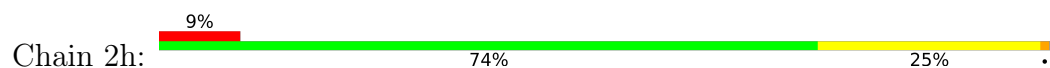


- Molecule 39: 30S ribosomal protein S8

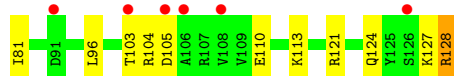




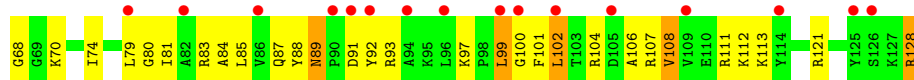
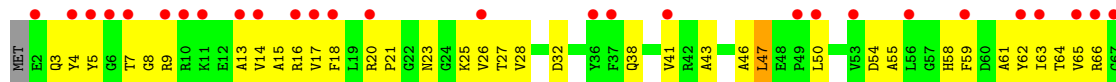
- Molecule 39: 30S ribosomal protein S8



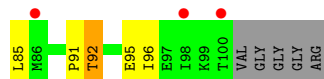
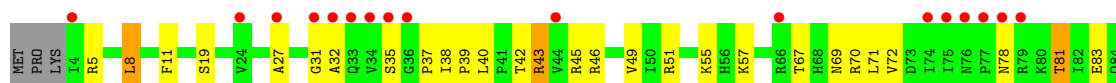
- Molecule 40: 30S ribosomal protein S9



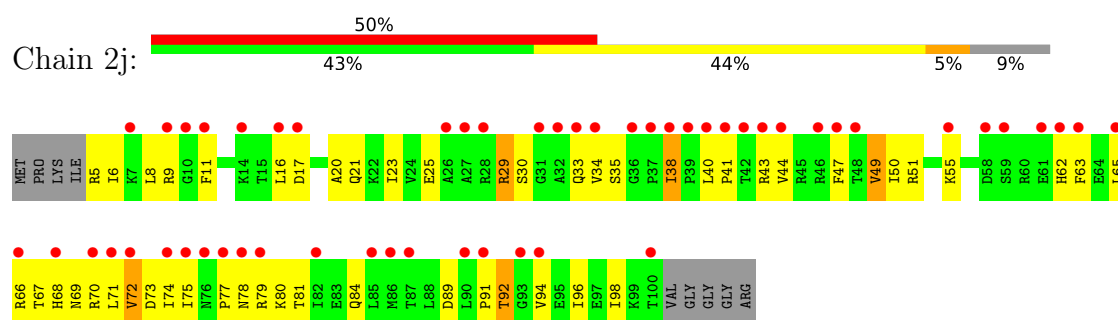
- Molecule 40: 30S ribosomal protein S9



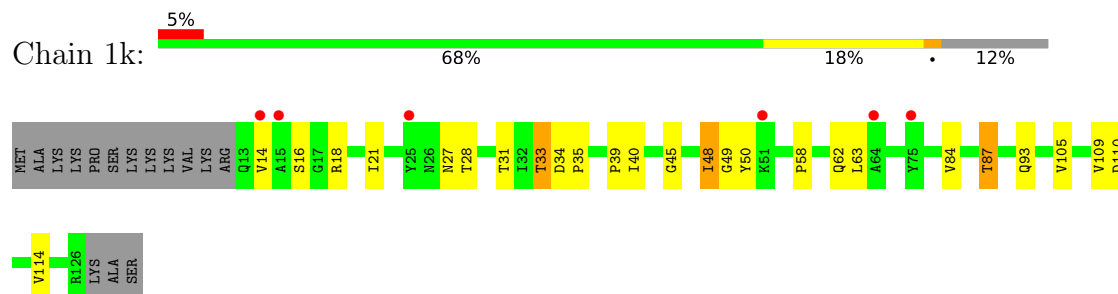
- Molecule 41: 30S ribosomal protein S10



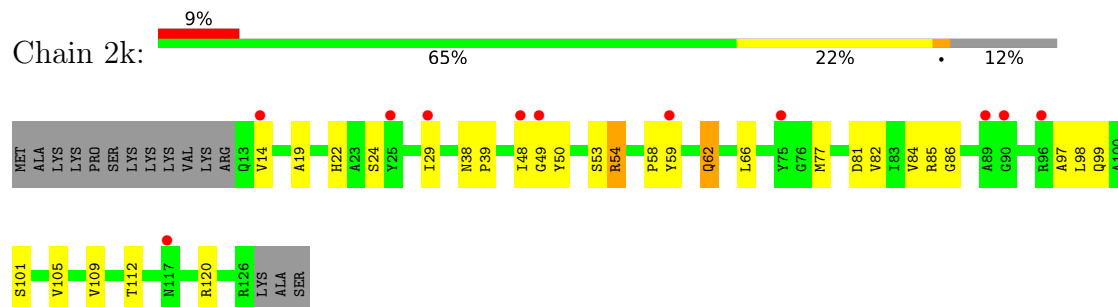
- Molecule 41: 30S ribosomal protein S10



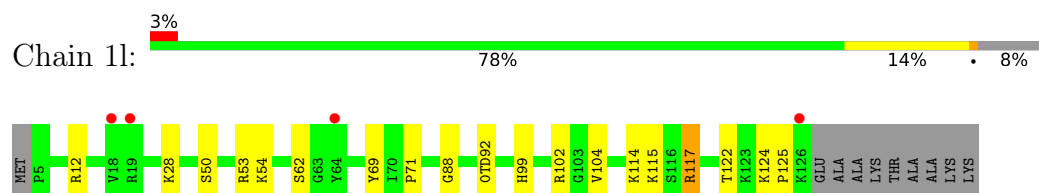
- Molecule 42: 30S ribosomal protein S11



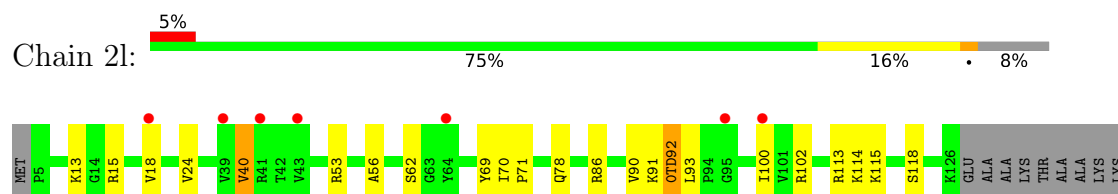
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

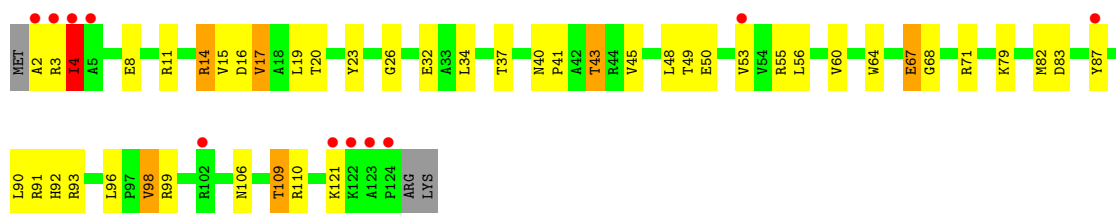


- Molecule 43: 30S ribosomal protein S12

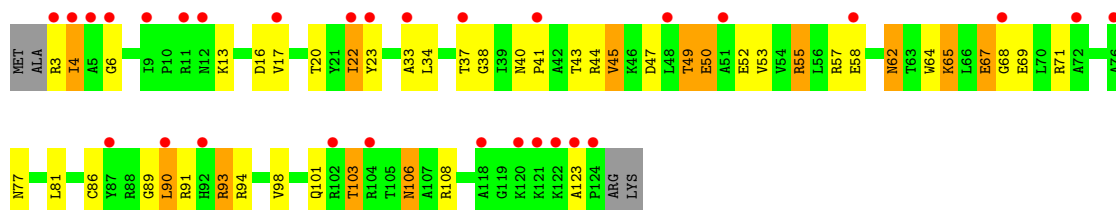


- Molecule 44: 30S ribosomal protein S13





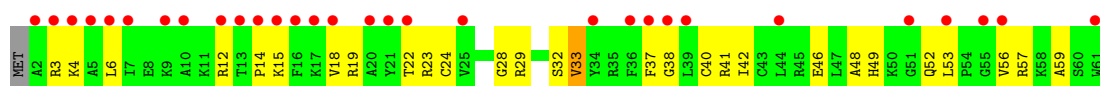
- Molecule 44: 30S ribosomal protein S13



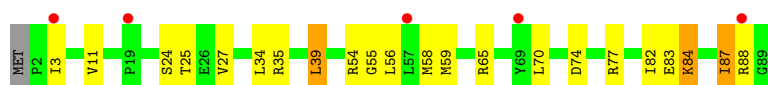
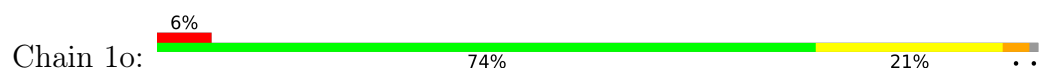
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



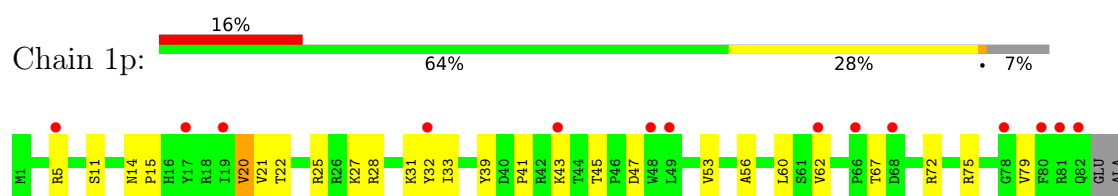
- Molecule 46: 30S ribosomal protein S15



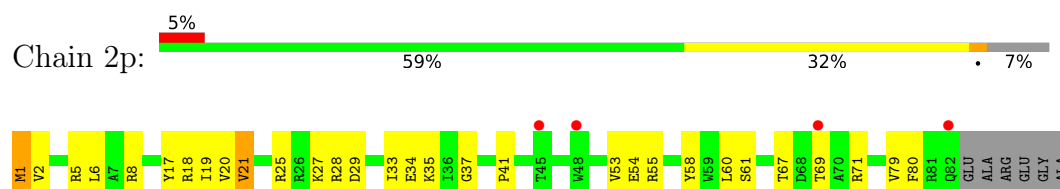
- Molecule 46: 30S ribosomal protein S15



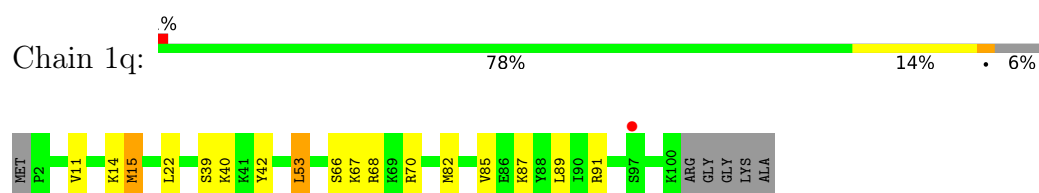
- Molecule 47: 30S ribosomal protein S16



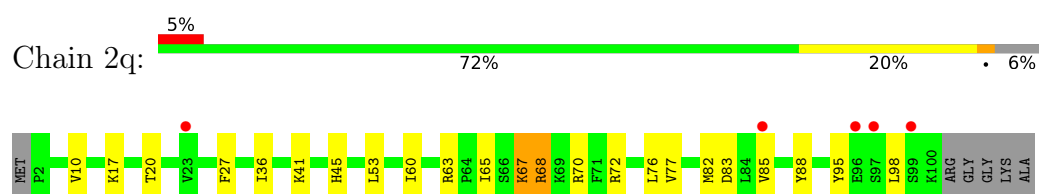
- Molecule 47: 30S ribosomal protein S16



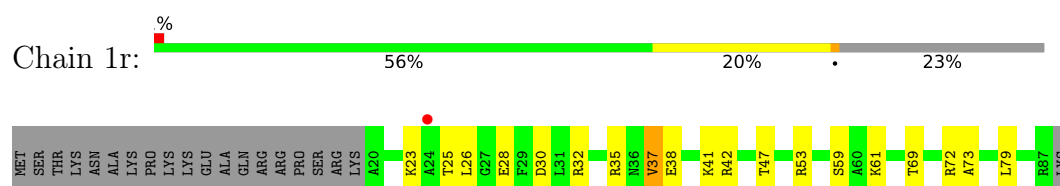
- Molecule 48: 30S ribosomal protein S17



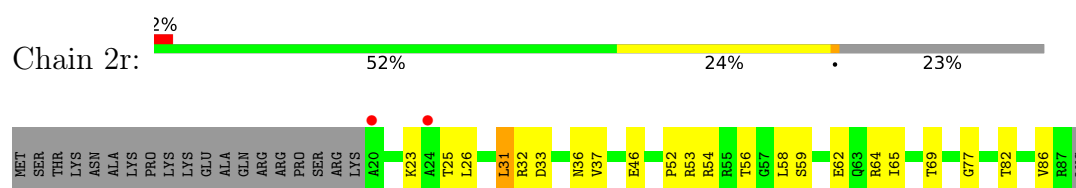
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

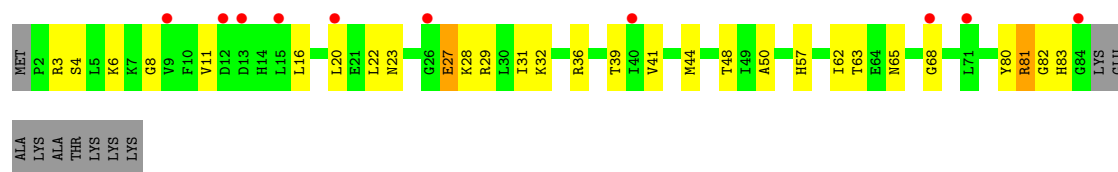


- Molecule 49: 30S ribosomal protein S18

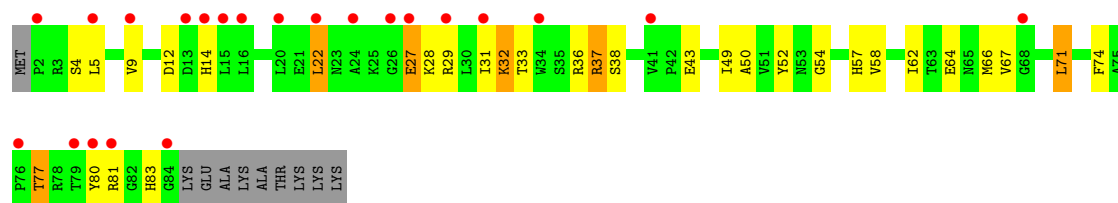


- Molecule 50: 30S ribosomal protein S19

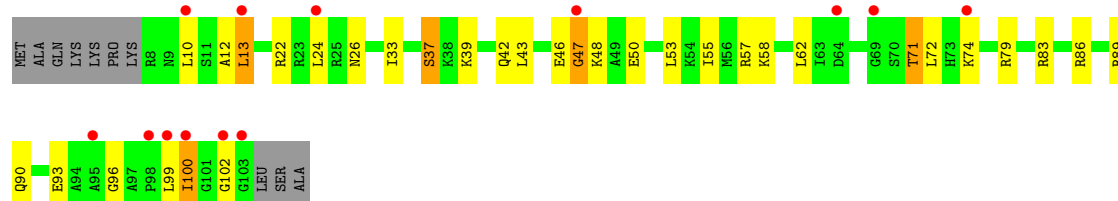




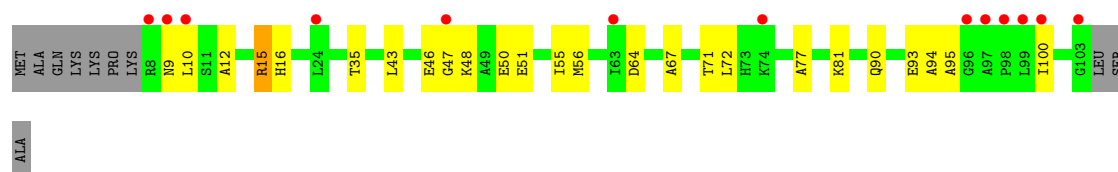
- Molecule 50: 30S ribosomal protein S19



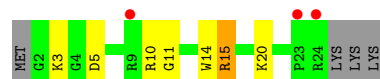
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

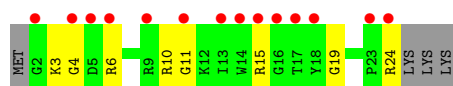


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

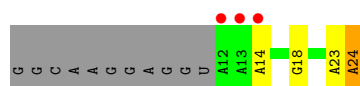




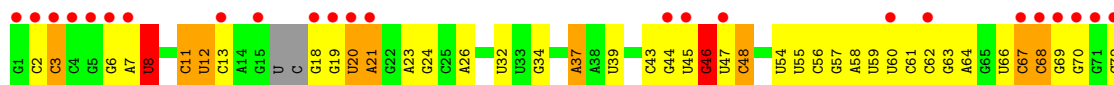
• Molecule 53: MF-mRNA



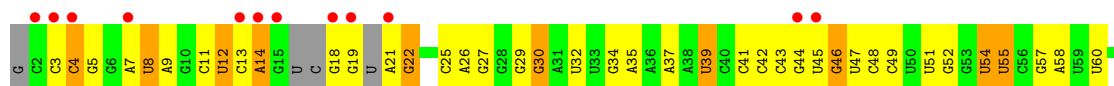
• Molecule 53: MF-mRNA



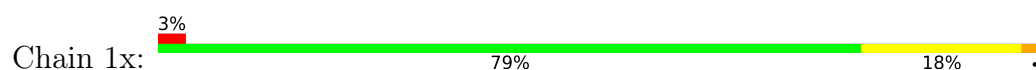
• Molecule 54: Aminoacylated Phe-tRNAphe



• Molecule 54: Aminoacylated Phe-tRNAphe



• Molecule 55: Aminoacylated fMet-tRNAmet

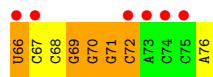
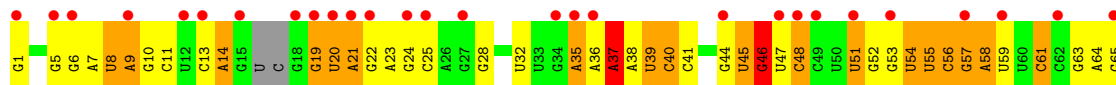
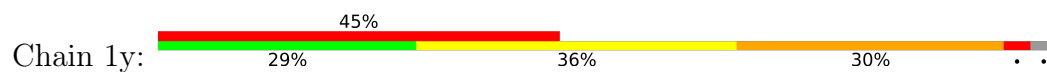


• Molecule 55: Aminoacylated fMet-tRNAmet

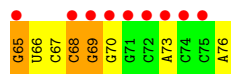
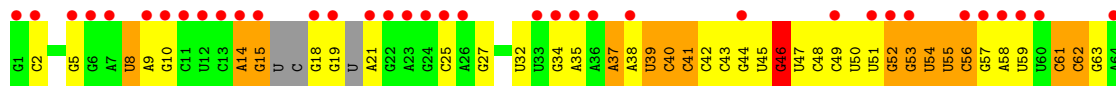




• Molecule 56: Deacylated tRNA^{phe}



• Molecule 56: Deacylated tRNA^{phe}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.54Å 448.51Å 620.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.20 – 2.40 147.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (147.20-2.40) 99.3 (147.20-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.260 0.221 , 0.261	Depositor DCC
R_{free} test set	111821 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	300319	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: 2MG, OMU, PSU, A1AE1, G7M, OMG, 5MC, 0TD, K, SF4, OMC, 4SU, M2G, FME, 5MU, MA6, 8AN, 4OC, MG, MIA, UR3, ZN, 2MA

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	0.31	0/68985	0.51	5/107677 (0.0%)
1	2A	0.24	0/67269	0.43	2/104999 (0.0%)
2	1B	0.25	0/2882	0.43	0/4494
2	2B	0.20	0/2879	0.39	0/4487
3	1D	0.29	0/2186	0.50	0/2944
3	2D	0.25	0/2186	0.48	0/2944
4	1E	0.30	0/1592	0.53	0/2149
4	2E	0.22	0/1592	0.45	0/2149
5	1F	0.29	0/1619	0.54	0/2193
5	2F	0.22	0/1615	0.47	0/2188
6	1G	0.24	0/1448	0.52	1/1957 (0.1%)
6	2G	0.19	0/1453	0.44	0/1963
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.20	0/1356	0.37	0/1834
8	1I	0.21	0/1112	0.43	0/1514
8	2I	0.22	0/1079	0.41	0/1475
9	1N	0.28	0/1144	0.49	0/1543
9	2N	0.20	0/1144	0.42	0/1543
10	1O	0.29	0/943	0.48	0/1269
10	2O	0.22	0/943	0.41	0/1269
11	1P	0.27	0/1152	0.60	0/1533
11	2P	0.23	0/1152	0.52	0/1533
12	1Q	0.29	0/1143	0.52	0/1527
12	2Q	0.21	0/1143	0.43	0/1527
13	1R	0.32	0/982	0.51	0/1312
13	2R	0.24	0/982	0.47	0/1312
14	1S	0.23	0/883	0.49	0/1176
14	2S	0.22	0/880	0.47	0/1172
15	1T	0.27	0/1105	0.51	0/1477
15	2T	0.22	0/1097	0.42	0/1468
16	1U	0.31	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.22	0/977	0.43	0/1301
17	1V	0.28	0/782	0.51	0/1049
17	2V	0.21	0/782	0.40	0/1049
18	1W	0.32	0/897	0.49	0/1205
18	2W	0.23	0/897	0.41	0/1205
19	1X	0.28	0/764	0.54	2/1025 (0.2%)
19	2X	0.22	0/764	0.49	2/1025 (0.2%)
20	1Y	0.25	0/819	0.50	0/1095
20	2Y	0.21	0/819	0.44	0/1095
21	1Z	0.24	0/1267	0.46	0/1717
21	2Z	0.22	0/1299	0.44	0/1763
22	10	0.30	0/662	0.50	0/881
22	20	0.22	0/662	0.45	0/881
23	11	0.27	0/762	0.46	0/1014
23	21	0.27	0/762	0.41	0/1014
24	12	0.26	0/590	0.47	0/781
24	22	0.20	0/590	0.38	0/781
25	13	0.27	0/474	0.52	0/635
25	23	0.20	0/469	0.43	0/630
26	14	0.26	0/565	0.58	0/761
26	24	0.25	0/545	0.51	0/737
27	15	0.30	0/469	0.54	0/635
27	25	0.23	0/469	0.43	0/635
28	16	0.30	0/460	0.50	0/613
28	26	0.25	0/456	0.47	0/608
29	17	0.32	0/426	0.54	0/561
29	27	0.28	0/426	0.53	0/561
30	18	0.27	0/525	0.50	0/691
30	28	0.21	0/525	0.44	0/691
31	19	0.30	0/310	0.56	0/407
31	29	0.20	0/310	0.46	0/407
32	1a	0.22	0/35795	0.41	2/55864 (0.0%)
32	2a	0.21	0/35886	0.39	3/56005 (0.0%)
33	1b	0.23	0/1881	0.48	0/2542
33	2b	0.22	0/1860	0.47	0/2518
34	1c	0.21	0/1572	0.41	0/2126
34	2c	0.22	0/1566	0.43	0/2119
35	1d	0.22	0/1685	0.45	0/2262
35	2d	0.22	0/1704	0.45	0/2284
36	1e	0.21	0/1145	0.45	0/1543
36	2e	0.23	0/1149	0.50	0/1548
37	1f	0.21	0/823	0.41	0/1115
37	2f	0.22	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1250	0.40	0/1679
38	2g	0.20	0/1254	0.42	0/1683
39	1h	0.20	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.40	0/1494
40	1i	0.22	0/1002	0.49	0/1346
40	2i	0.23	0/997	0.51	0/1343
41	1j	0.22	0/722	0.45	0/982
41	2j	0.23	0/727	0.47	0/988
42	1k	0.20	0/844	0.41	0/1145
42	2k	0.19	0/848	0.38	0/1149
43	1l	0.24	0/937	0.44	0/1260
43	2l	0.20	0/937	0.42	0/1260
44	1m	0.21	0/969	0.50	1/1302 (0.1%)
44	2m	0.21	0/961	0.48	0/1291
45	1n	0.21	0/501	0.44	0/664
45	2n	0.22	0/501	0.49	0/664
46	1o	0.22	0/739	0.39	0/985
46	2o	0.20	0/739	0.41	0/985
47	1p	0.22	0/697	0.47	0/939
47	2p	0.21	0/693	0.47	0/935
48	1q	0.21	0/836	0.43	0/1117
48	2q	0.20	0/836	0.46	1/1117 (0.1%)
49	1r	0.21	0/560	0.40	0/746
49	2r	0.19	0/560	0.40	0/746
50	1s	0.22	0/667	0.49	0/900
50	2s	0.23	0/661	0.54	0/893
51	1t	0.22	0/730	0.48	0/965
51	2t	0.23	0/729	0.48	1/965 (0.1%)
52	1u	0.21	0/203	0.49	0/266
52	2u	0.29	0/203	0.48	0/266
53	1v	0.22	0/310	0.35	0/480
53	2v	0.20	0/310	0.38	0/480
54	1w	0.31	1/1581 (0.1%)	0.44	0/2458
54	2w	0.31	2/1531 (0.1%)	0.42	0/2379
55	1x	0.31	1/1723 (0.1%)	0.45	0/2684
55	2x	0.27	0/1723	0.41	0/2684
56	1y	0.35	2/1606 (0.1%)	0.45	0/2497
56	2y	0.34	2/1583 (0.1%)	0.44	0/2459
All	All	0.25	8/316584 (0.0%)	0.45	20/473955 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
26	24	0	1
33	1b	0	1
51	1t	0	1
All	All	0	5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	8	4SU	O3'-P	5.61	1.61	1.56
56	1y	46	G7M	O3'-P	5.49	1.61	1.56
54	2w	46	G7M	O3'-P	5.47	1.61	1.56
56	2y	46	G7M	O3'-P	5.39	1.61	1.56
55	1x	8	4SU	O3'-P	5.31	1.61	1.56

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	7.62	120.93	109.50
6	1G	127	GLY	N-CA-C	-6.19	105.94	114.67
1	2A	1992	G	C2'-C3'-O3'	6.13	118.70	109.50
32	2a	1272	G	N1-C2-N2	-5.79	98.82	116.20
1	1A	512	G	O4'-C1'-N9	5.72	116.79	108.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
33	1b	126	GLU	Peptide
51	1t	99	LEU	Peptide
26	24	59	PHE	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61854	0	31201	523	0
1	2A	60324	0	30433	607	0
2	1B	2577	0	1305	23	0
2	2B	2575	0	1303	31	0
3	1D	2136	0	2218	31	0
3	2D	2136	0	2218	33	0
4	1E	1559	0	1618	23	0
4	2E	1559	0	1618	36	0
5	1F	1584	0	1625	35	0
5	2F	1580	0	1619	37	0
6	1G	1423	0	1436	39	0
6	2G	1428	0	1438	41	0
7	1H	1330	0	1407	23	0
7	2H	1330	0	1407	27	0
8	1I	1097	0	1140	37	0
8	2I	1064	0	1082	22	1
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	20	0
10	2O	933	0	996	22	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	29	0
12	1Q	1122	0	1179	14	0
12	2Q	1122	0	1179	24	0
13	1R	968	0	1033	11	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	12	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	17	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	15	0
17	1V	771	0	830	9	0
17	2V	771	0	830	9	0
18	1W	886	0	940	9	0
18	2W	886	0	940	12	0
19	1X	750	0	814	7	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	33	0
21	2Z	1271	0	1273	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	10	653	0	674	10	0
22	20	653	0	674	13	0
23	11	755	0	826	10	0
23	21	755	0	826	11	0
24	12	588	0	643	2	0
24	22	588	0	643	12	0
25	13	469	0	518	8	0
25	23	464	0	514	9	0
26	14	552	0	533	34	0
26	24	532	0	503	19	0
27	15	455	0	465	4	0
27	25	455	0	465	10	0
28	16	453	0	473	9	0
28	26	449	0	469	8	0
29	17	418	0	467	8	0
29	27	418	0	467	6	0
30	18	517	0	582	12	0
30	28	517	0	582	13	0
31	19	307	0	335	4	0
31	29	307	0	335	4	0
32	1a	32246	0	16295	334	1
32	2a	32327	0	16338	425	0
33	1b	1846	0	1867	59	0
33	2b	1825	0	1828	76	0
34	1c	1548	0	1535	30	0
34	2c	1542	0	1517	53	0
35	1d	1655	0	1672	31	0
35	2d	1674	0	1714	48	0
36	1e	1129	0	1185	28	0
36	2e	1133	0	1191	38	0
37	1f	810	0	804	13	0
37	2f	816	0	808	14	0
38	1g	1231	0	1238	15	0
38	2g	1235	0	1249	24	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	23	0
40	1i	983	0	986	20	0
40	2i	978	0	966	49	0
41	1j	709	0	650	25	0
41	2j	714	0	672	38	0
42	1k	829	0	825	13	0
42	2k	833	0	836	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1l	932	0	981	11	0
43	2l	932	0	980	15	0
44	1m	958	0	1002	27	0
44	2m	950	0	988	38	0
45	1n	492	0	529	11	0
45	2n	492	0	529	22	0
46	1o	728	0	760	13	0
46	2o	728	0	760	20	0
47	1p	681	0	697	12	0
47	2p	677	0	686	18	0
48	1q	823	0	891	12	0
48	2q	823	0	891	12	0
49	1r	555	0	618	12	0
49	2r	555	0	618	15	0
50	1s	652	0	662	18	0
50	2s	646	0	644	24	0
51	1t	728	0	798	18	0
51	2t	727	0	796	13	0
52	1u	199	0	208	6	0
52	2u	199	0	208	7	0
53	1v	277	0	140	1	0
53	2v	277	0	140	4	0
54	1w	1592	0	817	24	0
54	2w	1544	0	783	21	0
55	1x	1646	0	838	10	0
55	2x	1646	0	838	22	0
56	1y	1585	0	803	39	0
56	2y	1565	0	794	33	0
57	10	11	0	0	0	0
57	11	6	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	14	1	0	0	0	0
57	15	7	0	0	0	0
57	16	1	0	0	0	0
57	17	7	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1093	0	0	0	0
57	1B	36	0	0	0	0
57	1D	14	0	0	0	0
57	1E	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1F	14	0	0	0	0
57	1G	4	0	0	0	0
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	7	0	0	0	0
57	1O	6	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	8	0	0	0	0
57	1R	3	0	0	0	0
57	1S	3	0	0	0	0
57	1T	4	0	0	0	0
57	1U	9	0	0	0	0
57	1V	8	0	0	0	0
57	1W	6	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	214	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	1	0	0	0	0
57	1h	1	0	0	0	0
57	1k	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	2	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	8	0	0	0	0
57	1x	14	0	0	0	0
57	20	4	0	0	0	0
57	21	1	0	0	0	0
57	23	3	0	0	0	0
57	25	5	0	0	0	0
57	26	1	0	0	0	0
57	27	3	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	854	0	0	0	0
57	2B	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2D	8	0	0	0	0
57	2E	11	0	0	0	0
57	2F	5	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	2	0	0	0	0
57	2R	2	0	0	0	0
57	2T	3	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	210	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	5	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	3	0	0	0	0
57	2w	7	0	0	0	0
57	2x	7	0	0	0	0
57	2y	5	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	76	0	0	0	0
59	2A	76	0	0	1	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	4	0
62	1w	11	0	8	1	0
62	2w	11	0	8	1	0
63	1x	10	0	10	0	0
63	2x	10	0	10	0	0
64	10	12	0	0	0	0
64	11	11	0	0	0	0
64	12	3	0	0	0	0
64	13	5	0	0	1	0
64	14	1	0	0	0	0
64	15	9	0	0	0	0
64	16	1	0	0	0	0
64	17	11	0	0	0	0
64	18	11	0	0	0	0
64	1A	2061	0	0	63	0
64	1B	60	0	0	3	0
64	1D	29	0	0	1	0
64	1E	27	0	0	1	0
64	1F	16	0	0	1	0
64	1G	1	0	0	0	0
64	1H	1	0	0	0	0
64	1N	5	0	0	0	0
64	1O	6	0	0	0	0
64	1P	22	0	0	1	0
64	1Q	9	0	0	0	0
64	1R	10	0	0	1	0
64	1S	4	0	0	0	0
64	1T	8	0	0	1	0
64	1U	10	0	0	0	0
64	1V	8	0	0	0	0
64	1W	9	0	0	1	0
64	1X	6	0	0	0	0
64	1Y	3	0	0	1	0
64	1Z	1	0	0	0	0
64	1a	388	0	0	22	0
64	1b	1	0	0	0	0
64	1c	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	1d	2	0	0	1	0
64	1e	3	0	0	0	0
64	1f	1	0	0	0	0
64	1g	1	0	0	0	0
64	1i	1	0	0	0	0
64	1j	2	0	0	0	0
64	1l	7	0	0	0	0
64	1m	1	0	0	0	0
64	1n	2	0	0	0	0
64	1o	1	0	0	0	0
64	1p	1	0	0	0	0
64	1q	2	0	0	0	0
64	1u	1	0	0	1	0
64	1v	5	0	0	0	0
64	1w	14	0	0	2	0
64	1x	15	0	0	1	0
64	1y	1	0	0	0	0
64	20	3	0	0	0	0
64	21	11	0	0	0	0
64	23	2	0	0	1	0
64	25	2	0	0	0	0
64	27	5	0	0	0	0
64	28	3	0	0	0	0
64	29	1	0	0	0	0
64	2A	1142	0	0	70	0
64	2B	19	0	0	0	0
64	2D	23	0	0	0	0
64	2E	12	0	0	0	0
64	2F	12	0	0	0	0
64	2I	2	0	0	0	0
64	2O	2	0	0	0	0
64	2P	11	0	0	0	0
64	2Q	2	0	0	0	0
64	2R	3	0	0	0	0
64	2T	5	0	0	0	0
64	2U	3	0	0	0	0
64	2V	1	0	0	0	0
64	2X	3	0	0	0	0
64	2Y	1	0	0	0	0
64	2Z	1	0	0	0	0
64	2a	221	0	0	12	0
64	2c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	2d	2	0	0	0	0
64	2g	1	0	0	0	0
64	2j	3	0	0	2	0
64	2l	4	0	0	1	0
64	2p	2	0	0	0	0
64	2q	1	0	0	0	0
64	2r	1	0	0	0	0
64	2t	1	0	0	0	0
64	2v	2	0	0	0	0
64	2w	3	0	0	0	0
64	2x	7	0	0	0	0
64	2y	2	0	0	0	0
All	All	300319	0	196751	3569	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3569 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.13	1.41
1:1A:1082:U:N3	1:1A:1086:A:N6	1.99	1.09
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.42	1.01
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	1.00
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.30	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:358:U:OP1	8:2I:121:LYS:NZ[2_655]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	25	38
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	25	38
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	25	38
5	2F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	25	38
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	4	4
7	1H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
7	2H	172/180 (96%)	153 (89%)	18 (10%)	1 (1%)	22	33
8	1I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	18 (12%)	3 (2%)	5	7
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	19	29
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
11	1P	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	13
11	2P	147/150 (98%)	132 (90%)	12 (8%)	3 (2%)	6	8
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	14	22
15	1T	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	16	26
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	13	20
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	12	18
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	13	20
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	13	20
21	1Z	148/206 (72%)	136 (92%)	11 (7%)	1 (1%)	19	29
21	2Z	156/206 (76%)	131 (84%)	20 (13%)	5 (3%)	3	3
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	12	18
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	18
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	57 (85%)	4 (6%)	6 (9%)	0	0
26	24	67/71 (94%)	49 (73%)	14 (21%)	4 (6%)	1	0
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	57 (100%)	0	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	196 (86%)	26 (11%)	7 (3%)	3	3
33	2b	229/256 (90%)	194 (85%)	30 (13%)	5 (2%)	5	6
34	1c	204/239 (85%)	193 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	178 (87%)	23 (11%)	3 (2%)	8	12
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	25	38
35	2d	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	13	20
36	1e	146/162 (90%)	137 (94%)	6 (4%)	3 (2%)	5	7
36	2e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	19	29
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
38	2g	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	19	29
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	8	11
40	2i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	26
41	1j	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	12	18
41	2j	94/105 (90%)	77 (82%)	13 (14%)	4 (4%)	2	1
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	7	9
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	22
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	26
44	1m	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	7	10
44	2m	120/126 (95%)	103 (86%)	14 (12%)	3 (2%)	4	5
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	11	16
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	4 (4%)	2 (2%)	5	7
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	11	16
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	4	5
51	1t	94/106 (89%)	82 (87%)	10 (11%)	2 (2%)	5	7
51	2t	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	12	18
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10564 (93%)	713 (6%)	93 (1%)	16	26

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	45	LEU
40	1i	54	ASP
44	1m	67	GLU
5	2F	130	ALA
6	2G	51	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	209 (97%)	6 (3%)	38	59
3	2D	215/218 (99%)	205 (95%)	10 (5%)	22	38
4	1E	164/166 (99%)	156 (95%)	8 (5%)	21	36
4	2E	164/166 (99%)	152 (93%)	12 (7%)	11	20
5	1F	160/166 (96%)	142 (89%)	18 (11%)	4	7
5	2F	159/166 (96%)	147 (92%)	12 (8%)	11	18
6	1G	143/156 (92%)	130 (91%)	13 (9%)	7	12
6	2G	143/156 (92%)	123 (86%)	20 (14%)	3	3
7	1H	144/148 (97%)	136 (94%)	8 (6%)	17	30
7	2H	144/148 (97%)	132 (92%)	12 (8%)	9	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1I	113/124 (91%)	95 (84%)	18 (16%)	2	2
8	2I	105/124 (85%)	90 (86%)	15 (14%)	2	3
9	1N	118/119 (99%)	112 (95%)	6 (5%)	20	35
9	2N	118/119 (99%)	114 (97%)	4 (3%)	32	52
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	57
10	2O	100/100 (100%)	93 (93%)	7 (7%)	12	21
11	1P	115/116 (99%)	107 (93%)	8 (7%)	12	21
11	2P	115/116 (99%)	107 (93%)	8 (7%)	12	21
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	18	32
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	23	40
13	1R	101/101 (100%)	96 (95%)	5 (5%)	20	36
13	2R	101/101 (100%)	96 (95%)	5 (5%)	20	36
14	1S	86/88 (98%)	79 (92%)	7 (8%)	9	15
14	2S	85/88 (97%)	72 (85%)	13 (15%)	2	3
15	1T	115/127 (91%)	112 (97%)	3 (3%)	41	62
15	2T	113/127 (89%)	110 (97%)	3 (3%)	40	60
16	1U	93/94 (99%)	89 (96%)	4 (4%)	25	42
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	54
17	1V	80/82 (98%)	74 (92%)	6 (8%)	11	18
17	2V	80/82 (98%)	74 (92%)	6 (8%)	11	18
18	1W	90/92 (98%)	86 (96%)	4 (4%)	24	41
18	2W	90/92 (98%)	84 (93%)	6 (7%)	13	23
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	74 (96%)	3 (4%)	27	46
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	7	11
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	5	8
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	8	12
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	7	11
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	56
22	20	65/67 (97%)	64 (98%)	1 (2%)	60	77
23	11	80/83 (96%)	76 (95%)	4 (5%)	20	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	21	80/83 (96%)	76 (95%)	4 (5%)	20	36
24	12	65/67 (97%)	61 (94%)	4 (6%)	15	26
24	22	65/67 (97%)	61 (94%)	4 (6%)	15	26
25	13	51/52 (98%)	48 (94%)	3 (6%)	16	28
25	23	50/52 (96%)	46 (92%)	4 (8%)	10	16
26	14	59/63 (94%)	45 (76%)	14 (24%)	0	0
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	1
27	15	50/52 (96%)	48 (96%)	2 (4%)	27	45
27	25	50/52 (96%)	48 (96%)	2 (4%)	27	45
28	16	51/52 (98%)	46 (90%)	5 (10%)	6	10
28	26	50/52 (96%)	47 (94%)	3 (6%)	16	27
29	17	41/42 (98%)	36 (88%)	5 (12%)	4	5
29	27	41/42 (98%)	36 (88%)	5 (12%)	4	5
30	18	54/55 (98%)	52 (96%)	2 (4%)	29	48
30	28	54/55 (98%)	52 (96%)	2 (4%)	29	48
31	19	34/34 (100%)	32 (94%)	2 (6%)	16	28
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	168 (88%)	24 (12%)	3	5
33	2b	187/220 (85%)	162 (87%)	25 (13%)	3	4
34	1c	142/188 (76%)	126 (89%)	16 (11%)	4	7
34	2c	140/188 (74%)	132 (94%)	8 (6%)	17	29
35	1d	169/181 (93%)	153 (90%)	16 (10%)	7	11
35	2d	173/181 (96%)	156 (90%)	17 (10%)	6	10
36	1e	113/123 (92%)	106 (94%)	7 (6%)	15	26
36	2e	114/123 (93%)	104 (91%)	10 (9%)	8	13
37	1f	84/90 (93%)	76 (90%)	8 (10%)	7	11
37	2f	85/90 (94%)	78 (92%)	7 (8%)	9	15
38	1g	119/127 (94%)	106 (89%)	13 (11%)	5	7
38	2g	120/127 (94%)	108 (90%)	12 (10%)	6	9
39	1h	114/119 (96%)	106 (93%)	8 (7%)	12	21
39	2h	114/119 (96%)	111 (97%)	3 (3%)	41	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	1i	90/99 (91%)	83 (92%)	7 (8%)	10	17
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	2
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	3
41	2j	69/92 (75%)	62 (90%)	7 (10%)	6	9
42	1k	82/99 (83%)	74 (90%)	8 (10%)	6	10
42	2k	83/99 (84%)	73 (88%)	10 (12%)	4	5
43	1l	96/108 (89%)	94 (98%)	2 (2%)	48	69
43	2l	96/108 (89%)	92 (96%)	4 (4%)	25	43
44	1m	93/101 (92%)	83 (89%)	10 (11%)	5	7
44	2m	92/101 (91%)	74 (80%)	18 (20%)	1	1
45	1n	49/50 (98%)	43 (88%)	6 (12%)	4	5
45	2n	49/50 (98%)	42 (86%)	7 (14%)	2	3
46	1o	78/80 (98%)	71 (91%)	7 (9%)	8	12
46	2o	78/80 (98%)	75 (96%)	3 (4%)	28	47
47	1p	69/74 (93%)	60 (87%)	9 (13%)	3	4
47	2p	68/74 (92%)	58 (85%)	10 (15%)	2	3
48	1q	94/97 (97%)	89 (95%)	5 (5%)	19	33
48	2q	94/97 (97%)	91 (97%)	3 (3%)	34	54
49	1r	59/77 (77%)	55 (93%)	4 (7%)	13	22
49	2r	59/77 (77%)	55 (93%)	4 (7%)	13	22
50	1s	69/80 (86%)	64 (93%)	5 (7%)	12	20
50	2s	67/80 (84%)	60 (90%)	7 (10%)	5	8
51	1t	70/82 (85%)	65 (93%)	5 (7%)	12	20
51	2t	70/82 (85%)	64 (91%)	6 (9%)	8	14
52	1u	18/22 (82%)	16 (89%)	2 (11%)	5	7
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8570 (92%)	733 (8%)	10	16

5 of 733 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	2R	73	VAL
33	2b	149	LEU

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Mol	Chain	Res	Type
14	2S	75	GLU
13	2R	36	THR
21	2Z	154	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
36	2e	73	ASN
51	2t	16	HIS
40	2i	3	GLN
42	2k	62	GLN
39	1h	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	423 (14%)	30 (1%)
1	2A	2791/2915 (95%)	450 (16%)	25 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	22 (18%)	0
32	1a	1497/1521 (98%)	231 (15%)	0
32	2a	1501/1521 (98%)	266 (17%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	26 (38%)	0
55	1x	75/77 (97%)	4 (5%)	0
55	2x	75/77 (97%)	6 (8%)	0
56	1y	72/76 (94%)	31 (43%)	0
56	2y	70/76 (92%)	26 (37%)	0
All	All	9346/9620 (97%)	1521 (16%)	55 (0%)

5 of 1521 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	72	U

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2629	A
1	2A	528	A
1	2A	2756	U
1	2A	1992	G
1	1A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.96	4 (19%)
1	OMU	2A	2552	57,1	19,22,23	1.12	1 (5%)	25,31,34	1.81	5 (20%)
54	PSU	1w	39	54	18,21,22	1.43	3 (16%)	21,30,33	1.63	3 (14%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.90	0
54	G7M	1w	46	54	20,26,27	1.22	2 (10%)	16,39,42	0.59	0
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.18	3 (11%)
43	0TD	1l	92	43	8,9,10	4.43	3 (37%)	6,11,13	7.28	2 (33%)
1	MA6	2A	2058	1	19,26,27	1.00	2 (10%)	18,38,41	2.00	4 (22%)
1	PSU	2A	2605	1	18,21,22	1.25	1 (5%)	21,30,33	2.07	4 (19%)
54	G7M	2w	46	54	20,26,27	1.23	1 (5%)	16,39,42	0.68	0
54	PSU	1w	55	54	18,21,22	1.33	2 (11%)	21,30,33	2.00	3 (14%)
56	MIA	2y	37	56	17,24,32	1.02	1 (5%)	16,35,47	1.30	2 (12%)
1	MA6	1A	2058	57,1	19,26,27	1.01	1 (5%)	18,38,41	1.91	4 (22%)
1	2MA	1A	2503	57,1	18,25,26	0.74	0	20,37,40	1.96	4 (20%)
32	PSU	1a	516	32	18,21,22	1.34	2 (11%)	21,30,33	1.90	5 (23%)
56	PSU	1y	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.93	4 (19%)
55	8AN	2x	76	57,55,63	17,24,25	1.15	2 (11%)	13,35,38	3.48	3 (23%)
54	5MU	1w	54	54	19,22,23	1.32	3 (15%)	27,32,35	2.17	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	1y	39	56	18,21,22	1.45	2 (11%)	21,30,33	1.71	3 (14%)
1	5MC	2A	1962	57,1	19,22,23	1.89	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.25	4 (15%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.14	5 (23%)
56	PSU	2y	55	56	18,21,22	1.42	2 (11%)	21,30,33	1.98	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.09	1 (5%)	26,32,35	1.82	3 (11%)
32	5MC	1a	967	32	19,22,23	1.65	3 (15%)	26,32,35	1.04	2 (7%)
54	4SU	1w	8	54	18,21,22	1.72	4 (22%)	25,30,33	1.78	5 (20%)
32	5MC	2a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.29	3 (11%)
32	G7M	1a	527	57,32	20,26,27	1.18	2 (10%)	16,39,42	0.66	0
56	G7M	2y	46	56	20,26,27	1.38	2 (10%)	16,39,42	0.65	0
55	5MC	1x	32	55	19,22,23	1.60	3 (15%)	26,32,35	1.28	3 (11%)
56	G7M	1y	46	56	20,26,27	1.37	1 (5%)	16,39,42	0.45	0
32	MA6	1a	1518	32	19,26,27	1.03	2 (10%)	18,38,41	2.07	3 (16%)
32	M2G	2a	966	32	20,27,28	1.32	3 (15%)	19,40,43	1.04	1 (5%)
1	5MU	2A	1939	1	19,22,23	1.44	6 (31%)	27,32,35	2.32	6 (22%)
54	8AN	2w	76	1,62,54	17,24,25	1.39	4 (23%)	13,35,38	1.94	1 (7%)
56	PSU	2y	32	56	18,21,22	1.35	2 (11%)	21,30,33	1.95	3 (14%)
1	5MC	1A	1942	1	19,22,23	1.85	3 (15%)	26,32,35	1.33	4 (15%)
32	G7M	2a	527	57,32	20,26,27	1.27	2 (10%)	16,39,42	0.53	0
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.96	4 (19%)
32	MA6	1a	1519	32	19,26,27	1.06	2 (10%)	18,38,41	1.95	3 (16%)
56	4SU	2y	8	56	18,21,22	1.76	4 (22%)	25,30,33	2.32	5 (20%)
1	PSU	1A	2605	57,1	18,21,22	1.52	3 (16%)	21,30,33	2.02	4 (19%)
1	5MU	1A	1915	1	19,22,23	1.44	6 (31%)	27,32,35	2.15	7 (25%)
32	5MC	2a	967	32	19,22,23	1.68	2 (10%)	26,32,35	1.04	2 (7%)
54	MIA	2w	37	54,53	19,27,32	1.88	3 (15%)	18,39,47	1.32	3 (16%)
1	5MC	1A	1962	57,1	19,22,23	1.79	3 (15%)	26,32,35	1.15	3 (11%)
1	OMG	2A	2251	55,1	19,26,27	0.90	1 (5%)	21,38,41	1.11	3 (14%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.18	6 (22%)
54	PSU	1w	32	57,54	18,21,22	1.34	2 (11%)	21,30,33	1.93	3 (14%)
32	M2G	1a	966	32	20,27,28	1.33	3 (15%)	19,40,43	1.02	2 (10%)
1	OMC	2A	1920	1	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	21,30,33	2.08	4 (19%)
56	5MU	2y	54	56	19,22,23	1.46	5 (26%)	27,32,35	1.78	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	57,1,55	19,26,27	0.95	1 (5%)	21,38,41	1.07	2 (9%)
32	2MG	1a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.33	3 (18%)
54	8AN	1w	76	1,62,54	17,24,25	1.43	4 (23%)	13,35,38	2.05	2 (15%)
56	5MU	1y	54	56	19,22,23	1.46	5 (26%)	27,32,35	2.07	6 (22%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.08	2 (8%)
32	PSU	2a	516	32	18,21,22	1.34	2 (11%)	21,30,33	2.09	5 (23%)
43	0TD	2l	92	43	8,9,10	4.56	1 (12%)	6,11,13	4.85	2 (33%)
56	PSU	2y	39	56	18,21,22	1.38	2 (11%)	21,30,33	1.77	4 (19%)
55	5MU	1x	54	57,55	19,22,23	1.42	4 (21%)	27,32,35	2.17	6 (22%)
32	5MC	2a	1407	57,32	19,22,23	1.54	3 (15%)	26,32,35	1.13	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	3 (14%)
55	4SU	1x	8	55	18,21,22	2.32	5 (27%)	25,30,33	1.73	7 (28%)
1	5MU	1A	1939	57,1	19,22,23	1.54	6 (31%)	27,32,35	2.20	6 (22%)
55	5MC	2x	32	55	19,22,23	1.68	3 (15%)	26,32,35	1.24	2 (7%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.06	4 (19%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.56	3 (18%)
55	8AN	1x	76	57,55,63	17,24,25	1.30	3 (17%)	13,35,38	4.12	4 (30%)
54	PSU	2w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.88	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.19	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.86	5 (19%)
56	4SU	1y	8	56	18,21,22	1.80	6 (33%)	25,30,33	1.90	5 (20%)
32	5MC	1a	1407	32	19,22,23	1.69	2 (10%)	26,32,35	1.17	4 (15%)
1	5MC	2A	1942	1	19,22,23	1.66	2 (10%)	26,32,35	1.08	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.30	6 (22%)
54	4SU	2w	8	54	18,21,22	1.75	4 (22%)	25,30,33	2.75	5 (20%)
54	MIA	1w	37	54	24,31,32	2.18	3 (12%)	22,44,47	2.42	7 (31%)
1	2MA	2A	2503	57,1	18,25,26	0.72	0	20,37,40	1.97	4 (20%)
56	MIA	1y	37	56	17,24,32	0.98	1 (5%)	16,35,47	1.32	1 (6%)
54	PSU	2w	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.93	3 (14%)
55	4SU	2x	8	57,55	18,21,22	2.16	5 (27%)	25,30,33	1.46	5 (20%)
1	OMU	1A	2552	57,1	19,22,23	1.20	2 (10%)	25,31,34	1.81	5 (20%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	1.08	3 (12%)
32	MA6	2a	1519	32	19,26,27	1.02	2 (10%)	18,38,41	1.95	3 (16%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.13	4 (19%)
54	5MU	2w	54	54	19,22,23	1.34	3 (15%)	27,32,35	1.83	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.96	3 (16%)
55	PSU	1x	55	57,55	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	MA6	2A	2058	1	-	0/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	0/3/25/34	0/3/3/3
1	MA6	1A	2058	57,1	-	0/7/29/30	0/3/3/3
1	2MA	1A	2503	57,1	-	1/3/25/26	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	57,55,63	-	3/3/25/26	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	3/3/25/26	0/3/3/3
56	G7M	2y	46	56	-	2/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	1/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
54	8AN	2w	76	1,62,54	-	0/3/25/26	0/3/3/3
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	3/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54,53	-	4/7/29/34	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/5/27/28	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	8AN	1w	76	1,62,54	-	0/3/25/26	0/3/3/3
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	57,32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
55	8AN	1x	76	57,55,63	-	3/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	1y	8	56	-	1/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	57,55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
55	PSU	1x	55	57,55	-	0/7/25/26	0/2/2/2

The worst 5 of 221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.43	1.69	1.82
43	1l	92	0TD	CB-SB	-11.78	1.70	1.82
1	2A	1962	5MC	C5-C4	7.11	1.49	1.44
54	1w	37	MIA	C13-C14	6.96	1.53	1.32
1	1A	1942	5MC	C5-C4	6.85	1.49	1.44

The worst 5 of 307 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.54	70.83	102.36
43	2l	92	0TD	CSB-SB-CB	-11.47	81.75	102.36
55	1x	76	8AN	O4'-C1'-N9	10.42	122.56	108.75
54	2w	8	4SU	C4-N3-C2	-8.85	118.83	127.31
55	2x	76	8AN	C4'-O4'-C1'	-8.47	102.16	109.92

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16

There are no ring outliers.

42 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	46	G7M	1	0
1	2A	2058	MA6	2	0
56	2y	37	MIA	1	0
1	1A	2058	MA6	1	0
55	2x	76	8AN	1	0
56	1y	39	PSU	1	0
55	2x	55	PSU	1	0
32	1a	967	5MC	1	0
54	1w	8	4SU	1	0
56	2y	46	G7M	1	0
56	1y	46	G7M	1	0
32	1a	1518	MA6	4	0
32	2a	966	M2G	1	0
1	2A	1939	5MU	1	0
54	2w	76	8AN	1	0
32	1a	1519	MA6	2	0
56	2y	8	4SU	2	0
32	2a	967	5MC	2	0
1	2A	2251	OMG	1	0
55	2x	54	5MU	3	0
32	1a	966	M2G	1	0
56	1y	55	PSU	2	0
56	2y	54	5MU	1	0
1	1A	2251	OMG	1	0
54	1w	76	8AN	1	0
56	1y	54	5MU	1	0
32	1a	1402	4OC	1	0
43	2l	92	0TD	1	0
56	2y	39	PSU	1	0
55	1x	8	4SU	2	0
1	1A	1939	5MU	1	0
54	2w	55	PSU	1	0
55	1x	76	8AN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	39	PSU	1	0
56	1y	8	4SU	1	0
54	1w	37	MIA	1	0
56	1y	37	MIA	4	0
55	2x	8	4SU	1	0
1	1A	2552	OMU	1	0
32	2a	1519	MA6	2	0
54	2w	54	5MU	1	0
32	2a	1518	MA6	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2755 ligands modelled in this entry, 2747 are monoatomic - leaving 8 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	$\# Z > 2$
63	FME	2x	108	55	8,9,10	0.36	0	8,9,11	1.31	2 (25%)
59	A1AE1	1A	4094	57	82,82,82	2.30	12 (14%)	116,122,122	2.14	33 (28%)
59	A1AE1	2A	3855	57	82,82,82	2.21	13 (15%)	116,122,122	2.21	31 (26%)
62	PHE	2w	108	54	10,11,12	1.63	1 (10%)	8,13,15	0.55	0
63	FME	1x	115	55	8,9,10	0.42	0	8,9,11	1.62	2 (25%)
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		
62	PHE	1w	109	54	10,11,12	1.55	1 (10%)	8,13,15	0.54	0

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
63	FME	2x	108	55	-	0/7/9/11	-
59	A1AE1	1A	4094	57	-	13/89/132/132	0/7/7/7
59	A1AE1	2A	3855	57	-	14/89/132/132	0/7/7/7
62	PHE	2w	108	54	-	3/5/6/8	0/1/1/1
63	FME	1x	115	55	-	1/7/9/11	-
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	303	35	-	-	0/6/5/5
62	PHE	1w	109	54	-	1/5/6/8	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4094	A1AE1	CAG-CAF	-12.78	1.41	1.53
59	2A	3855	A1AE1	CAG-CAF	-11.71	1.42	1.53
59	2A	3855	A1AE1	CAB-CAF	-7.13	1.40	1.52
59	1A	4094	A1AE1	CAB-CAF	-6.88	1.40	1.52
59	1A	4094	A1AE1	OBR-NBJ	5.87	1.54	1.40

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3855	A1AE1	CAB-CAF-NBJ	-12.26	117.17	126.21
59	1A	4094	A1AE1	CAB-CAF-NBJ	-10.52	118.45	126.21
59	1A	4094	A1AE1	OBB-CBT-NBV	6.79	122.08	111.01
59	2A	3855	A1AE1	OBB-CBT-NBV	6.34	121.34	111.01
59	1A	4094	A1AE1	CAK-OBB-CBT	-5.76	108.58	117.04

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

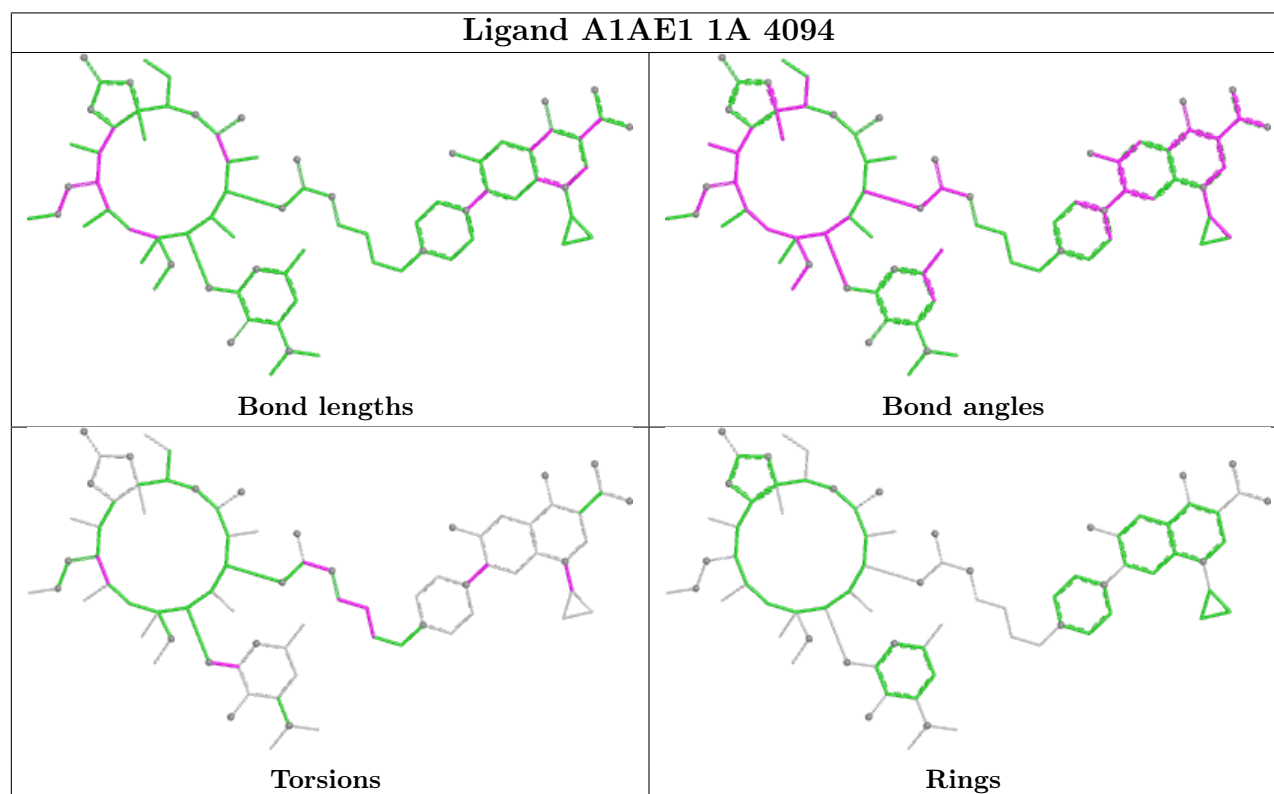
Mol	Chain	Res	Type	Atoms
62	1w	109	PHE	O-C-CA-CB
62	2w	108	PHE	O-C-CA-CB
59	1A	4094	A1AE1	CBZ-CBY-NBX-CCX
59	2A	3855	A1AE1	CBZ-CBY-NBX-CCX
59	1A	4094	A1AE1	CCJ-CCI-NCH-CCG

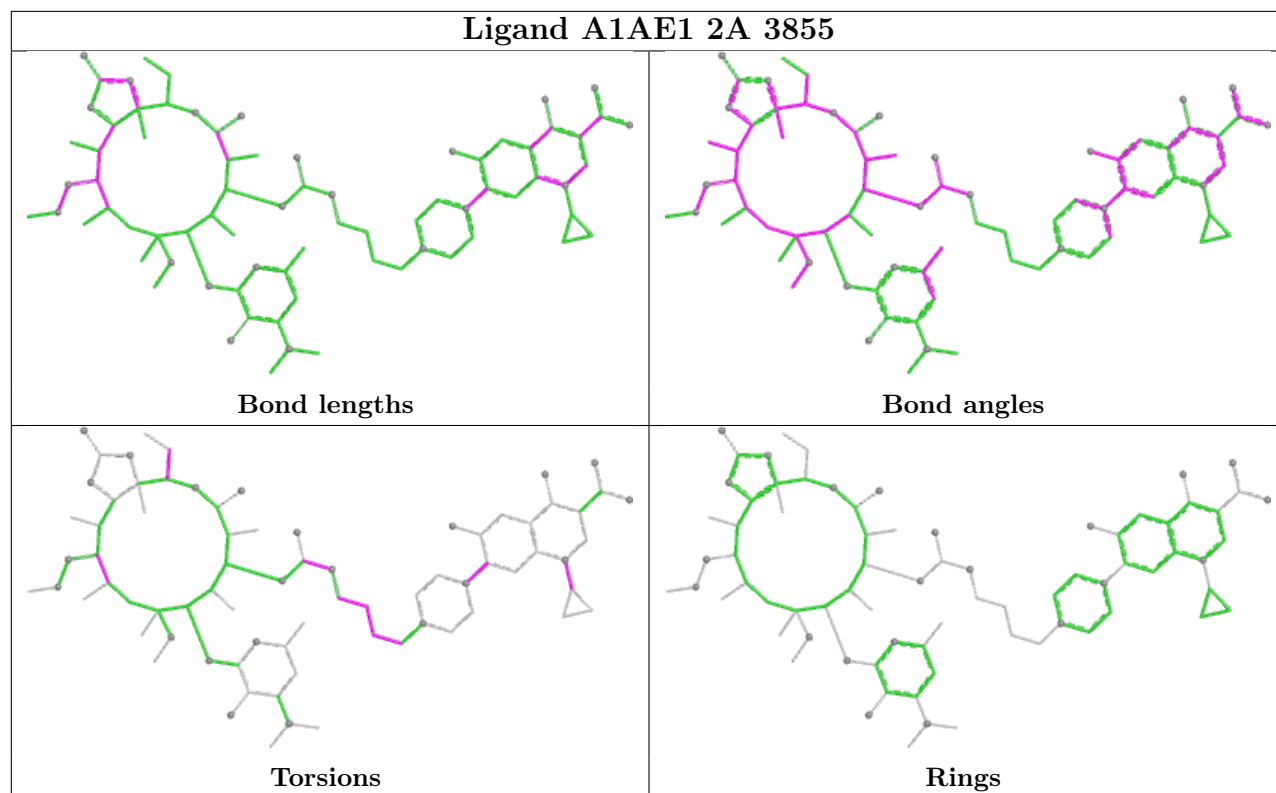
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2A	3855	A1AE1	1	0
62	2w	108	PHE	1	0
61	2d	303	SF4	4	0
62	1w	109	PHE	1	0

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%)	-0.34	215 (7%) 22 20	20, 37, 89, 98	0
1	2A	2788/2915 (95%)	0.16	173 (6%) 28 25	33, 55, 87, 97	0
2	1B	120/121 (99%)	-0.12	1 (0%) 82 80	34, 50, 65, 81	0
2	2B	120/121 (99%)	0.79	0 100 100	58, 69, 77, 84	0
3	1D	275/276 (99%)	-0.19	3 (1%) 77 75	24, 38, 52, 72	0
3	2D	275/276 (99%)	0.11	4 (1%) 71 68	30, 48, 59, 81	0
4	1E	204/206 (99%)	-0.15	2 (0%) 79 76	21, 40, 58, 72	0
4	2E	204/206 (99%)	0.44	2 (0%) 79 76	36, 57, 68, 75	0
5	1F	203/210 (96%)	-0.06	3 (1%) 71 68	20, 43, 66, 77	0
5	2F	203/210 (96%)	0.49	5 (2%) 58 55	33, 62, 75, 79	0
6	1G	181/182 (99%)	0.54	8 (4%) 39 37	42, 56, 69, 78	0
6	2G	181/182 (99%)	1.17	19 (10%) 13 11	58, 71, 79, 84	0
7	1H	174/180 (96%)	0.40	6 (3%) 48 45	40, 52, 64, 72	0
7	2H	174/180 (96%)	1.58	49 (28%) 1 2	65, 77, 83, 88	0
8	1I	146/148 (98%)	0.94	9 (6%) 28 25	46, 67, 76, 80	0
8	2I	146/148 (98%)	1.15	14 (9%) 15 13	50, 68, 76, 80	0
9	1N	140/140 (100%)	-0.08	2 (1%) 73 70	26, 39, 60, 69	0
9	2N	140/140 (100%)	0.69	5 (3%) 46 43	46, 61, 73, 82	0
10	1O	122/122 (100%)	-0.24	0 100 100	29, 40, 58, 62	0
10	2O	122/122 (100%)	0.39	0 100 100	47, 57, 67, 72	0
11	1P	149/150 (99%)	0.08	3 (2%) 64 61	22, 49, 67, 71	0
11	2P	149/150 (99%)	0.85	14 (9%) 15 14	37, 63, 77, 80	0
12	1Q	141/141 (100%)	-0.14	2 (1%) 73 70	25, 41, 56, 69	0
12	2Q	141/141 (100%)	0.90	12 (8%) 18 17	44, 62, 71, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.43	0 100 100	26, 35, 48, 56	0
13	2R	118/118 (100%)	0.28	0 100 100	41, 52, 62, 68	0
14	1S	110/112 (98%)	0.34	1 (0%) 81 78	39, 50, 61, 65	0
14	2S	110/112 (98%)	1.04	13 (11%) 10 9	58, 65, 73, 78	0
15	1T	131/146 (89%)	0.10	2 (1%) 71 68	33, 45, 66, 74	0
15	2T	131/146 (89%)	0.63	5 (3%) 44 42	50, 60, 71, 77	0
16	1U	116/118 (98%)	-0.49	0 100 100	23, 31, 47, 62	0
16	2U	116/118 (98%)	0.53	1 (0%) 81 78	43, 58, 69, 74	0
17	1V	101/101 (100%)	-0.34	1 (0%) 79 76	25, 39, 55, 65	0
17	2V	101/101 (100%)	0.86	2 (1%) 64 61	42, 66, 73, 80	0
18	1W	112/113 (99%)	-0.36	1 (0%) 81 78	26, 33, 50, 77	0
18	2W	112/113 (99%)	0.20	2 (1%) 67 63	41, 49, 62, 82	0
19	1X	95/96 (98%)	-0.05	3 (3%) 50 47	30, 41, 63, 77	0
19	2X	95/96 (98%)	0.42	2 (2%) 63 60	45, 57, 71, 78	0
20	1Y	107/110 (97%)	0.38	4 (3%) 45 43	39, 51, 63, 73	0
20	2Y	107/110 (97%)	1.10	14 (13%) 8 7	54, 66, 76, 80	0
21	1Z	154/206 (74%)	0.91	25 (16%) 5 5	41, 62, 78, 82	0
21	2Z	160/206 (77%)	1.80	50 (31%) 1 1	63, 75, 82, 88	0
22	10	83/85 (97%)	-0.08	1 (1%) 76 73	28, 37, 51, 64	0
22	20	83/85 (97%)	0.79	4 (4%) 36 34	38, 58, 66, 75	0
23	11	97/98 (98%)	0.34	2 (2%) 63 60	30, 50, 69, 75	0
23	21	97/98 (98%)	0.46	3 (3%) 51 48	40, 54, 69, 75	0
24	12	70/72 (97%)	0.29	3 (4%) 40 38	35, 49, 59, 68	0
24	22	70/72 (97%)	0.81	3 (4%) 40 38	58, 66, 74, 75	0
25	13	59/60 (98%)	-0.19	1 (1%) 69 65	25, 36, 60, 72	0
25	23	59/60 (98%)	0.70	4 (6%) 25 22	51, 61, 71, 77	0
26	14	69/71 (97%)	1.30	16 (23%) 2 3	49, 71, 81, 85	0
26	24	69/71 (97%)	1.74	22 (31%) 1 1	70, 77, 84, 87	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 65	22, 34, 53, 58	0
27	25	59/60 (98%)	0.25	3 (5%) 34 32	38, 49, 64, 75	0
28	16	53/54 (98%)	-0.14	0 100 100	33, 44, 56, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.59	2 (3%) 44 42	47, 57, 63, 66	0
29	17	48/49 (97%)	-0.29	3 (6%) 27 25	21, 29, 55, 62	0
29	27	48/49 (97%)	0.06	1 (2%) 63 60	32, 41, 61, 69	0
30	18	64/65 (98%)	-0.42	0 100 100	28, 36, 43, 57	0
30	28	64/65 (98%)	0.34	1 (1%) 70 67	44, 51, 58, 63	0
31	19	37/37 (100%)	-0.15	0 100 100	31, 39, 51, 58	0
31	29	37/37 (100%)	0.93	1 (2%) 56 53	58, 64, 72, 77	0
32	1a	1488/1521 (97%)	0.46	83 (5%) 31 28	36, 62, 85, 97	0
32	2a	1491/1521 (98%)	0.73	112 (7%) 22 20	45, 69, 86, 97	0
33	1b	231/256 (90%)	1.42	50 (21%) 3 3	60, 73, 80, 84	0
33	2b	231/256 (90%)	1.59	65 (28%) 2 2	64, 76, 81, 86	0
34	1c	206/239 (86%)	1.03	17 (8%) 19 17	56, 67, 77, 81	0
34	2c	206/239 (86%)	1.43	38 (18%) 4 4	65, 74, 81, 86	0
35	1d	208/209 (99%)	1.03	19 (9%) 16 14	53, 65, 72, 80	0
35	2d	208/209 (99%)	0.96	18 (8%) 17 16	55, 65, 73, 79	0
36	1e	148/162 (91%)	0.71	5 (3%) 48 45	48, 61, 69, 73	0
36	2e	148/162 (91%)	1.21	15 (10%) 14 12	59, 68, 74, 80	0
37	1f	100/101 (99%)	0.87	4 (4%) 43 40	54, 64, 70, 73	0
37	2f	100/101 (99%)	0.86	4 (4%) 43 40	55, 63, 71, 75	0
38	1g	155/156 (99%)	0.90	17 (10%) 12 10	57, 66, 78, 81	0
38	2g	155/156 (99%)	1.26	21 (13%) 8 7	65, 72, 78, 82	0
39	1h	137/138 (99%)	0.66	4 (2%) 54 50	51, 63, 70, 73	0
39	2h	137/138 (99%)	1.07	12 (8%) 17 16	60, 69, 75, 78	0
40	1i	127/128 (99%)	1.34	21 (16%) 5 5	51, 71, 77, 80	0
40	2i	127/128 (99%)	1.77	44 (34%) 1 1	62, 75, 81, 83	0
41	1j	97/105 (92%)	1.49	20 (20%) 3 3	53, 71, 81, 85	0
41	2j	96/105 (91%)	2.14	53 (55%) 0 0	66, 77, 83, 85	0
42	1k	114/129 (88%)	0.63	6 (5%) 33 30	42, 63, 71, 78	0
42	2k	114/129 (88%)	0.95	11 (9%) 15 13	54, 67, 74, 76	0
43	1l	121/132 (91%)	0.38	4 (3%) 49 46	42, 50, 61, 69	0
43	2l	121/132 (91%)	0.75	7 (5%) 30 27	53, 60, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.06	11 (8%) 17 15	50, 65, 72, 84	0
44	2m	122/126 (96%)	1.62	30 (24%) 2 2	65, 74, 78, 82	0
45	1n	60/61 (98%)	1.02	4 (6%) 25 23	55, 62, 68, 71	0
45	2n	60/61 (98%)	2.17	30 (50%) 0 0	68, 75, 79, 83	0
46	1o	88/89 (98%)	0.76	5 (5%) 30 28	45, 62, 70, 74	0
46	2o	88/89 (98%)	0.92	7 (7%) 20 18	56, 66, 75, 80	0
47	1p	82/88 (93%)	1.37	14 (17%) 5 5	54, 66, 71, 79	0
47	2p	82/88 (93%)	1.04	4 (4%) 36 33	56, 65, 72, 75	0
48	1q	99/105 (94%)	0.83	1 (1%) 79 76	55, 63, 71, 74	0
48	2q	99/105 (94%)	0.85	5 (5%) 34 32	59, 67, 74, 78	0
49	1r	68/88 (77%)	0.53	1 (1%) 71 68	52, 63, 72, 74	0
49	2r	68/88 (77%)	0.67	2 (2%) 54 50	58, 65, 73, 77	0
50	1s	83/93 (89%)	1.19	10 (12%) 10 8	60, 67, 74, 78	0
50	2s	83/93 (89%)	1.65	22 (26%) 2 2	71, 77, 81, 88	0
51	1t	96/106 (90%)	1.01	13 (13%) 8 7	57, 65, 74, 78	0
51	2t	96/106 (90%)	1.04	13 (13%) 8 7	57, 65, 75, 78	0
52	1u	23/27 (85%)	1.15	3 (13%) 9 7	54, 62, 66, 68	0
52	2u	23/27 (85%)	2.19	14 (60%) 0 0	66, 72, 75, 78	0
53	1v	13/24 (54%)	0.62	2 (15%) 6 6	47, 52, 82, 85	0
53	2v	13/24 (54%)	1.25	3 (23%) 2 3	57, 66, 86, 93	0
54	1w	66/76 (86%)	1.78	25 (37%) 1 1	29, 80, 90, 92	0
54	2w	64/76 (84%)	1.67	18 (28%) 2 2	45, 85, 90, 94	0
55	1x	72/77 (93%)	0.23	2 (2%) 55 51	25, 56, 75, 83	0
55	2x	72/77 (93%)	0.65	2 (2%) 55 51	39, 69, 80, 89	0
56	1y	67/76 (88%)	2.10	34 (50%) 0 0	61, 90, 95, 97	0
56	2y	66/76 (86%)	2.26	45 (68%) 0 0	67, 91, 94, 96	0
All	All	20871/21748 (95%)	0.48	1718 (8%) 19 17	20, 60, 82, 98	0

The worst 5 of 1718 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	652(U)	G	9.7
1	2A	652(V)	C	8.7

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Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	8.5
1	1A	652(C)	G	8.4
1	1A	653	A	8.4

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($\text{\AA}^2$)	Q<0.9
56	4SU	2y	8	20/21	0.42	0.22	89,98,103,117	0
56	G7M	1y	46	24/25	0.52	0.20	86,91,98,109	0
56	G7M	2y	46	24/25	0.52	0.18	80,89,97,113	0
56	PSU	2y	55	20/21	0.56	0.18	86,91,95,96	0
56	PSU	1y	55	20/21	0.61	0.15	85,89,96,106	0
56	MIA	2y	37	22/30	0.61	0.16	80,87,99,111	0
56	4SU	1y	8	20/21	0.64	0.16	87,92,102,110	0
56	5MU	1y	54	21/22	0.65	0.15	80,86,92,104	0
56	5MU	2y	54	21/22	0.66	0.18	83,89,100,110	0
56	PSU	2y	39	20/21	0.66	0.16	82,86,95,101	0
56	MIA	1y	37	22/30	0.69	0.15	81,86,92,99	0
54	G7M	2w	46	24/25	0.73	0.20	79,88,97,115	0
56	PSU	1y	39	20/21	0.74	0.16	78,84,91,95	0
54	G7M	1w	46	24/25	0.75	0.17	67,79,94,112	0
56	PSU	1y	32	20/21	0.78	0.14	74,84,96,96	0
56	PSU	2y	32	20/21	0.79	0.12	78,83,93,103	0
54	4SU	2w	8	20/21	0.80	0.17	82,87,99,99	0
54	PSU	2w	55	20/21	0.84	0.12	65,77,83,87	0
54	4SU	1w	8	20/21	0.85	0.16	75,79,87,88	0
54	MIA	2w	37	25/30	0.88	0.15	59,70,78,93	0
32	2MG	2a	1207	24/25	0.89	0.13	64,78,80,81	0
54	PSU	2w	32	20/21	0.89	0.13	64,77,81,82	0
43	0TD	2l	92	10/11	0.89	0.14	57,60,71,78	0
54	PSU	1w	55	20/21	0.90	0.11	49,68,71,73	0
55	PSU	2x	55	20/21	0.90	0.11	63,71,77,82	0
32	G7M	2a	527	24/25	0.90	0.14	55,60,65,72	0
54	5MU	2w	54	21/22	0.91	0.11	68,73,77,80	0
54	MIA	1w	37	29/30	0.91	0.17	44,53,68,84	0
55	4SU	2x	8	20/21	0.92	0.12	65,70,73,74	0
55	5MC	2x	32	21/22	0.92	0.13	59,64,69,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	967	21/22	0.92	0.13	58,64,70,74	0
1	5MU	2A	1915	21/22	0.92	0.11	57,63,68,68	0
54	PSU	2w	39	20/21	0.92	0.12	63,73,79,79	0
55	PSU	1x	55	20/21	0.93	0.10	57,59,70,74	0
43	0TD	1l	92	10/11	0.93	0.11	40,48,50,65	0
32	M2G	2a	966	25/26	0.93	0.14	55,62,73,76	0
55	5MU	2x	54	21/22	0.93	0.12	64,74,77,78	0
54	PSU	1w	32	20/21	0.94	0.12	56,61,67,68	0
55	4SU	1x	8	20/21	0.94	0.10	54,60,69,71	0
55	5MU	1x	54	21/22	0.94	0.10	58,63,68,72	0
1	PSU	2A	1917	20/21	0.94	0.09	51,58,67,68	0
32	5MC	2a	1400	21/22	0.94	0.14	55,62,69,73	0
32	PSU	2a	516	20/21	0.94	0.11	56,65,70,71	0
32	MA6	1a	1519	24/25	0.95	0.10	35,44,48,56	0
1	5MU	1A	1915	21/22	0.95	0.10	41,50,55,55	0
1	OMC	2A	1920	21/22	0.95	0.10	49,56,60,64	0
32	4OC	2a	1402	22/23	0.95	0.10	50,55,59,64	0
32	5MC	2a	1404	21/22	0.95	0.09	45,50,54,58	0
55	5MC	1x	32	21/22	0.95	0.11	45,51,57,63	0
32	2MG	1a	1207	24/25	0.95	0.10	60,65,68,69	0
1	PSU	2A	1911	20/21	0.95	0.09	49,59,65,65	0
1	5MC	2A	1962	21/22	0.96	0.09	41,49,52,65	0
54	8AN	2w	76	22/23	0.96	0.09	35,40,43,47	0
32	5MC	2a	1407	21/22	0.96	0.10	44,51,55,58	0
32	UR3	2a	1498	21/22	0.96	0.10	49,55,57,59	0
32	MA6	2a	1518	24/25	0.96	0.10	50,58,62,63	0
32	MA6	2a	1519	24/25	0.96	0.12	52,58,61,63	0
55	8AN	2x	76	22/23	0.96	0.09	33,39,45,58	0
32	5MC	1a	967	21/22	0.96	0.09	43,52,56,61	0
1	5MC	1A	1942	21/22	0.96	0.09	27,39,43,54	0
54	PSU	1w	39	20/21	0.96	0.08	51,59,64,74	0
32	PSU	1a	516	20/21	0.96	0.08	41,53,57,58	0
54	5MU	1w	54	21/22	0.96	0.10	39,55,65,68	0
32	G7M	1a	527	24/25	0.96	0.09	36,42,48,50	0
32	M2G	1a	966	25/26	0.96	0.10	43,50,54,56	0
1	MA6	2A	2058	24/25	0.97	0.09	31,40,49,56	0
1	OMU	2A	2552	21/22	0.97	0.08	38,44,48,54	0
1	PSU	2A	2605	20/21	0.97	0.07	34,40,42,43	0
1	PSU	1A	1911	20/21	0.97	0.08	41,45,50,52	0
55	8AN	1x	76	22/23	0.97	0.07	20,25,30,37	0
1	PSU	1A	1917	20/21	0.97	0.07	40,47,51,53	0
32	5MC	1a	1400	21/22	0.97	0.09	42,48,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.10	39,43,46,47	0
32	5MC	1a	1404	21/22	0.97	0.08	29,39,42,44	0
1	5MU	2A	1939	21/22	0.97	0.08	28,39,44,46	0
1	5MC	2A	1942	21/22	0.97	0.08	44,51,56,61	0
32	5MC	1a	1407	21/22	0.97	0.08	33,38,44,46	0
1	PSU	1A	2605	20/21	0.98	0.06	24,28,31,34	0
1	5MU	1A	1939	21/22	0.98	0.06	21,28,32,33	0
1	OMC	1A	1920	21/22	0.98	0.08	37,43,47,50	0
32	UR3	1a	1498	21/22	0.98	0.07	36,41,43,44	0
32	MA6	1a	1518	24/25	0.98	0.08	33,41,44,45	0
1	5MC	1A	1962	21/22	0.98	0.06	26,34,41,42	0
1	MA6	1A	2058	24/25	0.98	0.07	15,26,33,36	0
1	OMG	2A	2251	24/25	0.98	0.08	36,42,44,46	0
1	2MA	2A	2503	23/24	0.98	0.08	29,40,43,47	0
1	2MA	1A	2503	23/24	0.98	0.06	18,24,26,29	0
1	OMU	1A	2552	21/22	0.98	0.07	25,28,31,34	0
54	8AN	1w	76	22/23	0.99	0.06	19,25,26,27	0
1	OMG	1A	2251	24/25	0.99	0.04	21,24,27,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
57	MG	2A	3400	1/1	0.43	0.42	88,88,88,88	0
57	MG	10	108	1/1	0.47	0.41	62,62,62,62	0
57	MG	20	102	1/1	0.55	0.31	69,69,69,69	0
57	MG	2y	103	1/1	0.58	0.20	80,80,80,80	0
57	MG	1B	221	1/1	0.61	0.29	64,64,64,64	0
57	MG	2A	3642	1/1	0.61	0.26	66,66,66,66	0
57	MG	1A	3227	1/1	0.61	0.17	66,66,66,66	0
57	MG	1a	1761	1/1	0.61	0.22	73,73,73,73	0
57	MG	1A	4028	1/1	0.62	0.37	76,76,76,76	0
57	MG	2A	3747	1/1	0.64	0.22	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3655	1/1	0.64	0.24	53,53,53,53	0
57	MG	1A	3694	1/1	0.64	0.24	69,69,69,69	0
57	MG	1A	3970	1/1	0.65	0.27	61,61,61,61	0
57	MG	2A	3364	1/1	0.65	0.57	79,79,79,79	0
57	MG	2a	1618	1/1	0.65	0.34	80,80,80,80	0
57	MG	2A	3696	1/1	0.65	0.22	69,69,69,69	0
57	MG	2A	3614	1/1	0.66	0.29	67,67,67,67	0
57	MG	2A	3088	1/1	0.66	0.27	76,76,76,76	0
57	MG	2A	3763	1/1	0.66	0.20	64,64,64,64	0
57	MG	2y	105	1/1	0.66	0.33	82,82,82,82	0
57	MG	1A	3961	1/1	0.67	0.17	73,73,73,73	0
57	MG	1A	3481	1/1	0.67	0.22	59,59,59,59	0
57	MG	1a	1799	1/1	0.67	0.27	71,71,71,71	0
57	MG	2a	1782	1/1	0.68	0.29	73,73,73,73	0
57	MG	1A	4005	1/1	0.68	0.22	52,52,52,52	0
57	MG	1A	3660	1/1	0.68	0.27	72,72,72,72	0
57	MG	2a	1784	1/1	0.69	0.36	77,77,77,77	0
57	MG	2a	1793	1/1	0.69	0.35	73,73,73,73	0
57	MG	2v	103	1/1	0.69	0.31	78,78,78,78	0
57	MG	1A	3556	1/1	0.69	0.16	32,32,32,32	0
57	MG	1B	222	1/1	0.69	0.19	54,54,54,54	0
57	MG	2a	1619	1/1	0.70	0.18	68,68,68,68	0
57	MG	2a	1780	1/1	0.70	0.30	76,76,76,76	0
57	MG	2A	3647	1/1	0.70	0.20	69,69,69,69	0
57	MG	2A	3497	1/1	0.70	0.35	76,76,76,76	0
57	MG	2A	3345	1/1	0.71	0.27	77,77,77,77	0
57	MG	2A	3450	1/1	0.71	0.34	76,76,76,76	0
57	MG	1B	229	1/1	0.71	0.27	74,74,74,74	0
57	MG	2A	3591	1/1	0.71	0.26	66,66,66,66	0
57	MG	2a	1761	1/1	0.72	0.44	71,71,71,71	0
57	MG	1A	3985	1/1	0.72	0.17	59,59,59,59	0
57	MG	1A	3589	1/1	0.72	0.19	76,76,76,76	0
57	MG	1A	3465	1/1	0.72	0.25	74,74,74,74	0
57	MG	1B	230	1/1	0.72	0.17	73,73,73,73	0
57	MG	1U	209	1/1	0.72	0.42	64,64,64,64	0
57	MG	1A	4051	1/1	0.72	0.20	74,74,74,74	0
57	MG	2a	1706	1/1	0.72	0.27	76,76,76,76	0
57	MG	2A	3618	1/1	0.73	0.24	73,73,73,73	0
57	MG	1A	3535	1/1	0.73	0.21	65,65,65,65	0
57	MG	1E	313	1/1	0.73	0.28	66,66,66,66	0
57	MG	1T	202	1/1	0.73	0.23	66,66,66,66	0
57	MG	1A	3980	1/1	0.73	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3965	1/1	0.73	0.15	79,79,79,79	0
57	MG	1a	1649	1/1	0.74	0.23	68,68,68,68	0
57	MG	1A	4011	1/1	0.74	0.13	63,63,63,63	0
57	MG	1A	3367	1/1	0.74	0.25	68,68,68,68	0
57	MG	1A	4034	1/1	0.74	0.26	68,68,68,68	0
57	MG	2A	3588	1/1	0.74	0.26	73,73,73,73	0
57	MG	1A	3929	1/1	0.74	0.14	40,40,40,40	0
57	MG	2a	1766	1/1	0.74	0.20	71,71,71,71	0
57	MG	2A	3276	1/1	0.75	0.34	72,72,72,72	0
57	MG	1A	3941	1/1	0.75	0.22	48,48,48,48	0
57	MG	1A	3973	1/1	0.75	0.14	48,48,48,48	0
57	MG	1A	3918	1/1	0.75	0.22	74,74,74,74	0
57	MG	2a	1776	1/1	0.75	0.30	72,72,72,72	0
57	MG	2A	3690	1/1	0.75	0.14	64,64,64,64	0
57	MG	1A	3571	1/1	0.75	0.19	58,58,58,58	0
57	MG	1A	3997	1/1	0.75	0.23	59,59,59,59	0
57	MG	2A	3539	1/1	0.75	0.20	59,59,59,59	0
57	MG	2j	201	1/1	0.75	0.15	76,76,76,76	0
57	MG	2l	203	1/1	0.75	0.21	71,71,71,71	0
57	MG	2A	3818	1/1	0.75	0.23	73,73,73,73	0
57	MG	2w	107	1/1	0.75	0.27	79,79,79,79	0
57	MG	1x	107	1/1	0.75	0.14	70,70,70,70	0
57	MG	1B	207	1/1	0.75	0.21	69,69,69,69	0
57	MG	2A	3183	1/1	0.76	0.28	80,80,80,80	0
57	MG	2A	3718	1/1	0.76	0.18	44,44,44,44	0
57	MG	1A	3972	1/1	0.76	0.22	66,66,66,66	0
57	MG	2A	3277	1/1	0.76	0.41	79,79,79,79	0
57	MG	2A	3605	1/1	0.76	0.19	46,46,46,46	0
57	MG	2A	3841	1/1	0.76	0.19	68,68,68,68	0
57	MG	1A	3926	1/1	0.76	0.17	73,73,73,73	0
57	MG	1A	4077	1/1	0.76	0.19	64,64,64,64	0
57	MG	2l	205	1/1	0.76	0.25	72,72,72,72	0
57	MG	1A	3764	1/1	0.76	0.12	53,53,53,53	0
57	MG	1B	220	1/1	0.76	0.17	68,68,68,68	0
57	MG	2a	1721	1/1	0.76	0.28	75,75,75,75	0
57	MG	1A	3628	1/1	0.76	0.31	70,70,70,70	0
57	MG	2A	3712	1/1	0.77	0.19	39,39,39,39	0
57	MG	2a	1722	1/1	0.77	0.20	75,75,75,75	0
57	MG	2a	1735	1/1	0.77	0.14	85,85,85,85	0
57	MG	2A	3291	1/1	0.77	0.32	61,61,61,61	0
57	MG	2a	1603	1/1	0.77	0.17	76,76,76,76	0
57	MG	2a	1767	1/1	0.77	0.22	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3318	1/1	0.77	0.20	78,78,78,78	0
57	MG	2A	3569	1/1	0.77	0.18	71,71,71,71	0
57	MG	1a	1749	1/1	0.77	0.17	70,70,70,70	0
57	MG	2a	1716	1/1	0.78	0.26	79,79,79,79	0
57	MG	2A	3651	1/1	0.78	0.25	60,60,60,60	0
57	MG	2A	3512	1/1	0.78	0.17	53,53,53,53	0
57	MG	1A	3903	1/1	0.78	0.15	57,57,57,57	0
57	MG	2A	3547	1/1	0.78	0.17	61,61,61,61	0
57	MG	2A	3560	1/1	0.78	0.16	64,64,64,64	0
57	MG	2A	3563	1/1	0.78	0.18	60,60,60,60	0
57	MG	1A	3712	1/1	0.78	0.12	33,33,33,33	0
57	MG	2A	3805	1/1	0.78	0.21	68,68,68,68	0
57	MG	2A	3307	1/1	0.78	0.19	66,66,66,66	0
57	MG	2A	3821	1/1	0.78	0.24	72,72,72,72	0
57	MG	1A	3507	1/1	0.78	0.52	71,71,71,71	0
57	MG	2a	1797	1/1	0.78	0.36	74,74,74,74	0
57	MG	2A	3851	1/1	0.78	0.16	65,65,65,65	0
57	MG	1w	106	1/1	0.78	0.25	83,83,83,83	0
57	MG	1V	208	1/1	0.78	0.16	59,59,59,59	0
57	MG	1A	3892	1/1	0.78	0.11	70,70,70,70	0
57	MG	15	106	1/1	0.78	0.25	54,54,54,54	0
57	MG	1A	3897	1/1	0.78	0.22	59,59,59,59	0
57	MG	2a	1708	1/1	0.78	0.39	75,75,75,75	0
57	MG	2A	3355	1/1	0.79	0.30	71,71,71,71	0
57	MG	2a	1666	1/1	0.79	0.29	68,68,68,68	0
57	MG	1A	3547	1/1	0.79	0.17	64,64,64,64	0
57	MG	2A	3625	1/1	0.79	0.27	79,79,79,79	0
57	MG	2A	3101	1/1	0.79	0.19	73,73,73,73	0
57	MG	2A	3420	1/1	0.79	0.15	70,70,70,70	0
57	MG	2A	3106	1/1	0.79	0.19	76,76,76,76	0
57	MG	2A	3663	1/1	0.79	0.16	84,84,84,84	0
57	MG	2A	3469	1/1	0.79	0.34	78,78,78,78	0
57	MG	2A	3149	1/1	0.79	0.42	79,79,79,79	0
57	MG	2A	3709	1/1	0.79	0.22	76,76,76,76	0
57	MG	2A	3502	1/1	0.79	0.17	57,57,57,57	0
57	MG	1A	3762	1/1	0.79	0.25	64,64,64,64	0
57	MG	1a	1696	1/1	0.79	0.22	60,60,60,60	0
57	MG	1A	3920	1/1	0.79	0.14	73,73,73,73	0
57	MG	2A	3556	1/1	0.79	0.17	78,78,78,78	0
57	MG	1A	3485	1/1	0.79	0.16	65,65,65,65	0
57	MG	2A	3299	1/1	0.79	0.22	71,71,71,71	0
57	MG	2A	3829	1/1	0.79	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3477	1/1	0.79	0.29	74,74,74,74	0
57	MG	1A	3188	1/1	0.79	0.15	74,74,74,74	0
57	MG	1B	228	1/1	0.79	0.17	67,67,67,67	0
57	MG	2A	3598	1/1	0.79	0.21	51,51,51,51	0
57	MG	2A	3354	1/1	0.79	0.25	74,74,74,74	0
57	MG	1A	3438	1/1	0.80	0.17	63,63,63,63	0
57	MG	1a	1737	1/1	0.80	0.22	60,60,60,60	0
57	MG	2B	210	1/1	0.80	0.17	82,82,82,82	0
57	MG	1A	3478	1/1	0.80	0.18	70,70,70,70	0
57	MG	2A	3579	1/1	0.80	0.16	54,54,54,54	0
57	MG	2a	1610	1/1	0.80	0.34	70,70,70,70	0
57	MG	1A	3888	1/1	0.80	0.16	65,65,65,65	0
57	MG	1A	3702	1/1	0.80	0.16	68,68,68,68	0
57	MG	2a	1660	1/1	0.80	0.27	70,70,70,70	0
57	MG	1O	206	1/1	0.80	0.29	66,66,66,66	0
57	MG	2a	1684	1/1	0.80	0.31	69,69,69,69	0
57	MG	2a	1689	1/1	0.80	0.29	67,67,67,67	0
57	MG	1A	3976	1/1	0.80	0.22	60,60,60,60	0
57	MG	2A	3611	1/1	0.80	0.17	65,65,65,65	0
57	MG	2A	3346	1/1	0.80	0.16	67,67,67,67	0
57	MG	2A	3073	1/1	0.80	0.18	57,57,57,57	0
57	MG	1A	3375	1/1	0.80	0.25	68,68,68,68	0
57	MG	1B	214	1/1	0.80	0.16	61,61,61,61	0
57	MG	2A	3386	1/1	0.80	0.31	67,67,67,67	0
57	MG	2A	3392	1/1	0.80	0.16	65,65,65,65	0
57	MG	1A	3948	1/1	0.80	0.14	68,68,68,68	0
57	MG	2A	3403	1/1	0.80	0.14	70,70,70,70	0
57	MG	2A	3124	1/1	0.80	0.12	71,71,71,71	0
57	MG	2A	3704	1/1	0.80	0.09	82,82,82,82	0
57	MG	2A	3434	1/1	0.80	0.21	61,61,61,61	0
57	MG	1A	3754	1/1	0.80	0.23	58,58,58,58	0
57	MG	1A	3964	1/1	0.80	0.19	59,59,59,59	0
57	MG	2A	3186	1/1	0.80	0.12	69,69,69,69	0
57	MG	2A	3217	1/1	0.80	0.17	67,67,67,67	0
57	MG	2A	3235	1/1	0.80	0.42	76,76,76,76	0
57	MG	2A	3243	1/1	0.80	0.29	65,65,65,65	0
57	MG	2A	3272	1/1	0.80	0.15	71,71,71,71	0
57	MG	2A	3274	1/1	0.80	0.14	69,69,69,69	0
57	MG	2y	104	1/1	0.80	0.28	82,82,82,82	0
57	MG	2A	3832	1/1	0.80	0.17	64,64,64,64	0
57	MG	1A	3746	1/1	0.81	0.20	64,64,64,64	0
57	MG	2A	3670	1/1	0.81	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1670	1/1	0.81	0.41	74,74,74,74	0
57	MG	1A	4010	1/1	0.81	0.16	69,69,69,69	0
57	MG	1A	3632	1/1	0.81	0.12	66,66,66,66	0
57	MG	2a	1690	1/1	0.81	0.26	64,64,64,64	0
57	MG	2a	1695	1/1	0.81	0.28	68,68,68,68	0
57	MG	1A	3267	1/1	0.81	0.16	66,66,66,66	0
57	MG	2A	3343	1/1	0.81	0.10	81,81,81,81	0
57	MG	1A	3164	1/1	0.81	0.20	73,73,73,73	0
57	MG	1a	1744	1/1	0.81	0.18	68,68,68,68	0
57	MG	1A	4046	1/1	0.81	0.19	72,72,72,72	0
57	MG	2a	1728	1/1	0.81	0.15	68,68,68,68	0
57	MG	2A	3760	1/1	0.81	0.22	76,76,76,76	0
57	MG	2A	3761	1/1	0.81	0.20	72,72,72,72	0
57	MG	2A	3571	1/1	0.81	0.24	70,70,70,70	0
57	MG	2A	3205	1/1	0.81	0.22	69,69,69,69	0
57	MG	1A	3812	1/1	0.81	0.19	57,57,57,57	0
57	MG	2A	3372	1/1	0.81	0.22	74,74,74,74	0
57	MG	1A	4055	1/1	0.81	0.12	59,59,59,59	0
57	MG	2a	1783	1/1	0.81	0.32	65,65,65,65	0
57	MG	1A	3853	1/1	0.81	0.14	45,45,45,45	0
57	MG	2a	1787	1/1	0.81	0.24	62,62,62,62	0
57	MG	2A	3255	1/1	0.81	0.17	68,68,68,68	0
57	MG	2A	3263	1/1	0.81	0.38	73,73,73,73	0
57	MG	2a	1798	1/1	0.81	0.26	68,68,68,68	0
57	MG	2B	202	1/1	0.81	0.17	67,67,67,67	0
57	MG	1A	3925	1/1	0.81	0.14	74,74,74,74	0
57	MG	2N	201	1/1	0.81	0.13	76,76,76,76	0
57	MG	2A	3623	1/1	0.81	0.21	66,66,66,66	0
57	MG	1x	111	1/1	0.81	0.24	71,71,71,71	0
57	MG	2A	3046	1/1	0.81	0.29	68,68,68,68	0
57	MG	1A	4004	1/1	0.81	0.13	37,37,37,37	0
57	MG	2A	3278	1/1	0.81	0.25	73,73,73,73	0
57	MG	1A	3341	1/1	0.82	0.15	65,65,65,65	0
57	MG	2A	3621	1/1	0.82	0.22	69,69,69,69	0
57	MG	1A	3669	1/1	0.82	0.21	59,59,59,59	0
57	MG	1A	3874	1/1	0.82	0.13	48,48,48,48	0
57	MG	1A	4031	1/1	0.82	0.13	54,54,54,54	0
57	MG	1A	3887	1/1	0.82	0.13	32,32,32,32	0
57	MG	1A	3306	1/1	0.82	0.34	71,71,71,71	0
57	MG	2B	201	1/1	0.82	0.23	67,67,67,67	0
57	MG	1A	3933	1/1	0.82	0.13	36,36,36,36	0
57	MG	2a	1765	1/1	0.82	0.26	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	104	1/1	0.82	0.18	69,69,69,69	0
57	MG	2F	3302	1/1	0.82	0.17	56,56,56,56	0
57	MG	2A	3678	1/1	0.82	0.21	70,70,70,70	0
57	MG	1A	3788	1/1	0.82	0.23	73,73,73,73	0
57	MG	20	104	1/1	0.82	0.19	67,67,67,67	0
57	MG	1A	4060	1/1	0.82	0.18	47,47,47,47	0
57	MG	2a	1606	1/1	0.82	0.19	70,70,70,70	0
57	MG	2A	3375	1/1	0.82	0.21	78,78,78,78	0
57	MG	2a	1613	1/1	0.82	0.14	70,70,70,70	0
57	MG	1A	3987	1/1	0.82	0.14	36,36,36,36	0
57	MG	1A	3791	1/1	0.82	0.12	52,52,52,52	0
57	MG	2a	1807	1/1	0.82	0.12	78,78,78,78	0
57	MG	2a	1620	1/1	0.82	0.22	65,65,65,65	0
57	MG	2a	1643	1/1	0.82	0.36	84,84,84,84	0
57	MG	14	101	1/1	0.82	0.16	71,71,71,71	0
57	MG	2v	102	1/1	0.82	0.26	68,68,68,68	0
57	MG	2A	3093	1/1	0.82	0.21	60,60,60,60	0
57	MG	1A	3792	1/1	0.82	0.16	68,68,68,68	0
57	MG	2A	3290	1/1	0.82	0.20	71,71,71,71	0
57	MG	1A	3904	1/1	0.82	0.13	36,36,36,36	0
57	MG	2A	3794	1/1	0.82	0.19	50,50,50,50	0
57	MG	2A	3171	1/1	0.83	0.14	50,50,50,50	0
57	MG	2A	3332	1/1	0.83	0.29	68,68,68,68	0
57	MG	2A	3341	1/1	0.83	0.34	62,62,62,62	0
57	MG	1a	1762	1/1	0.83	0.16	47,47,47,47	0
57	MG	1a	1777	1/1	0.83	0.15	71,71,71,71	0
57	MG	2a	1703	1/1	0.83	0.21	70,70,70,70	0
57	MG	2A	3201	1/1	0.83	0.21	76,76,76,76	0
57	MG	2A	3581	1/1	0.83	0.26	62,62,62,62	0
57	MG	2a	1713	1/1	0.83	0.23	72,72,72,72	0
57	MG	1A	3636	1/1	0.83	0.14	34,34,34,34	0
57	MG	1A	3506	1/1	0.83	0.20	67,67,67,67	0
57	MG	2A	3359	1/1	0.83	0.30	69,69,69,69	0
57	MG	1A	3966	1/1	0.83	0.10	66,66,66,66	0
57	MG	2A	3238	1/1	0.83	0.16	73,73,73,73	0
57	MG	2a	1752	1/1	0.83	0.14	68,68,68,68	0
57	MG	2A	3835	1/1	0.83	0.20	67,67,67,67	0
57	MG	2A	3840	1/1	0.83	0.32	71,71,71,71	0
57	MG	1a	1662	1/1	0.83	0.15	58,58,58,58	0
57	MG	2A	3849	1/1	0.83	0.18	61,61,61,61	0
57	MG	1A	3968	1/1	0.83	0.14	65,65,65,65	0
57	MG	1a	1721	1/1	0.83	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3264	1/1	0.83	0.19	62,62,62,62	0
57	MG	1a	1723	1/1	0.83	0.24	67,67,67,67	0
57	MG	1a	1730	1/1	0.83	0.21	61,61,61,61	0
57	MG	1A	3163	1/1	0.83	0.17	67,67,67,67	0
57	MG	2a	1792	1/1	0.83	0.14	64,64,64,64	0
57	MG	2A	3448	1/1	0.83	0.33	75,75,75,75	0
57	MG	1A	3418	1/1	0.83	0.23	75,75,75,75	0
57	MG	2A	3665	1/1	0.83	0.21	67,67,67,67	0
57	MG	1a	1747	1/1	0.83	0.17	65,65,65,65	0
57	MG	2A	3672	1/1	0.83	0.17	62,62,62,62	0
57	MG	1A	4090	1/1	0.83	0.21	60,60,60,60	0
57	MG	2A	3679	1/1	0.83	0.20	50,50,50,50	0
57	MG	2A	3146	1/1	0.83	0.23	69,69,69,69	0
57	MG	2A	3695	1/1	0.83	0.19	69,69,69,69	0
57	MG	1l	105	1/1	0.83	0.20	76,76,76,76	0
57	MG	2a	1653	1/1	0.83	0.30	68,68,68,68	0
57	MG	2A	3168	1/1	0.83	0.15	60,60,60,60	0
57	MG	2A	3310	1/1	0.83	0.16	68,68,68,68	0
57	MG	2A	3301	1/1	0.84	0.22	66,66,66,66	0
57	MG	2A	3169	1/1	0.84	0.16	64,64,64,64	0
57	MG	1A	3320	1/1	0.84	0.17	61,61,61,61	0
57	MG	1B	225	1/1	0.84	0.17	57,57,57,57	0
57	MG	2A	3720	1/1	0.84	0.17	60,60,60,60	0
57	MG	2A	3320	1/1	0.84	0.14	62,62,62,62	0
57	MG	2A	3327	1/1	0.84	0.20	68,68,68,68	0
57	MG	1A	3423	1/1	0.84	0.14	59,59,59,59	0
57	MG	2A	3335	1/1	0.84	0.19	70,70,70,70	0
57	MG	2A	3188	1/1	0.84	0.23	61,61,61,61	0
57	MG	2A	3578	1/1	0.84	0.12	37,37,37,37	0
57	MG	1a	1641	1/1	0.84	0.20	64,64,64,64	0
57	MG	1w	108	1/1	0.84	0.20	80,80,80,80	0
57	MG	2A	3826	1/1	0.84	0.18	68,68,68,68	0
57	MG	2A	3206	1/1	0.84	0.17	74,74,74,74	0
57	MG	2A	3348	1/1	0.84	0.31	67,67,67,67	0
57	MG	2A	3834	1/1	0.84	0.24	73,73,73,73	0
57	MG	1A	3797	1/1	0.84	0.18	53,53,53,53	0
57	MG	2A	3231	1/1	0.84	0.18	70,70,70,70	0
57	MG	1a	1659	1/1	0.84	0.25	73,73,73,73	0
57	MG	1A	3758	1/1	0.84	0.13	71,71,71,71	0
57	MG	2A	3022	1/1	0.84	0.18	74,74,74,74	0
57	MG	2A	3038	1/1	0.84	0.38	75,75,75,75	0
57	MG	1A	3424	1/1	0.84	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	303	1/1	0.84	0.15	72,72,72,72	0
57	MG	2B	216	1/1	0.84	0.14	61,61,61,61	0
57	MG	1G	203	1/1	0.84	0.13	67,67,67,67	0
57	MG	2A	3402	1/1	0.84	0.34	63,63,63,63	0
57	MG	1A	4024	1/1	0.84	0.21	61,61,61,61	0
57	MG	2a	1795	1/1	0.84	0.18	69,69,69,69	0
57	MG	2A	3413	1/1	0.84	0.32	74,74,74,74	0
57	MG	1A	3366	1/1	0.84	0.30	70,70,70,70	0
57	MG	1A	4029	1/1	0.84	0.18	79,79,79,79	0
57	MG	2a	1810	1/1	0.84	0.36	68,68,68,68	0
57	MG	2A	3671	1/1	0.84	0.36	67,67,67,67	0
57	MG	2A	3442	1/1	0.84	0.20	68,68,68,68	0
57	MG	1A	3785	1/1	0.84	0.17	58,58,58,58	0
57	MG	1W	205	1/1	0.84	0.20	43,43,43,43	0
57	MG	2A	3462	1/1	0.84	0.21	68,68,68,68	0
57	MG	2w	102	1/1	0.84	0.11	78,78,78,78	0
57	MG	2w	103	1/1	0.84	0.20	75,75,75,75	0
57	MG	2a	1629	1/1	0.84	0.15	86,86,86,86	0
57	MG	2x	106	1/1	0.84	0.12	40,40,40,40	0
57	MG	2a	1637	1/1	0.84	0.29	71,71,71,71	0
57	MG	1a	1758	1/1	0.84	0.17	55,55,55,55	0
57	MG	1A	3395	1/1	0.84	0.13	71,71,71,71	0
57	MG	2A	3635	1/1	0.85	0.18	62,62,62,62	0
57	MG	2A	3639	1/1	0.85	0.15	57,57,57,57	0
57	MG	1A	3868	1/1	0.85	0.10	54,54,54,54	0
57	MG	2a	1607	1/1	0.85	0.35	68,68,68,68	0
57	MG	1a	1804	1/1	0.85	0.16	69,69,69,69	0
57	MG	1a	1807	1/1	0.85	0.12	78,78,78,78	0
57	MG	1a	1809	1/1	0.85	0.15	64,64,64,64	0
57	MG	2A	3664	1/1	0.85	0.12	69,69,69,69	0
57	MG	1A	3870	1/1	0.85	0.10	28,28,28,28	0
57	MG	2A	3669	1/1	0.85	0.24	77,77,77,77	0
57	MG	2a	1634	1/1	0.85	0.29	63,63,63,63	0
57	MG	1A	3938	1/1	0.85	0.17	47,47,47,47	0
57	MG	1a	1640	1/1	0.85	0.18	67,67,67,67	0
57	MG	1x	106	1/1	0.85	0.17	69,69,69,69	0
57	MG	2a	1655	1/1	0.85	0.16	64,64,64,64	0
57	MG	1A	3760	1/1	0.85	0.23	70,70,70,70	0
57	MG	1A	3684	1/1	0.85	0.10	51,51,51,51	0
57	MG	2a	1668	1/1	0.85	0.18	61,61,61,61	0
57	MG	2A	3680	1/1	0.85	0.19	64,64,64,64	0
57	MG	2a	1675	1/1	0.85	0.26	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3229	1/1	0.85	0.14	65,65,65,65	0
57	MG	1A	4019	1/1	0.85	0.11	54,54,54,54	0
57	MG	1a	1668	1/1	0.85	0.19	74,74,74,74	0
57	MG	2A	3701	1/1	0.85	0.18	73,73,73,73	0
57	MG	2A	3702	1/1	0.85	0.19	63,63,63,63	0
57	MG	2A	3050	1/1	0.85	0.21	65,65,65,65	0
57	MG	2A	3706	1/1	0.85	0.23	71,71,71,71	0
57	MG	2a	1710	1/1	0.85	0.18	64,64,64,64	0
57	MG	2A	3708	1/1	0.85	0.16	75,75,75,75	0
57	MG	2A	3054	1/1	0.85	0.16	66,66,66,66	0
57	MG	2A	3710	1/1	0.85	0.13	68,68,68,68	0
57	MG	2A	3289	1/1	0.85	0.21	70,70,70,70	0
57	MG	2A	3500	1/1	0.85	0.33	74,74,74,74	0
57	MG	2A	3062	1/1	0.85	0.10	55,55,55,55	0
57	MG	2A	3741	1/1	0.85	0.17	67,67,67,67	0
57	MG	2a	1754	1/1	0.85	0.18	69,69,69,69	0
57	MG	1a	1695	1/1	0.85	0.27	64,64,64,64	0
57	MG	2A	3753	1/1	0.85	0.12	65,65,65,65	0
57	MG	1A	3212	1/1	0.85	0.23	71,71,71,71	0
57	MG	1A	3065	1/1	0.85	0.26	62,62,62,62	0
57	MG	1A	3736	1/1	0.85	0.20	76,76,76,76	0
57	MG	2a	1779	1/1	0.85	0.22	70,70,70,70	0
57	MG	2A	3765	1/1	0.85	0.13	83,83,83,83	0
57	MG	2A	3784	1/1	0.85	0.12	72,72,72,72	0
57	MG	1A	3742	1/1	0.85	0.11	26,26,26,26	0
57	MG	2A	3804	1/1	0.85	0.17	45,45,45,45	0
57	MG	1A	3914	1/1	0.85	0.23	65,65,65,65	0
57	MG	2A	3134	1/1	0.85	0.32	69,69,69,69	0
57	MG	2A	3138	1/1	0.85	0.29	65,65,65,65	0
57	MG	2A	3330	1/1	0.85	0.29	79,79,79,79	0
57	MG	1A	3585	1/1	0.85	0.14	56,56,56,56	0
57	MG	1A	3410	1/1	0.85	0.22	59,59,59,59	0
57	MG	2A	3584	1/1	0.85	0.23	67,67,67,67	0
57	MG	2A	3339	1/1	0.85	0.22	73,73,73,73	0
57	MG	2f	202	1/1	0.85	0.21	75,75,75,75	0
57	MG	2A	3162	1/1	0.85	0.15	67,67,67,67	0
57	MG	1A	3923	1/1	0.85	0.13	75,75,75,75	0
57	MG	1A	4058	1/1	0.85	0.20	64,64,64,64	0
57	MG	1a	1759	1/1	0.85	0.12	62,62,62,62	0
57	MG	1A	3850	1/1	0.85	0.12	41,41,41,41	0
57	MG	1A	3595	1/1	0.85	0.16	69,69,69,69	0
57	MG	1A	4088	1/1	0.85	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3193	1/1	0.85	0.22	66,66,66,66	0
57	MG	2E	309	1/1	0.85	0.20	56,56,56,56	0
57	MG	2y	101	1/1	0.85	0.13	80,80,80,80	0
57	MG	1a	1791	1/1	0.85	0.16	56,56,56,56	0
57	MG	2A	3627	1/1	0.85	0.14	67,67,67,67	0
57	MG	2A	3632	1/1	0.85	0.14	74,74,74,74	0
57	MG	1a	1752	1/1	0.86	0.14	75,75,75,75	0
57	MG	2a	1616	1/1	0.86	0.16	60,60,60,60	0
57	MG	2A	3684	1/1	0.86	0.12	67,67,67,67	0
57	MG	1a	1753	1/1	0.86	0.13	54,54,54,54	0
57	MG	1A	3487	1/1	0.86	0.19	64,64,64,64	0
57	MG	2a	1622	1/1	0.86	0.24	72,72,72,72	0
57	MG	2A	3293	1/1	0.86	0.21	61,61,61,61	0
57	MG	2A	3697	1/1	0.86	0.17	64,64,64,64	0
57	MG	2a	1636	1/1	0.86	0.23	70,70,70,70	0
57	MG	1A	3861	1/1	0.86	0.12	42,42,42,42	0
57	MG	2a	1641	1/1	0.86	0.24	67,67,67,67	0
57	MG	1A	3637	1/1	0.86	0.11	27,27,27,27	0
57	MG	2A	3703	1/1	0.86	0.23	59,59,59,59	0
57	MG	2A	3304	1/1	0.86	0.12	63,63,63,63	0
57	MG	2a	1657	1/1	0.86	0.17	68,68,68,68	0
57	MG	1a	1612	1/1	0.86	0.32	66,66,66,66	0
57	MG	1a	1633	1/1	0.86	0.25	63,63,63,63	0
57	MG	1A	3492	1/1	0.86	0.26	61,61,61,61	0
57	MG	2A	3166	1/1	0.86	0.21	74,74,74,74	0
57	MG	1A	3579	1/1	0.86	0.17	55,55,55,55	0
57	MG	2A	3572	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3577	1/1	0.86	0.10	44,44,44,44	0
57	MG	2A	3723	1/1	0.86	0.14	57,57,57,57	0
57	MG	2a	1691	1/1	0.86	0.16	62,62,62,62	0
57	MG	2a	1694	1/1	0.86	0.37	71,71,71,71	0
57	MG	2A	3724	1/1	0.86	0.16	55,55,55,55	0
57	MG	1a	1645	1/1	0.86	0.33	67,67,67,67	0
57	MG	2a	1704	1/1	0.86	0.22	75,75,75,75	0
57	MG	1E	311	1/1	0.86	0.09	25,25,25,25	0
57	MG	2A	3749	1/1	0.86	0.14	67,67,67,67	0
57	MG	1a	1650	1/1	0.86	0.16	59,59,59,59	0
57	MG	2A	3758	1/1	0.86	0.10	77,77,77,77	0
57	MG	1a	1814	1/1	0.86	0.14	58,58,58,58	0
57	MG	2a	1719	1/1	0.86	0.22	58,58,58,58	0
57	MG	1A	4067	1/1	0.86	0.25	64,64,64,64	0
57	MG	1A	3726	1/1	0.86	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1724	1/1	0.86	0.22	77,77,77,77	0
57	MG	1x	101	1/1	0.86	0.30	70,70,70,70	0
57	MG	2A	3774	1/1	0.86	0.14	53,53,53,53	0
57	MG	2a	1737	1/1	0.86	0.22	80,80,80,80	0
57	MG	2A	3203	1/1	0.86	0.17	64,64,64,64	0
57	MG	2A	3609	1/1	0.86	0.13	68,68,68,68	0
57	MG	2a	1760	1/1	0.86	0.17	54,54,54,54	0
57	MG	2A	3798	1/1	0.86	0.10	57,57,57,57	0
57	MG	1A	3810	1/1	0.86	0.16	70,70,70,70	0
57	MG	1A	4089	1/1	0.86	0.21	64,64,64,64	0
57	MG	1Q	205	1/1	0.86	0.14	58,58,58,58	0
57	MG	2A	3620	1/1	0.86	0.13	66,66,66,66	0
57	MG	1a	1702	1/1	0.86	0.29	76,76,76,76	0
57	MG	2A	3360	1/1	0.86	0.18	62,62,62,62	0
57	MG	1A	3734	1/1	0.86	0.08	39,39,39,39	0
57	MG	2A	3833	1/1	0.86	0.22	70,70,70,70	0
57	MG	1A	3814	1/1	0.86	0.21	45,45,45,45	0
57	MG	2a	1786	1/1	0.86	0.29	68,68,68,68	0
57	MG	1A	3840	1/1	0.86	0.11	23,23,23,23	0
57	MG	2A	3839	1/1	0.86	0.17	67,67,67,67	0
57	MG	2A	3247	1/1	0.86	0.35	67,67,67,67	0
57	MG	2A	3249	1/1	0.86	0.23	77,77,77,77	0
57	MG	1A	3981	1/1	0.86	0.14	51,51,51,51	0
57	MG	2A	3643	1/1	0.86	0.20	70,70,70,70	0
57	MG	2a	1804	1/1	0.86	0.26	65,65,65,65	0
57	MG	2a	1806	1/1	0.86	0.26	67,67,67,67	0
57	MG	2A	3856	1/1	0.86	0.20	69,69,69,69	0
57	MG	2A	3644	1/1	0.86	0.21	72,72,72,72	0
57	MG	1a	1739	1/1	0.86	0.18	55,55,55,55	0
57	MG	2B	206	1/1	0.86	0.23	66,66,66,66	0
57	MG	2A	3057	1/1	0.86	0.28	71,71,71,71	0
57	MG	2A	3660	1/1	0.86	0.19	64,64,64,64	0
57	MG	2q	202	1/1	0.86	0.20	74,74,74,74	0
57	MG	2A	3268	1/1	0.86	0.22	64,64,64,64	0
57	MG	1a	1742	1/1	0.86	0.18	66,66,66,66	0
57	MG	2A	3425	1/1	0.86	0.19	68,68,68,68	0
57	MG	2A	3067	1/1	0.86	0.33	71,71,71,71	0
57	MG	1X	107	1/1	0.86	0.15	56,56,56,56	0
57	MG	2a	1602	1/1	0.86	0.11	79,79,79,79	0
57	MG	1Y	201	1/1	0.86	0.13	56,56,56,56	0
57	MG	1A	3404	1/1	0.86	0.19	67,67,67,67	0
57	MG	2A	3286	1/1	0.86	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3467	1/1	0.86	0.21	60,60,60,60	0
57	MG	1A	3352	1/1	0.87	0.15	59,59,59,59	0
57	MG	1A	3393	1/1	0.87	0.20	57,57,57,57	0
57	MG	1A	3427	1/1	0.87	0.18	66,66,66,66	0
57	MG	2a	1624	1/1	0.87	0.13	71,71,71,71	0
57	MG	2A	3251	1/1	0.87	0.27	64,64,64,64	0
57	MG	1A	3359	1/1	0.87	0.11	51,51,51,51	0
57	MG	1A	3494	1/1	0.87	0.17	65,65,65,65	0
57	MG	2A	3470	1/1	0.87	0.19	66,66,66,66	0
57	MG	2A	3473	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3479	1/1	0.87	0.12	53,53,53,53	0
57	MG	1A	3696	1/1	0.87	0.11	45,45,45,45	0
57	MG	1x	109	1/1	0.87	0.26	66,66,66,66	0
57	MG	1a	1654	1/1	0.87	0.13	57,57,57,57	0
57	MG	2A	3507	1/1	0.87	0.10	40,40,40,40	0
57	MG	2A	3007	1/1	0.87	0.26	63,63,63,63	0
57	MG	2A	3525	1/1	0.87	0.18	52,52,52,52	0
57	MG	1A	3699	1/1	0.87	0.12	54,54,54,54	0
57	MG	2a	1673	1/1	0.87	0.24	61,61,61,61	0
57	MG	1A	3449	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3043	1/1	0.87	0.17	58,58,58,58	0
57	MG	2A	3743	1/1	0.87	0.12	63,63,63,63	0
57	MG	1A	3994	1/1	0.87	0.13	60,60,60,60	0
57	MG	1a	1670	1/1	0.87	0.13	62,62,62,62	0
57	MG	1a	1682	1/1	0.87	0.21	67,67,67,67	0
57	MG	2A	3755	1/1	0.87	0.13	47,47,47,47	0
57	MG	2a	1702	1/1	0.87	0.29	67,67,67,67	0
57	MG	2A	3757	1/1	0.87	0.14	46,46,46,46	0
57	MG	1a	1692	1/1	0.87	0.22	65,65,65,65	0
57	MG	1A	3704	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3064	1/1	0.87	0.17	73,73,73,73	0
57	MG	1A	3806	1/1	0.87	0.10	42,42,42,42	0
57	MG	1A	3607	1/1	0.87	0.09	26,26,26,26	0
57	MG	2A	3079	1/1	0.87	0.18	60,60,60,60	0
57	MG	1a	1717	1/1	0.87	0.16	74,74,74,74	0
57	MG	2A	3787	1/1	0.87	0.08	58,58,58,58	0
57	MG	2A	3090	1/1	0.87	0.15	72,72,72,72	0
57	MG	1A	3717	1/1	0.87	0.08	20,20,20,20	0
57	MG	2A	3800	1/1	0.87	0.13	68,68,68,68	0
57	MG	2a	1732	1/1	0.87	0.15	67,67,67,67	0
57	MG	1D	310	1/1	0.87	0.17	51,51,51,51	0
57	MG	1a	1727	1/1	0.87	0.30	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1738	1/1	0.87	0.10	66,66,66,66	0
57	MG	1A	3613	1/1	0.87	0.07	37,37,37,37	0
57	MG	2A	3819	1/1	0.87	0.13	68,68,68,68	0
57	MG	2A	3610	1/1	0.87	0.24	54,54,54,54	0
57	MG	1a	1731	1/1	0.87	0.11	55,55,55,55	0
57	MG	2a	1764	1/1	0.87	0.28	80,80,80,80	0
57	MG	1A	3829	1/1	0.87	0.08	21,21,21,21	0
57	MG	1E	315	1/1	0.87	0.12	58,58,58,58	0
57	MG	1A	4020	1/1	0.87	0.09	28,28,28,28	0
57	MG	2a	1772	1/1	0.87	0.15	60,60,60,60	0
57	MG	2A	3154	1/1	0.87	0.22	67,67,67,67	0
57	MG	1A	4021	1/1	0.87	0.09	27,27,27,27	0
57	MG	1A	3363	1/1	0.87	0.19	61,61,61,61	0
57	MG	1A	3934	1/1	0.87	0.17	55,55,55,55	0
57	MG	1A	3848	1/1	0.87	0.17	58,58,58,58	0
57	MG	1A	3524	1/1	0.87	0.22	59,59,59,59	0
57	MG	1A	3131	1/1	0.87	0.22	51,51,51,51	0
57	MG	2A	3184	1/1	0.87	0.18	64,64,64,64	0
57	MG	1A	4045	1/1	0.87	0.20	60,60,60,60	0
57	MG	1A	3743	1/1	0.87	0.09	25,25,25,25	0
57	MG	2B	205	1/1	0.87	0.21	63,63,63,63	0
57	MG	2A	3381	1/1	0.87	0.23	50,50,50,50	0
57	MG	2A	3648	1/1	0.87	0.25	58,58,58,58	0
57	MG	2a	1801	1/1	0.87	0.19	72,72,72,72	0
57	MG	2B	212	1/1	0.87	0.25	71,71,71,71	0
57	MG	2B	215	1/1	0.87	0.19	72,72,72,72	0
57	MG	2A	3649	1/1	0.87	0.16	58,58,58,58	0
57	MG	2a	1809	1/1	0.87	0.21	57,57,57,57	0
57	MG	2B	218	1/1	0.87	0.24	68,68,68,68	0
57	MG	2A	3383	1/1	0.87	0.22	39,39,39,39	0
57	MG	2F	3301	1/1	0.87	0.11	59,59,59,59	0
57	MG	1A	3962	1/1	0.87	0.14	73,73,73,73	0
57	MG	2A	3390	1/1	0.87	0.23	67,67,67,67	0
57	MG	2V	202	1/1	0.87	0.14	62,62,62,62	0
57	MG	1A	3863	1/1	0.87	0.22	62,62,62,62	0
57	MG	1a	1789	1/1	0.87	0.10	69,69,69,69	0
57	MG	11	103	1/1	0.87	0.15	62,62,62,62	0
57	MG	1A	3244	1/1	0.87	0.26	63,63,63,63	0
57	MG	2w	104	1/1	0.87	0.15	72,72,72,72	0
57	MG	2A	3410	1/1	0.87	0.29	69,69,69,69	0
57	MG	1A	3869	1/1	0.87	0.14	67,67,67,67	0
57	MG	1A	4061	1/1	0.87	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2y	102	1/1	0.87	0.14	82,82,82,82	0
57	MG	1a	1602	1/1	0.87	0.19	60,60,60,60	0
57	MG	2A	3428	1/1	0.87	0.13	71,71,71,71	0
57	MG	1A	3646	1/1	0.87	0.24	64,64,64,64	0
57	MG	1A	3365	1/1	0.88	0.28	70,70,70,70	0
57	MG	26	101	1/1	0.88	0.22	64,64,64,64	0
57	MG	1A	3787	1/1	0.88	0.24	63,63,63,63	0
57	MG	2A	3141	1/1	0.88	0.17	58,58,58,58	0
57	MG	1A	3416	1/1	0.88	0.20	64,64,64,64	0
57	MG	1a	1757	1/1	0.88	0.16	72,72,72,72	0
57	MG	2A	3352	1/1	0.88	0.18	65,65,65,65	0
57	MG	1A	4068	1/1	0.88	0.13	47,47,47,47	0
57	MG	2A	3659	1/1	0.88	0.16	56,56,56,56	0
57	MG	1A	3896	1/1	0.88	0.13	52,52,52,52	0
57	MG	1A	3206	1/1	0.88	0.12	51,51,51,51	0
57	MG	1A	3902	1/1	0.88	0.09	38,38,38,38	0
57	MG	1a	1763	1/1	0.88	0.15	49,49,49,49	0
57	MG	2A	3369	1/1	0.88	0.23	62,62,62,62	0
57	MG	2a	1625	1/1	0.88	0.15	71,71,71,71	0
57	MG	1A	3332	1/1	0.88	0.17	57,57,57,57	0
57	MG	2A	3178	1/1	0.88	0.23	64,64,64,64	0
57	MG	2A	3180	1/1	0.88	0.22	65,65,65,65	0
57	MG	2A	3182	1/1	0.88	0.14	63,63,63,63	0
57	MG	2a	1640	1/1	0.88	0.15	65,65,65,65	0
57	MG	1a	1788	1/1	0.88	0.30	75,75,75,75	0
57	MG	1A	3372	1/1	0.88	0.12	55,55,55,55	0
57	MG	2a	1644	1/1	0.88	0.32	81,81,81,81	0
57	MG	2A	3185	1/1	0.88	0.39	75,75,75,75	0
57	MG	2A	3397	1/1	0.88	0.33	62,62,62,62	0
57	MG	2A	3692	1/1	0.88	0.15	55,55,55,55	0
57	MG	1B	208	1/1	0.88	0.24	71,71,71,71	0
57	MG	1a	1793	1/1	0.88	0.14	70,70,70,70	0
57	MG	2A	3189	1/1	0.88	0.21	60,60,60,60	0
57	MG	2A	3404	1/1	0.88	0.26	62,62,62,62	0
57	MG	1a	1798	1/1	0.88	0.19	59,59,59,59	0
57	MG	1A	3908	1/1	0.88	0.08	43,43,43,43	0
57	MG	1a	1802	1/1	0.88	0.11	66,66,66,66	0
57	MG	1B	215	1/1	0.88	0.11	59,59,59,59	0
57	MG	1A	3910	1/1	0.88	0.14	48,48,48,48	0
57	MG	2A	3212	1/1	0.88	0.16	63,63,63,63	0
57	MG	2A	3214	1/1	0.88	0.16	62,62,62,62	0
57	MG	1A	3069	1/1	0.88	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1696	1/1	0.88	0.16	67,67,67,67	0
57	MG	2a	1698	1/1	0.88	0.23	72,72,72,72	0
57	MG	2a	1701	1/1	0.88	0.18	63,63,63,63	0
57	MG	1a	1653	1/1	0.88	0.24	61,61,61,61	0
57	MG	1f	3101	1/1	0.88	0.16	48,48,48,48	0
57	MG	1A	3714	1/1	0.88	0.13	38,38,38,38	0
57	MG	1A	3387	1/1	0.88	0.15	53,53,53,53	0
57	MG	1A	3276	1/1	0.88	0.23	66,66,66,66	0
57	MG	1a	1664	1/1	0.88	0.29	60,60,60,60	0
57	MG	1A	3924	1/1	0.88	0.15	58,58,58,58	0
57	MG	2A	3254	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	3298	1/1	0.88	0.18	52,52,52,52	0
57	MG	2A	3501	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3257	1/1	0.88	0.15	59,59,59,59	0
57	MG	2A	3503	1/1	0.88	0.24	61,61,61,61	0
57	MG	2A	3261	1/1	0.88	0.13	66,66,66,66	0
57	MG	1x	108	1/1	0.88	0.14	67,67,67,67	0
57	MG	1D	302	1/1	0.88	0.24	60,60,60,60	0
57	MG	2A	3532	1/1	0.88	0.10	40,40,40,40	0
57	MG	2A	3266	1/1	0.88	0.13	68,68,68,68	0
57	MG	2a	1750	1/1	0.88	0.14	78,78,78,78	0
57	MG	2A	3778	1/1	0.88	0.14	39,39,39,39	0
57	MG	2A	3781	1/1	0.88	0.12	46,46,46,46	0
57	MG	2A	3544	1/1	0.88	0.16	57,57,57,57	0
57	MG	1a	1688	1/1	0.88	0.15	71,71,71,71	0
57	MG	1A	3835	1/1	0.88	0.10	44,44,44,44	0
57	MG	1A	3476	1/1	0.88	0.12	68,68,68,68	0
57	MG	2A	3030	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3565	1/1	0.88	0.11	39,39,39,39	0
57	MG	2a	1769	1/1	0.88	0.17	68,68,68,68	0
57	MG	2A	3568	1/1	0.88	0.21	56,56,56,56	0
57	MG	1A	3847	1/1	0.88	0.19	68,68,68,68	0
57	MG	2a	1777	1/1	0.88	0.16	67,67,67,67	0
57	MG	1a	1697	1/1	0.88	0.22	63,63,63,63	0
57	MG	1A	3551	1/1	0.88	0.16	52,52,52,52	0
57	MG	2a	1781	1/1	0.88	0.22	62,62,62,62	0
57	MG	2A	3574	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3287	1/1	0.88	0.18	76,76,76,76	0
57	MG	2A	3830	1/1	0.88	0.11	58,58,58,58	0
57	MG	1a	1709	1/1	0.88	0.10	52,52,52,52	0
57	MG	1a	1716	1/1	0.88	0.13	60,60,60,60	0
57	MG	2a	1789	1/1	0.88	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3240	1/1	0.88	0.14	56,56,56,56	0
57	MG	2A	3583	1/1	0.88	0.16	47,47,47,47	0
57	MG	1A	4030	1/1	0.88	0.14	63,63,63,63	0
57	MG	1N	201	1/1	0.88	0.12	47,47,47,47	0
57	MG	2A	3066	1/1	0.88	0.23	58,58,58,58	0
57	MG	1O	205	1/1	0.88	0.11	67,67,67,67	0
57	MG	2A	3850	1/1	0.88	0.13	56,56,56,56	0
57	MG	2a	1805	1/1	0.88	0.28	68,68,68,68	0
57	MG	1A	3557	1/1	0.88	0.15	57,57,57,57	0
57	MG	1A	3406	1/1	0.88	0.18	71,71,71,71	0
57	MG	2A	3317	1/1	0.88	0.27	73,73,73,73	0
57	MG	1A	3680	1/1	0.88	0.14	60,60,60,60	0
57	MG	2e	201	1/1	0.88	0.10	63,63,63,63	0
57	MG	2A	3319	1/1	0.88	0.13	78,78,78,78	0
57	MG	2g	201	1/1	0.88	0.14	77,77,77,77	0
57	MG	1A	3574	1/1	0.88	0.08	35,35,35,35	0
57	MG	2B	207	1/1	0.88	0.12	69,69,69,69	0
57	MG	1a	1741	1/1	0.88	0.17	66,66,66,66	0
57	MG	1A	3685	1/1	0.88	0.11	57,57,57,57	0
57	MG	2B	214	1/1	0.88	0.26	70,70,70,70	0
57	MG	1A	3686	1/1	0.88	0.18	59,59,59,59	0
57	MG	2A	3333	1/1	0.88	0.17	64,64,64,64	0
57	MG	2B	217	1/1	0.88	0.30	73,73,73,73	0
57	MG	2A	3116	1/1	0.88	0.16	58,58,58,58	0
57	MG	2A	3629	1/1	0.88	0.14	60,60,60,60	0
57	MG	2A	3338	1/1	0.88	0.13	58,58,58,58	0
57	MG	1A	3780	1/1	0.88	0.22	44,44,44,44	0
57	MG	2A	3636	1/1	0.88	0.15	60,60,60,60	0
57	MG	2T	203	1/1	0.88	0.22	69,69,69,69	0
57	MG	2A	3340	1/1	0.88	0.45	53,53,53,53	0
57	MG	2A	3640	1/1	0.88	0.15	67,67,67,67	0
57	MG	1w	104	1/1	0.89	0.14	72,72,72,72	0
57	MG	1A	3915	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	4033	1/1	0.89	0.13	55,55,55,55	0
57	MG	2A	3270	1/1	0.89	0.22	65,65,65,65	0
57	MG	2B	213	1/1	0.89	0.25	61,61,61,61	0
57	MG	1a	1603	1/1	0.89	0.22	65,65,65,65	0
57	MG	1A	3153	1/1	0.89	0.18	64,64,64,64	0
57	MG	1a	1630	1/1	0.89	0.22	66,66,66,66	0
57	MG	1A	3024	1/1	0.89	0.20	76,76,76,76	0
57	MG	1A	3282	1/1	0.89	0.09	36,36,36,36	0
57	MG	2D	307	1/1	0.89	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2E	307	1/1	0.89	0.10	36,36,36,36	0
57	MG	2A	3282	1/1	0.89	0.22	68,68,68,68	0
57	MG	2A	3284	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3291	1/1	0.89	0.25	60,60,60,60	0
57	MG	1x	110	1/1	0.89	0.11	27,27,27,27	0
57	MG	2Q	202	1/1	0.89	0.23	65,65,65,65	0
57	MG	2A	3288	1/1	0.89	0.18	62,62,62,62	0
57	MG	1A	3803	1/1	0.89	0.12	59,59,59,59	0
57	MG	1x	113	1/1	0.89	0.14	55,55,55,55	0
57	MG	2A	3001	1/1	0.89	0.36	64,64,64,64	0
57	MG	2A	3003	1/1	0.89	0.17	55,55,55,55	0
57	MG	28	101	1/1	0.89	0.21	68,68,68,68	0
57	MG	28	102	1/1	0.89	0.18	63,63,63,63	0
57	MG	1A	4056	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3582	1/1	0.89	0.14	55,55,55,55	0
57	MG	2a	1604	1/1	0.89	0.22	60,60,60,60	0
57	MG	1A	3409	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3232	1/1	0.89	0.18	64,64,64,64	0
57	MG	2a	1609	1/1	0.89	0.18	66,66,66,66	0
57	MG	2A	3308	1/1	0.89	0.17	61,61,61,61	0
57	MG	2a	1611	1/1	0.89	0.24	71,71,71,71	0
57	MG	2A	3626	1/1	0.89	0.14	58,58,58,58	0
57	MG	1a	1656	1/1	0.89	0.31	63,63,63,63	0
57	MG	2A	3314	1/1	0.89	0.13	57,57,57,57	0
57	MG	1a	1657	1/1	0.89	0.35	74,74,74,74	0
57	MG	1A	4062	1/1	0.89	0.17	41,41,41,41	0
57	MG	1a	1660	1/1	0.89	0.34	63,63,63,63	0
57	MG	2A	3637	1/1	0.89	0.12	58,58,58,58	0
57	MG	1A	3813	1/1	0.89	0.10	43,43,43,43	0
57	MG	2A	3325	1/1	0.89	0.16	64,64,64,64	0
57	MG	2a	1630	1/1	0.89	0.25	72,72,72,72	0
57	MG	2A	3641	1/1	0.89	0.16	65,65,65,65	0
57	MG	1A	3937	1/1	0.89	0.09	53,53,53,53	0
57	MG	2A	3329	1/1	0.89	0.15	74,74,74,74	0
57	MG	1a	1665	1/1	0.89	0.16	50,50,50,50	0
57	MG	1A	4073	1/1	0.89	0.09	73,73,73,73	0
57	MG	2a	1642	1/1	0.89	0.14	54,54,54,54	0
57	MG	1A	3705	1/1	0.89	0.09	25,25,25,25	0
57	MG	2A	3068	1/1	0.89	0.21	56,56,56,56	0
57	MG	2a	1651	1/1	0.89	0.35	74,74,74,74	0
57	MG	2A	3336	1/1	0.89	0.21	73,73,73,73	0
57	MG	2A	3652	1/1	0.89	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1672	1/1	0.89	0.33	65,65,65,65	0
57	MG	1a	1674	1/1	0.89	0.13	65,65,65,65	0
57	MG	1a	1678	1/1	0.89	0.19	55,55,55,55	0
57	MG	1A	3413	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3091	1/1	0.89	0.13	74,74,74,74	0
57	MG	1A	3600	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3953	1/1	0.89	0.13	40,40,40,40	0
57	MG	2a	1680	1/1	0.89	0.21	63,63,63,63	0
57	MG	1A	3956	1/1	0.89	0.08	41,41,41,41	0
57	MG	2a	1688	1/1	0.89	0.23	72,72,72,72	0
57	MG	1A	3300	1/1	0.89	0.17	55,55,55,55	0
57	MG	2A	3676	1/1	0.89	0.10	37,37,37,37	0
57	MG	1B	212	1/1	0.89	0.22	63,63,63,63	0
57	MG	2A	3129	1/1	0.89	0.14	66,66,66,66	0
57	MG	1A	3610	1/1	0.89	0.10	43,43,43,43	0
57	MG	1a	1706	1/1	0.89	0.20	65,65,65,65	0
57	MG	2A	3140	1/1	0.89	0.23	64,64,64,64	0
57	MG	1A	3730	1/1	0.89	0.07	71,71,71,71	0
57	MG	2A	3693	1/1	0.89	0.21	71,71,71,71	0
57	MG	1a	1715	1/1	0.89	0.15	60,60,60,60	0
57	MG	1A	3210	1/1	0.89	0.23	49,49,49,49	0
57	MG	2A	3153	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3382	1/1	0.89	0.34	55,55,55,55	0
57	MG	1A	3852	1/1	0.89	0.13	62,62,62,62	0
57	MG	2A	3385	1/1	0.89	0.29	58,58,58,58	0
57	MG	1A	3496	1/1	0.89	0.16	66,66,66,66	0
57	MG	1A	3969	1/1	0.89	0.09	49,49,49,49	0
57	MG	2a	1720	1/1	0.89	0.24	67,67,67,67	0
57	MG	1A	3023	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3394	1/1	0.89	0.31	63,63,63,63	0
57	MG	1A	3329	1/1	0.89	0.24	54,54,54,54	0
57	MG	1A	3744	1/1	0.89	0.11	42,42,42,42	0
57	MG	1B	234	1/1	0.89	0.17	70,70,70,70	0
57	MG	2A	3719	1/1	0.89	0.18	61,61,61,61	0
57	MG	1a	1738	1/1	0.89	0.11	72,72,72,72	0
57	MG	1A	3745	1/1	0.89	0.09	40,40,40,40	0
57	MG	1A	3978	1/1	0.89	0.08	40,40,40,40	0
57	MG	2A	3729	1/1	0.89	0.18	42,42,42,42	0
57	MG	2A	3740	1/1	0.89	0.11	56,56,56,56	0
57	MG	1A	3522	1/1	0.89	0.18	63,63,63,63	0
57	MG	1A	3748	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3984	1/1	0.89	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3880	1/1	0.89	0.10	43,43,43,43	0
57	MG	2A	3430	1/1	0.89	0.17	64,64,64,64	0
57	MG	1A	3886	1/1	0.89	0.09	30,30,30,30	0
57	MG	1A	3642	1/1	0.89	0.08	43,43,43,43	0
57	MG	2A	3445	1/1	0.89	0.28	65,65,65,65	0
57	MG	2a	1773	1/1	0.89	0.18	70,70,70,70	0
57	MG	2A	3759	1/1	0.89	0.13	65,65,65,65	0
57	MG	2A	3200	1/1	0.89	0.19	59,59,59,59	0
57	MG	1A	3755	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3999	1/1	0.89	0.11	56,56,56,56	0
57	MG	1A	3643	1/1	0.89	0.12	40,40,40,40	0
57	MG	2A	3770	1/1	0.89	0.17	61,61,61,61	0
57	MG	1Q	207	1/1	0.89	0.18	60,60,60,60	0
57	MG	2A	3777	1/1	0.89	0.12	61,61,61,61	0
57	MG	1A	3425	1/1	0.89	0.24	72,72,72,72	0
57	MG	1A	3379	1/1	0.89	0.14	67,67,67,67	0
57	MG	1A	3898	1/1	0.89	0.14	53,53,53,53	0
57	MG	2A	3481	1/1	0.89	0.30	55,55,55,55	0
57	MG	2A	3790	1/1	0.89	0.13	44,44,44,44	0
57	MG	2A	3791	1/1	0.89	0.12	60,60,60,60	0
57	MG	2A	3496	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3224	1/1	0.89	0.16	59,59,59,59	0
57	MG	1A	3430	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3802	1/1	0.89	0.14	74,74,74,74	0
57	MG	1A	3773	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3236	1/1	0.89	0.27	56,56,56,56	0
57	MG	2A	3807	1/1	0.89	0.11	40,40,40,40	0
57	MG	2A	3808	1/1	0.89	0.09	49,49,49,49	0
57	MG	1A	3777	1/1	0.89	0.19	60,60,60,60	0
57	MG	2A	3242	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3509	1/1	0.89	0.10	48,48,48,48	0
57	MG	2A	3511	1/1	0.89	0.16	54,54,54,54	0
57	MG	1Z	302	1/1	0.89	0.10	59,59,59,59	0
57	MG	2l	201	1/1	0.89	0.14	65,65,65,65	0
57	MG	2A	3522	1/1	0.89	0.16	44,44,44,44	0
57	MG	2l	204	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3245	1/1	0.89	0.14	62,62,62,62	0
57	MG	2A	3526	1/1	0.89	0.19	71,71,71,71	0
57	MG	2v	101	1/1	0.89	0.28	61,61,61,61	0
57	MG	2A	3527	1/1	0.89	0.15	60,60,60,60	0
57	MG	10	105	1/1	0.89	0.26	61,61,61,61	0
57	MG	2A	3538	1/1	0.89	0.17	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3907	1/1	0.89	0.12	50,50,50,50	0
57	MG	11	102	1/1	0.89	0.14	62,62,62,62	0
57	MG	1A	3245	1/1	0.89	0.10	49,49,49,49	0
57	MG	2A	3555	1/1	0.89	0.14	68,68,68,68	0
57	MG	1A	3555	1/1	0.89	0.12	58,58,58,58	0
57	MG	13	103	1/1	0.89	0.14	59,59,59,59	0
57	MG	2A	3259	1/1	0.89	0.41	68,68,68,68	0
57	MG	1A	3392	1/1	0.89	0.14	57,57,57,57	0
57	MG	15	105	1/1	0.89	0.12	47,47,47,47	0
57	MG	2A	3406	1/1	0.90	0.21	55,55,55,55	0
57	MG	2A	3005	1/1	0.90	0.26	60,60,60,60	0
57	MG	1A	4040	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3383	1/1	0.90	0.13	48,48,48,48	0
57	MG	1A	3630	1/1	0.90	0.11	40,40,40,40	0
57	MG	2A	3426	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3343	1/1	0.90	0.24	65,65,65,65	0
57	MG	1A	3955	1/1	0.90	0.10	50,50,50,50	0
57	MG	2A	3432	1/1	0.90	0.12	73,73,73,73	0
57	MG	2a	1614	1/1	0.90	0.12	67,67,67,67	0
57	MG	1A	3388	1/1	0.90	0.17	54,54,54,54	0
57	MG	2a	1617	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3681	1/1	0.90	0.17	66,66,66,66	0
57	MG	2A	3437	1/1	0.90	0.31	71,71,71,71	0
57	MG	2A	3689	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3256	1/1	0.90	0.12	71,71,71,71	0
57	MG	10	102	1/1	0.90	0.14	58,58,58,58	0
57	MG	1a	1725	1/1	0.90	0.14	61,61,61,61	0
57	MG	2a	1628	1/1	0.90	0.29	67,67,67,67	0
57	MG	1A	3518	1/1	0.90	0.12	51,51,51,51	0
57	MG	2A	3451	1/1	0.90	0.12	57,57,57,57	0
57	MG	2a	1633	1/1	0.90	0.35	62,62,62,62	0
57	MG	2A	3457	1/1	0.90	0.20	59,59,59,59	0
57	MG	2a	1635	1/1	0.90	0.23	70,70,70,70	0
57	MG	1A	3391	1/1	0.90	0.13	50,50,50,50	0
57	MG	1A	3429	1/1	0.90	0.15	68,68,68,68	0
57	MG	1a	1733	1/1	0.90	0.12	74,74,74,74	0
57	MG	1A	3876	1/1	0.90	0.10	61,61,61,61	0
57	MG	1A	3162	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3652	1/1	0.90	0.12	29,29,29,29	0
57	MG	1A	3431	1/1	0.90	0.20	65,65,65,65	0
57	MG	2a	1645	1/1	0.90	0.15	80,80,80,80	0
57	MG	1A	3657	1/1	0.90	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3890	1/1	0.90	0.09	53,53,53,53	0
57	MG	1A	3432	1/1	0.90	0.23	55,55,55,55	0
57	MG	2A	3279	1/1	0.90	0.13	62,62,62,62	0
57	MG	1A	3263	1/1	0.90	0.07	40,40,40,40	0
57	MG	2A	3100	1/1	0.90	0.28	69,69,69,69	0
57	MG	2A	3506	1/1	0.90	0.16	56,56,56,56	0
57	MG	2A	3726	1/1	0.90	0.15	61,61,61,61	0
57	MG	1a	1750	1/1	0.90	0.12	64,64,64,64	0
57	MG	2a	1674	1/1	0.90	0.30	70,70,70,70	0
57	MG	2A	3731	1/1	0.90	0.15	71,71,71,71	0
57	MG	2a	1677	1/1	0.90	0.17	64,64,64,64	0
57	MG	2A	3104	1/1	0.90	0.23	61,61,61,61	0
57	MG	2a	1682	1/1	0.90	0.37	64,64,64,64	0
57	MG	1a	1605	1/1	0.90	0.10	61,61,61,61	0
57	MG	2a	1687	1/1	0.90	0.16	73,73,73,73	0
57	MG	2A	3113	1/1	0.90	0.20	72,72,72,72	0
57	MG	2A	3519	1/1	0.90	0.12	64,64,64,64	0
57	MG	2A	3114	1/1	0.90	0.22	60,60,60,60	0
57	MG	2A	3751	1/1	0.90	0.16	50,50,50,50	0
57	MG	2A	3115	1/1	0.90	0.30	65,65,65,65	0
57	MG	1A	3784	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3121	1/1	0.90	0.35	70,70,70,70	0
57	MG	2A	3122	1/1	0.90	0.15	57,57,57,57	0
57	MG	2A	3537	1/1	0.90	0.08	49,49,49,49	0
57	MG	1a	1621	1/1	0.90	0.28	63,63,63,63	0
57	MG	1A	3362	1/1	0.90	0.14	52,52,52,52	0
57	MG	2A	3540	1/1	0.90	0.12	45,45,45,45	0
57	MG	2a	1705	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3543	1/1	0.90	0.09	47,47,47,47	0
57	MG	2a	1707	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3900	1/1	0.90	0.15	57,57,57,57	0
57	MG	2A	3773	1/1	0.90	0.08	38,38,38,38	0
57	MG	2A	3545	1/1	0.90	0.14	71,71,71,71	0
57	MG	1A	3983	1/1	0.90	0.17	55,55,55,55	0
57	MG	2a	1717	1/1	0.90	0.12	68,68,68,68	0
57	MG	2a	1718	1/1	0.90	0.19	78,78,78,78	0
57	MG	2A	3550	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3311	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3312	1/1	0.90	0.13	60,60,60,60	0
57	MG	1A	3464	1/1	0.90	0.15	53,53,53,53	0
57	MG	1A	3569	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3151	1/1	0.90	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3470	1/1	0.90	0.14	61,61,61,61	0
57	MG	1A	3303	1/1	0.90	0.12	61,61,61,61	0
57	MG	2A	3570	1/1	0.90	0.24	62,62,62,62	0
57	MG	1A	3269	1/1	0.90	0.12	64,64,64,64	0
57	MG	1A	3241	1/1	0.90	0.17	68,68,68,68	0
57	MG	2A	3164	1/1	0.90	0.10	69,69,69,69	0
57	MG	2A	3806	1/1	0.90	0.10	56,56,56,56	0
57	MG	2a	1759	1/1	0.90	0.15	52,52,52,52	0
57	MG	1A	3588	1/1	0.90	0.12	50,50,50,50	0
57	MG	1A	3480	1/1	0.90	0.15	53,53,53,53	0
57	MG	1a	1801	1/1	0.90	0.11	49,49,49,49	0
57	MG	1A	3593	1/1	0.90	0.11	39,39,39,39	0
57	MG	1a	1803	1/1	0.90	0.14	62,62,62,62	0
57	MG	1A	3411	1/1	0.90	0.23	50,50,50,50	0
57	MG	2A	3828	1/1	0.90	0.10	54,54,54,54	0
57	MG	1a	1805	1/1	0.90	0.15	70,70,70,70	0
57	MG	1E	310	1/1	0.90	0.16	60,60,60,60	0
57	MG	1A	3825	1/1	0.90	0.13	66,66,66,66	0
57	MG	1A	3279	1/1	0.90	0.26	62,62,62,62	0
57	MG	2A	3607	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3608	1/1	0.90	0.16	42,42,42,42	0
57	MG	1b	301	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	4023	1/1	0.90	0.13	47,47,47,47	0
57	MG	1a	1671	1/1	0.90	0.12	69,69,69,69	0
57	MG	2A	3844	1/1	0.90	0.12	61,61,61,61	0
57	MG	2A	3351	1/1	0.90	0.36	65,65,65,65	0
57	MG	2A	3615	1/1	0.90	0.24	70,70,70,70	0
57	MG	2a	1788	1/1	0.90	0.25	58,58,58,58	0
57	MG	2A	3617	1/1	0.90	0.15	63,63,63,63	0
57	MG	2A	3853	1/1	0.90	0.14	67,67,67,67	0
57	MG	2A	3192	1/1	0.90	0.17	62,62,62,62	0
57	MG	1A	3601	1/1	0.90	0.14	49,49,49,49	0
57	MG	2A	3195	1/1	0.90	0.35	68,68,68,68	0
57	MG	1w	107	1/1	0.90	0.09	79,79,79,79	0
57	MG	1G	202	1/1	0.90	0.21	62,62,62,62	0
57	MG	2a	1802	1/1	0.90	0.24	68,68,68,68	0
57	MG	1A	3928	1/1	0.90	0.12	26,26,26,26	0
57	MG	2B	208	1/1	0.90	0.14	57,57,57,57	0
57	MG	2B	209	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3368	1/1	0.90	0.11	67,67,67,67	0
57	MG	2A	3204	1/1	0.90	0.16	55,55,55,55	0
57	MG	1a	1679	1/1	0.90	0.32	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3373	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3140	1/1	0.90	0.09	49,49,49,49	0
57	MG	1a	1684	1/1	0.90	0.24	67,67,67,67	0
57	MG	1a	1686	1/1	0.90	0.10	55,55,55,55	0
57	MG	2A	3216	1/1	0.90	0.22	66,66,66,66	0
57	MG	2A	3384	1/1	0.90	0.25	54,54,54,54	0
57	MG	2E	303	1/1	0.90	0.14	65,65,65,65	0
57	MG	1N	207	1/1	0.90	0.16	47,47,47,47	0
57	MG	1A	3417	1/1	0.90	0.15	70,70,70,70	0
57	MG	2A	3226	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3645	1/1	0.90	0.13	48,48,48,48	0
57	MG	2A	3228	1/1	0.90	0.12	60,60,60,60	0
57	MG	2O	3900	1/1	0.90	0.12	60,60,60,60	0
57	MG	1A	3612	1/1	0.90	0.10	35,35,35,35	0
57	MG	2A	3234	1/1	0.90	0.17	81,81,81,81	0
57	MG	1x	112	1/1	0.90	0.11	69,69,69,69	0
57	MG	2x	105	1/1	0.90	0.24	67,67,67,67	0
57	MG	2A	3401	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3654	1/1	0.90	0.19	48,48,48,48	0
57	MG	25	105	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3288	1/1	0.90	0.16	44,44,44,44	0
57	MG	1A	3616	1/1	0.90	0.07	34,34,34,34	0
57	MG	1A	4039	1/1	0.90	0.14	41,41,41,41	0
59	A1AE1	2A	3855	76/76	0.90	0.15	46,60,66,71	0
57	MG	1A	3894	1/1	0.91	0.08	66,66,66,66	0
57	MG	1O	204	1/1	0.91	0.09	45,45,45,45	0
57	MG	20	103	1/1	0.91	0.28	70,70,70,70	0
57	MG	2A	3353	1/1	0.91	0.24	49,49,49,49	0
57	MG	25	101	1/1	0.91	0.08	68,68,68,68	0
57	MG	1A	3664	1/1	0.91	0.11	53,53,53,53	0
57	MG	1A	3774	1/1	0.91	0.16	48,48,48,48	0
57	MG	1A	3666	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3305	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3361	1/1	0.91	0.13	64,64,64,64	0
57	MG	2A	3159	1/1	0.91	0.22	59,59,59,59	0
57	MG	2A	3366	1/1	0.91	0.22	58,58,58,58	0
57	MG	2a	1605	1/1	0.91	0.34	72,72,72,72	0
57	MG	1A	3782	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	4014	1/1	0.91	0.08	47,47,47,47	0
57	MG	2a	1608	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	3783	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	3673	1/1	0.91	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3650	1/1	0.91	0.17	69,69,69,69	0
57	MG	1A	3679	1/1	0.91	0.16	74,74,74,74	0
57	MG	2A	3378	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3380	1/1	0.91	0.21	44,44,44,44	0
57	MG	2A	3655	1/1	0.91	0.10	69,69,69,69	0
57	MG	1A	3185	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3683	1/1	0.91	0.09	50,50,50,50	0
57	MG	1A	3912	1/1	0.91	0.13	57,57,57,57	0
57	MG	2a	1621	1/1	0.91	0.13	74,74,74,74	0
57	MG	1A	3790	1/1	0.91	0.09	53,53,53,53	0
57	MG	2a	1623	1/1	0.91	0.15	54,54,54,54	0
57	MG	1A	3584	1/1	0.91	0.14	39,39,39,39	0
57	MG	2A	3666	1/1	0.91	0.10	61,61,61,61	0
57	MG	10	110	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3388	1/1	0.91	0.13	37,37,37,37	0
57	MG	10	111	1/1	0.91	0.25	70,70,70,70	0
57	MG	1A	3916	1/1	0.91	0.10	66,66,66,66	0
57	MG	1a	1770	1/1	0.91	0.10	68,68,68,68	0
57	MG	1A	3313	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3399	1/1	0.91	0.18	52,52,52,52	0
57	MG	1a	1786	1/1	0.91	0.24	52,52,52,52	0
57	MG	1a	1787	1/1	0.91	0.29	56,56,56,56	0
57	MG	1A	3369	1/1	0.91	0.26	65,65,65,65	0
57	MG	2A	3687	1/1	0.91	0.16	75,75,75,75	0
57	MG	1A	4038	1/1	0.91	0.14	32,32,32,32	0
57	MG	1a	1790	1/1	0.91	0.26	59,59,59,59	0
57	MG	13	104	1/1	0.91	0.09	50,50,50,50	0
57	MG	2a	1647	1/1	0.91	0.10	64,64,64,64	0
57	MG	2a	1648	1/1	0.91	0.22	52,52,52,52	0
57	MG	1A	3921	1/1	0.91	0.15	67,67,67,67	0
57	MG	1A	3799	1/1	0.91	0.08	65,65,65,65	0
57	MG	2A	3416	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3417	1/1	0.91	0.15	65,65,65,65	0
57	MG	1A	3688	1/1	0.91	0.09	23,23,23,23	0
57	MG	2A	3207	1/1	0.91	0.21	47,47,47,47	0
57	MG	2a	1667	1/1	0.91	0.32	77,77,77,77	0
57	MG	15	107	1/1	0.91	0.12	63,63,63,63	0
57	MG	2a	1669	1/1	0.91	0.22	63,63,63,63	0
57	MG	18	105	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3705	1/1	0.91	0.20	67,67,67,67	0
57	MG	1A	3805	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3314	1/1	0.91	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3223	1/1	0.91	0.19	54,54,54,54	0
57	MG	2a	1679	1/1	0.91	0.23	55,55,55,55	0
57	MG	1a	1604	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3439	1/1	0.91	0.19	63,63,63,63	0
57	MG	2a	1683	1/1	0.91	0.12	68,68,68,68	0
57	MG	2A	3716	1/1	0.91	0.15	60,60,60,60	0
57	MG	1A	3808	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1609	1/1	0.91	0.40	61,61,61,61	0
57	MG	1a	1811	1/1	0.91	0.14	74,74,74,74	0
57	MG	1A	3373	1/1	0.91	0.23	58,58,58,58	0
57	MG	1a	1613	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	1693	1/1	0.91	0.12	67,67,67,67	0
57	MG	1e	201	1/1	0.91	0.12	68,68,68,68	0
57	MG	1A	4057	1/1	0.91	0.18	58,58,58,58	0
57	MG	2A	3241	1/1	0.91	0.14	48,48,48,48	0
57	MG	1n	101	1/1	0.91	0.37	65,65,65,65	0
57	MG	1v	101	1/1	0.91	0.20	68,68,68,68	0
57	MG	1a	1622	1/1	0.91	0.21	60,60,60,60	0
57	MG	2A	3745	1/1	0.91	0.16	72,72,72,72	0
57	MG	2A	3475	1/1	0.91	0.16	41,41,41,41	0
57	MG	2A	3748	1/1	0.91	0.09	48,48,48,48	0
57	MG	2A	3478	1/1	0.91	0.10	35,35,35,35	0
57	MG	1a	1623	1/1	0.91	0.25	63,63,63,63	0
57	MG	1A	3930	1/1	0.91	0.13	38,38,38,38	0
57	MG	2A	3486	1/1	0.91	0.17	68,68,68,68	0
57	MG	2a	1711	1/1	0.91	0.16	57,57,57,57	0
57	MG	2A	3489	1/1	0.91	0.09	46,46,46,46	0
57	MG	2A	3492	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3123	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3599	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3936	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3322	1/1	0.91	0.13	52,52,52,52	0
57	MG	1A	3203	1/1	0.91	0.23	53,53,53,53	0
57	MG	2A	3769	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3071	1/1	0.91	0.14	38,38,38,38	0
57	MG	1A	3713	1/1	0.91	0.13	34,34,34,34	0
57	MG	1A	4079	1/1	0.91	0.19	39,39,39,39	0
57	MG	2a	1734	1/1	0.91	0.16	65,65,65,65	0
57	MG	1A	3075	1/1	0.91	0.15	31,31,31,31	0
57	MG	1A	3843	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3080	1/1	0.91	0.16	58,58,58,58	0
57	MG	1B	206	1/1	0.91	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3960	1/1	0.91	0.08	54,54,54,54	0
57	MG	2a	1753	1/1	0.91	0.09	67,67,67,67	0
57	MG	1A	3348	1/1	0.91	0.10	50,50,50,50	0
57	MG	2a	1757	1/1	0.91	0.14	65,65,65,65	0
57	MG	2A	3275	1/1	0.91	0.29	63,63,63,63	0
57	MG	1A	3534	1/1	0.91	0.14	40,40,40,40	0
57	MG	2A	3797	1/1	0.91	0.08	56,56,56,56	0
57	MG	2a	1762	1/1	0.91	0.20	58,58,58,58	0
57	MG	2A	3529	1/1	0.91	0.09	55,55,55,55	0
57	MG	2A	3009	1/1	0.91	0.23	63,63,63,63	0
57	MG	1a	1666	1/1	0.91	0.26	63,63,63,63	0
57	MG	1B	213	1/1	0.91	0.14	56,56,56,56	0
57	MG	2A	3031	1/1	0.91	0.11	44,44,44,44	0
57	MG	2a	1771	1/1	0.91	0.33	67,67,67,67	0
57	MG	2A	3283	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1669	1/1	0.91	0.22	68,68,68,68	0
57	MG	1A	3294	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3538	1/1	0.91	0.18	43,43,43,43	0
57	MG	1A	3856	1/1	0.91	0.11	37,37,37,37	0
57	MG	1a	1673	1/1	0.91	0.25	62,62,62,62	0
57	MG	2A	3822	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3823	1/1	0.91	0.19	68,68,68,68	0
57	MG	1A	3967	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3059	1/1	0.91	0.23	61,61,61,61	0
57	MG	1a	1676	1/1	0.91	0.26	52,52,52,52	0
57	MG	2A	3297	1/1	0.91	0.21	60,60,60,60	0
57	MG	1A	3860	1/1	0.91	0.09	25,25,25,25	0
57	MG	2A	3566	1/1	0.91	0.17	60,60,60,60	0
57	MG	2a	1791	1/1	0.91	0.15	62,62,62,62	0
57	MG	1B	224	1/1	0.91	0.08	49,49,49,49	0
57	MG	1A	3546	1/1	0.91	0.25	54,54,54,54	0
57	MG	1B	227	1/1	0.91	0.09	40,40,40,40	0
57	MG	1A	3446	1/1	0.91	0.11	43,43,43,43	0
57	MG	1A	3448	1/1	0.91	0.15	69,69,69,69	0
57	MG	2A	3573	1/1	0.91	0.17	45,45,45,45	0
57	MG	2A	3848	1/1	0.91	0.23	62,62,62,62	0
57	MG	2A	3085	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3640	1/1	0.91	0.12	29,29,29,29	0
57	MG	1a	1693	1/1	0.91	0.30	64,64,64,64	0
57	MG	1A	3353	1/1	0.91	0.29	38,38,38,38	0
57	MG	1B	236	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3094	1/1	0.91	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3096	1/1	0.91	0.19	58,58,58,58	0
57	MG	2A	3323	1/1	0.91	0.17	61,61,61,61	0
57	MG	1A	3401	1/1	0.91	0.18	43,43,43,43	0
57	MG	2A	3326	1/1	0.91	0.30	69,69,69,69	0
57	MG	1A	3248	1/1	0.91	0.25	53,53,53,53	0
57	MG	1E	308	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3105	1/1	0.91	0.17	66,66,66,66	0
57	MG	1A	3558	1/1	0.91	0.12	40,40,40,40	0
57	MG	2A	3112	1/1	0.91	0.20	58,58,58,58	0
57	MG	1a	1711	1/1	0.91	0.17	46,46,46,46	0
57	MG	1A	3224	1/1	0.91	0.16	68,68,68,68	0
57	MG	2A	3337	1/1	0.91	0.24	60,60,60,60	0
57	MG	2A	3616	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	3759	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3166	1/1	0.91	0.10	57,57,57,57	0
57	MG	2w	105	1/1	0.91	0.22	51,51,51,51	0
57	MG	1a	1718	1/1	0.91	0.19	55,55,55,55	0
57	MG	2x	101	1/1	0.91	0.19	41,41,41,41	0
57	MG	2x	103	1/1	0.91	0.27	69,69,69,69	0
57	MG	1A	3364	1/1	0.91	0.30	47,47,47,47	0
57	MG	1F	313	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3624	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3344	1/1	0.91	0.18	60,60,60,60	0
57	MG	1A	3988	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3662	1/1	0.91	0.17	59,59,59,59	0
57	MG	1A	3996	1/1	0.91	0.06	14,14,14,14	0
57	MG	2A	3631	1/1	0.91	0.13	58,58,58,58	0
57	MG	1a	1810	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3376	1/1	0.92	0.26	65,65,65,65	0
57	MG	1A	3456	1/1	0.92	0.16	59,59,59,59	0
57	MG	2A	3379	1/1	0.92	0.33	53,53,53,53	0
57	MG	1a	1812	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	3457	1/1	0.92	0.11	66,66,66,66	0
57	MG	1a	1658	1/1	0.92	0.26	64,64,64,64	0
57	MG	2A	3646	1/1	0.92	0.12	49,49,49,49	0
57	MG	1d	301	1/1	0.92	0.14	59,59,59,59	0
57	MG	1A	3239	1/1	0.92	0.18	62,62,62,62	0
57	MG	1A	3905	1/1	0.92	0.13	64,64,64,64	0
57	MG	1h	201	1/1	0.92	0.10	72,72,72,72	0
57	MG	1B	235	1/1	0.92	0.12	48,48,48,48	0
57	MG	2A	3389	1/1	0.92	0.10	49,49,49,49	0
57	MG	1A	3346	1/1	0.92	0.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3210	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3657	1/1	0.92	0.10	61,61,61,61	0
57	MG	1A	3399	1/1	0.92	0.21	44,44,44,44	0
57	MG	1A	4006	1/1	0.92	0.08	44,44,44,44	0
57	MG	2a	1615	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3661	1/1	0.92	0.11	69,69,69,69	0
57	MG	1A	3473	1/1	0.92	0.13	60,60,60,60	0
57	MG	1A	3119	1/1	0.92	0.16	54,54,54,54	0
57	MG	1A	3271	1/1	0.92	0.10	28,28,28,28	0
57	MG	1x	102	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3272	1/1	0.92	0.24	48,48,48,48	0
57	MG	1x	105	1/1	0.92	0.12	56,56,56,56	0
57	MG	1A	3592	1/1	0.92	0.08	31,31,31,31	0
57	MG	2A	3409	1/1	0.92	0.13	51,51,51,51	0
57	MG	1A	3061	1/1	0.92	0.23	48,48,48,48	0
57	MG	2a	1627	1/1	0.92	0.14	58,58,58,58	0
57	MG	1F	304	1/1	0.92	0.09	65,65,65,65	0
57	MG	2A	3415	1/1	0.92	0.23	64,64,64,64	0
57	MG	1A	3312	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3002	1/1	0.92	0.10	48,48,48,48	0
57	MG	2A	3240	1/1	0.92	0.23	67,67,67,67	0
57	MG	2A	3685	1/1	0.92	0.09	42,42,42,42	0
57	MG	1A	4026	1/1	0.92	0.27	67,67,67,67	0
57	MG	1a	1680	1/1	0.92	0.18	57,57,57,57	0
57	MG	2a	1638	1/1	0.92	0.29	65,65,65,65	0
57	MG	2a	1639	1/1	0.92	0.24	66,66,66,66	0
57	MG	1a	1681	1/1	0.92	0.35	57,57,57,57	0
57	MG	1A	3706	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3246	1/1	0.92	0.12	60,60,60,60	0
57	MG	1N	205	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3435	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3004	1/1	0.92	0.30	63,63,63,63	0
57	MG	2A	3699	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3250	1/1	0.92	0.17	57,57,57,57	0
57	MG	2A	3441	1/1	0.92	0.14	53,53,53,53	0
57	MG	2a	1652	1/1	0.92	0.10	75,75,75,75	0
57	MG	1a	1685	1/1	0.92	0.17	58,58,58,58	0
57	MG	2a	1654	1/1	0.92	0.15	64,64,64,64	0
57	MG	1A	3280	1/1	0.92	0.21	55,55,55,55	0
57	MG	2A	3446	1/1	0.92	0.19	51,51,51,51	0
57	MG	1O	201	1/1	0.92	0.10	68,68,68,68	0
57	MG	2a	1661	1/1	0.92	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1662	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	1690	1/1	0.92	0.22	56,56,56,56	0
57	MG	2A	3023	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3456	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3258	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3713	1/1	0.92	0.11	56,56,56,56	0
57	MG	2A	3028	1/1	0.92	0.24	67,67,67,67	0
57	MG	2A	3717	1/1	0.92	0.40	48,48,48,48	0
57	MG	2A	3260	1/1	0.92	0.16	58,58,58,58	0
57	MG	2a	1676	1/1	0.92	0.18	62,62,62,62	0
57	MG	1A	3822	1/1	0.92	0.17	40,40,40,40	0
57	MG	1A	3415	1/1	0.92	0.17	37,37,37,37	0
57	MG	2A	3034	1/1	0.92	0.09	39,39,39,39	0
57	MG	1A	3828	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3606	1/1	0.92	0.07	28,28,28,28	0
57	MG	1A	3832	1/1	0.92	0.13	22,22,22,22	0
57	MG	2A	3730	1/1	0.92	0.09	57,57,57,57	0
57	MG	2A	3047	1/1	0.92	0.09	52,52,52,52	0
57	MG	2A	3485	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3273	1/1	0.92	0.16	59,59,59,59	0
57	MG	2A	3742	1/1	0.92	0.15	65,65,65,65	0
57	MG	1S	3603	1/1	0.92	0.09	59,59,59,59	0
57	MG	1T	201	1/1	0.92	0.10	57,57,57,57	0
57	MG	1A	3316	1/1	0.92	0.11	62,62,62,62	0
57	MG	2A	3058	1/1	0.92	0.23	60,60,60,60	0
57	MG	1A	3317	1/1	0.92	0.16	61,61,61,61	0
57	MG	2A	3750	1/1	0.92	0.12	64,64,64,64	0
57	MG	1A	4041	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3280	1/1	0.92	0.16	63,63,63,63	0
57	MG	1A	4042	1/1	0.92	0.19	66,66,66,66	0
57	MG	2A	3504	1/1	0.92	0.14	53,53,53,53	0
57	MG	2A	3065	1/1	0.92	0.23	65,65,65,65	0
57	MG	1A	3319	1/1	0.92	0.19	69,69,69,69	0
57	MG	1A	3419	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3509	1/1	0.92	0.11	50,50,50,50	0
57	MG	2A	3762	1/1	0.92	0.11	74,74,74,74	0
57	MG	2A	3070	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	1722	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3074	1/1	0.92	0.15	53,53,53,53	0
57	MG	1A	3627	1/1	0.92	0.07	29,29,29,29	0
57	MG	2A	3082	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3514	1/1	0.92	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3949	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3004	1/1	0.92	0.13	43,43,43,43	0
57	MG	2a	1723	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3533	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3535	1/1	0.92	0.25	59,59,59,59	0
57	MG	2a	1730	1/1	0.92	0.10	64,64,64,64	0
57	MG	2a	1731	1/1	0.92	0.14	62,62,62,62	0
57	MG	1A	3371	1/1	0.92	0.16	66,66,66,66	0
57	MG	2A	3789	1/1	0.92	0.15	61,61,61,61	0
57	MG	2A	3305	1/1	0.92	0.26	54,54,54,54	0
57	MG	1A	3523	1/1	0.92	0.20	59,59,59,59	0
57	MG	1A	3101	1/1	0.92	0.11	46,46,46,46	0
57	MG	2a	1749	1/1	0.92	0.20	68,68,68,68	0
57	MG	2A	3796	1/1	0.92	0.10	75,75,75,75	0
57	MG	2A	3541	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3095	1/1	0.92	0.13	49,49,49,49	0
57	MG	11	104	1/1	0.92	0.08	45,45,45,45	0
57	MG	1A	3529	1/1	0.92	0.09	40,40,40,40	0
57	MG	12	102	1/1	0.92	0.13	49,49,49,49	0
57	MG	2A	3548	1/1	0.92	0.19	63,63,63,63	0
57	MG	2A	3549	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	3866	1/1	0.92	0.10	39,39,39,39	0
57	MG	2a	1763	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3553	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3810	1/1	0.92	0.10	41,41,41,41	0
57	MG	2A	3815	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	4072	1/1	0.92	0.19	58,58,58,58	0
57	MG	1A	3324	1/1	0.92	0.19	57,57,57,57	0
57	MG	2a	1770	1/1	0.92	0.19	65,65,65,65	0
57	MG	2A	3820	1/1	0.92	0.15	60,60,60,60	0
57	MG	2A	3557	1/1	0.92	0.26	65,65,65,65	0
57	MG	2A	3111	1/1	0.92	0.18	42,42,42,42	0
57	MG	1a	1748	1/1	0.92	0.09	69,69,69,69	0
57	MG	1A	3756	1/1	0.92	0.08	42,42,42,42	0
57	MG	1A	3238	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3330	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3328	1/1	0.92	0.21	67,67,67,67	0
57	MG	2A	3831	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3545	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3331	1/1	0.92	0.21	59,59,59,59	0
57	MG	1A	4093	1/1	0.92	0.25	53,53,53,53	0
57	MG	1B	202	1/1	0.92	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3837	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	3884	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3885	1/1	0.92	0.07	48,48,48,48	0
57	MG	1A	3656	1/1	0.92	0.17	57,57,57,57	0
57	MG	1B	210	1/1	0.92	0.15	60,60,60,60	0
57	MG	1a	1776	1/1	0.92	0.09	67,67,67,67	0
57	MG	1B	211	1/1	0.92	0.17	50,50,50,50	0
57	MG	1A	3385	1/1	0.92	0.14	57,57,57,57	0
57	MG	2a	1799	1/1	0.92	0.24	67,67,67,67	0
57	MG	2A	3342	1/1	0.92	0.10	70,70,70,70	0
57	MG	1A	3548	1/1	0.92	0.21	51,51,51,51	0
57	MG	2A	3592	1/1	0.92	0.17	41,41,41,41	0
57	MG	1a	1624	1/1	0.92	0.26	60,60,60,60	0
57	MG	2A	3604	1/1	0.92	0.13	61,61,61,61	0
57	MG	1a	1625	1/1	0.92	0.22	53,53,53,53	0
57	MG	1A	3776	1/1	0.92	0.15	60,60,60,60	0
57	MG	2A	3347	1/1	0.92	0.22	72,72,72,72	0
57	MG	1a	1632	1/1	0.92	0.25	67,67,67,67	0
57	MG	1a	1792	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3264	1/1	0.92	0.15	58,58,58,58	0
57	MG	1a	1637	1/1	0.92	0.15	54,54,54,54	0
57	MG	1a	1638	1/1	0.92	0.23	58,58,58,58	0
57	MG	2A	3173	1/1	0.92	0.24	66,66,66,66	0
57	MG	2A	3356	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3357	1/1	0.92	0.13	69,69,69,69	0
57	MG	2A	3619	1/1	0.92	0.14	52,52,52,52	0
57	MG	2r	101	1/1	0.92	0.14	72,72,72,72	0
57	MG	2t	201	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3358	1/1	0.92	0.18	70,70,70,70	0
57	MG	2A	3176	1/1	0.92	0.12	43,43,43,43	0
57	MG	2D	308	1/1	0.92	0.07	27,27,27,27	0
57	MG	2w	101	1/1	0.92	0.29	67,67,67,67	0
57	MG	2E	302	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3982	1/1	0.92	0.08	33,33,33,33	0
57	MG	2E	306	1/1	0.92	0.12	56,56,56,56	0
57	MG	1A	3439	1/1	0.92	0.13	58,58,58,58	0
57	MG	2A	3362	1/1	0.92	0.16	66,66,66,66	0
57	MG	1A	3665	1/1	0.92	0.20	50,50,50,50	0
57	MG	1B	223	1/1	0.92	0.15	64,64,64,64	0
57	MG	1A	3333	1/1	0.92	0.17	46,46,46,46	0
57	MG	1a	1806	1/1	0.92	0.14	54,54,54,54	0
57	MG	2P	201	1/1	0.92	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2P	202	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3370	1/1	0.92	0.13	68,68,68,68	0
57	MG	2A	3371	1/1	0.92	0.13	69,69,69,69	0
57	MG	1A	3336	1/1	0.92	0.20	45,45,45,45	0
59	A1AE1	1A	4094	76/76	0.92	0.12	29,49,58,64	0
57	MG	1A	3297	1/1	0.92	0.28	60,60,60,60	0
57	MG	1A	3796	1/1	0.93	0.09	20,20,20,20	0
57	MG	1a	1800	1/1	0.93	0.18	67,67,67,67	0
57	MG	20	101	1/1	0.93	0.11	58,58,58,58	0
57	MG	1A	3445	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3798	1/1	0.93	0.12	65,65,65,65	0
57	MG	2A	3374	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	3337	1/1	0.93	0.17	59,59,59,59	0
57	MG	25	103	1/1	0.93	0.13	58,58,58,58	0
57	MG	1A	3800	1/1	0.93	0.10	20,20,20,20	0
57	MG	2A	3377	1/1	0.93	0.18	45,45,45,45	0
57	MG	1a	1626	1/1	0.93	0.15	52,52,52,52	0
57	MG	1a	1627	1/1	0.93	0.24	61,61,61,61	0
57	MG	2A	3191	1/1	0.93	0.15	59,59,59,59	0
57	MG	1a	1629	1/1	0.93	0.20	48,48,48,48	0
57	MG	1A	3801	1/1	0.93	0.09	25,25,25,25	0
57	MG	1A	3304	1/1	0.93	0.18	65,65,65,65	0
57	MG	2A	3197	1/1	0.93	0.08	47,47,47,47	0
57	MG	1A	3678	1/1	0.93	0.07	27,27,27,27	0
57	MG	1A	4092	1/1	0.93	0.26	61,61,61,61	0
57	MG	1A	3150	1/1	0.93	0.18	38,38,38,38	0
57	MG	1a	1639	1/1	0.93	0.14	61,61,61,61	0
57	MG	2A	3656	1/1	0.93	0.09	36,36,36,36	0
57	MG	2a	1612	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	3453	1/1	0.93	0.10	48,48,48,48	0
57	MG	1B	204	1/1	0.93	0.18	56,56,56,56	0
57	MG	2A	3393	1/1	0.93	0.26	64,64,64,64	0
57	MG	1A	3560	1/1	0.93	0.08	44,44,44,44	0
57	MG	2A	3662	1/1	0.93	0.12	60,60,60,60	0
57	MG	2A	3208	1/1	0.93	0.22	58,58,58,58	0
57	MG	1a	1646	1/1	0.93	0.18	49,49,49,49	0
57	MG	2A	3211	1/1	0.93	0.17	64,64,64,64	0
57	MG	1A	3566	1/1	0.93	0.09	53,53,53,53	0
57	MG	2A	3667	1/1	0.93	0.13	69,69,69,69	0
57	MG	1A	3275	1/1	0.93	0.14	59,59,59,59	0
57	MG	1a	1651	1/1	0.93	0.27	68,68,68,68	0
57	MG	1w	105	1/1	0.93	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3942	1/1	0.93	0.07	12,12,12,12	0
57	MG	2A	3675	1/1	0.93	0.14	38,38,38,38	0
57	MG	1A	3946	1/1	0.93	0.09	61,61,61,61	0
57	MG	1a	1655	1/1	0.93	0.22	64,64,64,64	0
57	MG	2a	1632	1/1	0.93	0.26	48,48,48,48	0
57	MG	1A	3394	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3414	1/1	0.93	0.29	53,53,53,53	0
57	MG	2A	3230	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3683	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	3818	1/1	0.93	0.17	38,38,38,38	0
57	MG	2A	3232	1/1	0.93	0.12	64,64,64,64	0
57	MG	2A	3686	1/1	0.93	0.12	44,44,44,44	0
57	MG	2A	3419	1/1	0.93	0.12	63,63,63,63	0
57	MG	2A	3233	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3460	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3575	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3427	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3826	1/1	0.93	0.07	34,34,34,34	0
57	MG	1A	3827	1/1	0.93	0.08	37,37,37,37	0
57	MG	2A	3239	1/1	0.93	0.19	61,61,61,61	0
57	MG	2a	1649	1/1	0.93	0.14	70,70,70,70	0
57	MG	2a	1650	1/1	0.93	0.08	60,60,60,60	0
57	MG	2A	3433	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3307	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3398	1/1	0.93	0.18	61,61,61,61	0
57	MG	1A	3830	1/1	0.93	0.06	28,28,28,28	0
57	MG	1A	3350	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3472	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3311	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3443	1/1	0.93	0.09	35,35,35,35	0
57	MG	1A	3841	1/1	0.93	0.15	76,76,76,76	0
57	MG	1A	3083	1/1	0.93	0.20	42,42,42,42	0
57	MG	2A	3711	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3447	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3356	1/1	0.93	0.08	37,37,37,37	0
57	MG	2A	3715	1/1	0.93	0.09	47,47,47,47	0
57	MG	2a	1671	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3449	1/1	0.93	0.31	68,68,68,68	0
57	MG	1A	3407	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3168	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3851	1/1	0.93	0.21	24,24,24,24	0
57	MG	2A	3010	1/1	0.93	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3722	1/1	0.93	0.09	56,56,56,56	0
57	MG	2A	3459	1/1	0.93	0.25	45,45,45,45	0
57	MG	2A	3015	1/1	0.93	0.15	67,67,67,67	0
57	MG	2A	3017	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3728	1/1	0.93	0.15	42,42,42,42	0
57	MG	1A	3977	1/1	0.93	0.11	58,58,58,58	0
57	MG	1A	3597	1/1	0.93	0.09	34,34,34,34	0
57	MG	1A	3718	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3719	1/1	0.93	0.09	21,21,21,21	0
57	MG	2A	3476	1/1	0.93	0.17	53,53,53,53	0
57	MG	2A	3477	1/1	0.93	0.19	69,69,69,69	0
57	MG	1A	3857	1/1	0.93	0.13	33,33,33,33	0
57	MG	1A	3361	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3267	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1697	1/1	0.93	0.10	63,63,63,63	0
57	MG	1A	3182	1/1	0.93	0.09	44,44,44,44	0
57	MG	2a	1699	1/1	0.93	0.20	62,62,62,62	0
57	MG	1A	3486	1/1	0.93	0.21	50,50,50,50	0
57	MG	1a	1689	1/1	0.93	0.14	64,64,64,64	0
57	MG	2A	3490	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3864	1/1	0.93	0.07	32,32,32,32	0
57	MG	2A	3493	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3756	1/1	0.93	0.13	40,40,40,40	0
57	MG	2A	3495	1/1	0.93	0.08	35,35,35,35	0
57	MG	1A	3735	1/1	0.93	0.09	26,26,26,26	0
57	MG	2a	1709	1/1	0.93	0.16	48,48,48,48	0
57	MG	2A	3051	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	3867	1/1	0.93	0.10	48,48,48,48	0
57	MG	1G	204	1/1	0.93	0.19	60,60,60,60	0
57	MG	2a	1715	1/1	0.93	0.19	61,61,61,61	0
57	MG	1A	3281	1/1	0.93	0.17	53,53,53,53	0
57	MG	1A	3491	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3060	1/1	0.93	0.16	55,55,55,55	0
57	MG	1A	3609	1/1	0.93	0.09	55,55,55,55	0
57	MG	1A	3247	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3508	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3286	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3285	1/1	0.93	0.13	56,56,56,56	0
57	MG	1A	3877	1/1	0.93	0.10	72,72,72,72	0
57	MG	2A	3779	1/1	0.93	0.09	41,41,41,41	0
57	MG	2a	1729	1/1	0.93	0.09	60,60,60,60	0
57	MG	2A	3780	1/1	0.93	0.25	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1714	1/1	0.93	0.13	68,68,68,68	0
57	MG	1A	3495	1/1	0.93	0.09	61,61,61,61	0
57	MG	1A	3881	1/1	0.93	0.11	58,58,58,58	0
57	MG	1A	4013	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3070	1/1	0.93	0.16	40,40,40,40	0
57	MG	2A	3292	1/1	0.93	0.19	67,67,67,67	0
57	MG	2a	1744	1/1	0.93	0.14	68,68,68,68	0
57	MG	2a	1745	1/1	0.93	0.12	61,61,61,61	0
57	MG	2a	1746	1/1	0.93	0.13	76,76,76,76	0
57	MG	1A	3753	1/1	0.93	0.27	29,29,29,29	0
57	MG	2A	3295	1/1	0.93	0.15	65,65,65,65	0
57	MG	1A	3262	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3187	1/1	0.93	0.14	60,60,60,60	0
57	MG	1V	203	1/1	0.93	0.35	45,45,45,45	0
57	MG	2A	3302	1/1	0.93	0.09	38,38,38,38	0
57	MG	2a	1758	1/1	0.93	0.19	50,50,50,50	0
57	MG	2A	3803	1/1	0.93	0.08	57,57,57,57	0
57	MG	1a	1726	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3422	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3306	1/1	0.93	0.17	53,53,53,53	0
57	MG	1W	201	1/1	0.93	0.11	57,57,57,57	0
57	MG	1A	3325	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3309	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3812	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	4025	1/1	0.93	0.25	56,56,56,56	0
57	MG	2a	1768	1/1	0.93	0.18	70,70,70,70	0
57	MG	1A	3635	1/1	0.93	0.12	34,34,34,34	0
57	MG	2A	3098	1/1	0.93	0.16	48,48,48,48	0
57	MG	1Z	301	1/1	0.93	0.14	63,63,63,63	0
57	MG	2A	3554	1/1	0.93	0.14	65,65,65,65	0
57	MG	2A	3315	1/1	0.93	0.14	69,69,69,69	0
57	MG	2a	1775	1/1	0.93	0.19	64,64,64,64	0
57	MG	1A	3295	1/1	0.93	0.17	53,53,53,53	0
57	MG	2A	3102	1/1	0.93	0.17	55,55,55,55	0
57	MG	2a	1778	1/1	0.93	0.13	55,55,55,55	0
57	MG	1a	1740	1/1	0.93	0.09	57,57,57,57	0
57	MG	1A	3519	1/1	0.93	0.11	39,39,39,39	0
57	MG	2A	3322	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3638	1/1	0.93	0.07	30,30,30,30	0
57	MG	2A	3324	1/1	0.93	0.31	51,51,51,51	0
57	MG	2A	3110	1/1	0.93	0.10	73,73,73,73	0
57	MG	2a	1785	1/1	0.93	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3046	1/1	0.93	0.09	24,24,24,24	0
57	MG	1a	1746	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3426	1/1	0.93	0.13	67,67,67,67	0
57	MG	1A	3901	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	3233	1/1	0.93	0.14	72,72,72,72	0
57	MG	1A	3644	1/1	0.93	0.10	34,34,34,34	0
57	MG	2A	3120	1/1	0.93	0.19	71,71,71,71	0
57	MG	1A	3779	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3580	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3376	1/1	0.93	0.16	53,53,53,53	0
57	MG	1A	3146	1/1	0.93	0.14	57,57,57,57	0
57	MG	2a	1800	1/1	0.93	0.19	55,55,55,55	0
57	MG	2A	3852	1/1	0.93	0.13	69,69,69,69	0
57	MG	2A	3126	1/1	0.93	0.12	59,59,59,59	0
57	MG	2a	1803	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3854	1/1	0.93	0.11	68,68,68,68	0
57	MG	2A	3586	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3127	1/1	0.93	0.13	49,49,49,49	0
57	MG	2A	3128	1/1	0.93	0.14	51,51,51,51	0
57	MG	2B	203	1/1	0.93	0.23	68,68,68,68	0
57	MG	2B	204	1/1	0.93	0.15	73,73,73,73	0
57	MG	2d	302	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3382	1/1	0.93	0.13	57,57,57,57	0
57	MG	2A	3593	1/1	0.93	0.17	71,71,71,71	0
57	MG	1A	3302	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	4048	1/1	0.93	0.15	32,32,32,32	0
57	MG	1A	3911	1/1	0.93	0.17	48,48,48,48	0
57	MG	1A	3544	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3144	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3659	1/1	0.93	0.08	63,63,63,63	0
57	MG	1A	3437	1/1	0.93	0.16	39,39,39,39	0
57	MG	2A	3349	1/1	0.93	0.22	57,57,57,57	0
57	MG	1a	1601	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1778	1/1	0.93	0.10	63,63,63,63	0
57	MG	2A	3156	1/1	0.93	0.21	58,58,58,58	0
57	MG	2D	306	1/1	0.93	0.17	62,62,62,62	0
57	MG	1a	1779	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	3334	1/1	0.93	0.28	47,47,47,47	0
57	MG	1A	4059	1/1	0.93	0.20	34,34,34,34	0
57	MG	1A	3204	1/1	0.93	0.14	50,50,50,50	0
57	MG	2E	304	1/1	0.93	0.15	63,63,63,63	0
57	MG	2w	106	1/1	0.93	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3167	1/1	0.93	0.13	49,49,49,49	0
57	MG	2A	3622	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3919	1/1	0.93	0.11	49,49,49,49	0
57	MG	2E	310	1/1	0.93	0.14	45,45,45,45	0
57	MG	1a	1606	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	3443	1/1	0.93	0.18	52,52,52,52	0
57	MG	2F	3303	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3172	1/1	0.93	0.25	69,69,69,69	0
57	MG	1a	1611	1/1	0.93	0.12	64,64,64,64	0
57	MG	1A	4063	1/1	0.93	0.20	60,60,60,60	0
57	MG	2A	3177	1/1	0.93	0.17	45,45,45,45	0
57	MG	1A	3793	1/1	0.93	0.14	50,50,50,50	0
57	MG	1O	203	1/1	0.94	0.18	59,59,59,59	0
57	MG	2A	3248	1/1	0.94	0.21	68,68,68,68	0
57	MG	2A	3024	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3668	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3027	1/1	0.94	0.16	55,55,55,55	0
57	MG	1a	1687	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3253	1/1	0.94	0.11	62,62,62,62	0
57	MG	1A	3692	1/1	0.94	0.22	58,58,58,58	0
57	MG	1A	3177	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3695	1/1	0.94	0.14	41,41,41,41	0
57	MG	1a	1691	1/1	0.94	0.14	55,55,55,55	0
57	MG	2A	3440	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3042	1/1	0.94	0.15	65,65,65,65	0
57	MG	1A	3475	1/1	0.94	0.10	69,69,69,69	0
57	MG	2A	3044	1/1	0.94	0.14	67,67,67,67	0
57	MG	1A	3697	1/1	0.94	0.09	62,62,62,62	0
57	MG	1S	3601	1/1	0.94	0.20	46,46,46,46	0
57	MG	1A	3178	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3701	1/1	0.94	0.08	29,29,29,29	0
57	MG	2A	3052	1/1	0.94	0.21	69,69,69,69	0
57	MG	1A	3615	1/1	0.94	0.09	31,31,31,31	0
57	MG	1a	1705	1/1	0.94	0.19	66,66,66,66	0
57	MG	2A	3452	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3694	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3271	1/1	0.94	0.10	70,70,70,70	0
57	MG	1T	204	1/1	0.94	0.14	55,55,55,55	0
57	MG	1U	204	1/1	0.94	0.16	37,37,37,37	0
57	MG	1A	4032	1/1	0.94	0.12	55,55,55,55	0
57	MG	2A	3463	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3465	1/1	0.94	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3054	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3428	1/1	0.94	0.14	66,66,66,66	0
57	MG	1A	4035	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3549	1/1	0.94	0.07	23,23,23,23	0
57	MG	1X	105	1/1	0.94	0.11	51,51,51,51	0
57	MG	1a	1720	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3708	1/1	0.94	0.09	25,25,25,25	0
57	MG	1A	3811	1/1	0.94	0.07	25,25,25,25	0
57	MG	1A	3086	1/1	0.94	0.11	42,42,42,42	0
57	MG	2A	3480	1/1	0.94	0.09	22,22,22,22	0
57	MG	2A	3714	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3554	1/1	0.94	0.10	30,30,30,30	0
57	MG	2A	3081	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	4043	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3488	1/1	0.94	0.08	55,55,55,55	0
57	MG	10	103	1/1	0.94	0.10	45,45,45,45	0
57	MG	1A	3042	1/1	0.94	0.07	29,29,29,29	0
57	MG	1A	3815	1/1	0.94	0.12	34,34,34,34	0
57	MG	1a	1732	1/1	0.94	0.20	72,72,72,72	0
57	MG	2a	1656	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3816	1/1	0.94	0.13	36,36,36,36	0
57	MG	1A	3817	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3727	1/1	0.94	0.10	39,39,39,39	0
57	MG	2A	3294	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3498	1/1	0.94	0.07	29,29,29,29	0
57	MG	1A	4052	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3296	1/1	0.94	0.15	69,69,69,69	0
57	MG	2A	3733	1/1	0.94	0.12	71,71,71,71	0
57	MG	2A	3735	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3736	1/1	0.94	0.12	67,67,67,67	0
57	MG	1A	3716	1/1	0.94	0.08	34,34,34,34	0
57	MG	1A	3005	1/1	0.94	0.16	64,64,64,64	0
57	MG	2A	3300	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3277	1/1	0.94	0.13	59,59,59,59	0
57	MG	1A	3403	1/1	0.94	0.14	36,36,36,36	0
57	MG	2a	1678	1/1	0.94	0.18	53,53,53,53	0
57	MG	2A	3746	1/1	0.94	0.15	66,66,66,66	0
57	MG	1A	3639	1/1	0.94	0.09	52,52,52,52	0
57	MG	2a	1681	1/1	0.94	0.16	53,53,53,53	0
57	MG	1a	1745	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3510	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3729	1/1	0.94	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1685	1/1	0.94	0.33	57,57,57,57	0
57	MG	2a	1686	1/1	0.94	0.22	63,63,63,63	0
57	MG	1A	3488	1/1	0.94	0.25	56,56,56,56	0
57	MG	2A	3515	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3732	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3520	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3521	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3190	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3940	1/1	0.94	0.11	49,49,49,49	0
57	MG	17	103	1/1	0.94	0.24	52,52,52,52	0
57	MG	17	106	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3528	1/1	0.94	0.06	36,36,36,36	0
57	MG	1a	1756	1/1	0.94	0.09	61,61,61,61	0
57	MG	18	101	1/1	0.94	0.18	52,52,52,52	0
57	MG	2A	3766	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3192	1/1	0.94	0.08	48,48,48,48	0
57	MG	18	106	1/1	0.94	0.16	62,62,62,62	0
57	MG	2A	3772	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3536	1/1	0.94	0.11	68,68,68,68	0
57	MG	19	101	1/1	0.94	0.24	54,54,54,54	0
57	MG	2A	3123	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	4069	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3836	1/1	0.94	0.11	29,29,29,29	0
57	MG	1a	1768	1/1	0.94	0.21	60,60,60,60	0
57	MG	1A	3944	1/1	0.94	0.06	27,27,27,27	0
57	MG	1a	1771	1/1	0.94	0.09	68,68,68,68	0
57	MG	1A	3197	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3738	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	4082	1/1	0.94	0.20	38,38,38,38	0
57	MG	1A	4083	1/1	0.94	0.20	42,42,42,42	0
57	MG	1a	1783	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	4087	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3645	1/1	0.94	0.06	21,21,21,21	0
57	MG	1A	3844	1/1	0.94	0.13	55,55,55,55	0
57	MG	1a	1619	1/1	0.94	0.08	50,50,50,50	0
57	MG	1a	1620	1/1	0.94	0.24	64,64,64,64	0
57	MG	1A	3845	1/1	0.94	0.08	31,31,31,31	0
57	MG	2A	3562	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3846	1/1	0.94	0.08	49,49,49,49	0
57	MG	2A	3564	1/1	0.94	0.19	65,65,65,65	0
57	MG	1A	3957	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3165	1/1	0.94	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3567	1/1	0.94	0.17	61,61,61,61	0
57	MG	2a	1736	1/1	0.94	0.11	60,60,60,60	0
57	MG	1a	1796	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3959	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1739	1/1	0.94	0.14	60,60,60,60	0
57	MG	2a	1740	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3161	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3648	1/1	0.94	0.08	33,33,33,33	0
57	MG	1A	3650	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3048	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3747	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3175	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3126	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3827	1/1	0.94	0.19	57,57,57,57	0
57	MG	2a	1755	1/1	0.94	0.22	59,59,59,59	0
57	MG	1A	3377	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3583	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3658	1/1	0.94	0.09	41,41,41,41	0
57	MG	1a	1808	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3081	1/1	0.94	0.09	61,61,61,61	0
57	MG	1B	217	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3587	1/1	0.94	0.07	36,36,36,36	0
57	MG	1A	3862	1/1	0.94	0.15	37,37,37,37	0
57	MG	1A	3513	1/1	0.94	0.24	53,53,53,53	0
57	MG	1A	3586	1/1	0.94	0.08	26,26,26,26	0
57	MG	1a	1647	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3190	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3601	1/1	0.94	0.08	43,43,43,43	0
57	MG	2A	3846	1/1	0.94	0.08	69,69,69,69	0
57	MG	2A	3847	1/1	0.94	0.12	66,66,66,66	0
57	MG	2A	3602	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3603	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3365	1/1	0.94	0.15	75,75,75,75	0
57	MG	1A	3455	1/1	0.94	0.08	55,55,55,55	0
57	MG	2A	3606	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3367	1/1	0.94	0.24	71,71,71,71	0
57	MG	1A	3761	1/1	0.94	0.11	31,31,31,31	0
57	MG	1A	3318	1/1	0.94	0.25	50,50,50,50	0
57	MG	1a	1652	1/1	0.94	0.13	56,56,56,56	0
57	MG	2A	3196	1/1	0.94	0.20	63,63,63,63	0
57	MG	2A	3612	1/1	0.94	0.15	60,60,60,60	0
57	MG	1k	201	1/1	0.94	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3198	1/1	0.94	0.16	70,70,70,70	0
57	MG	1l	3200	1/1	0.94	0.06	73,73,73,73	0
57	MG	1A	3138	1/1	0.94	0.07	36,36,36,36	0
57	MG	1A	3765	1/1	0.94	0.09	39,39,39,39	0
57	MG	1w	101	1/1	0.94	0.14	51,51,51,51	0
57	MG	1w	103	1/1	0.94	0.23	63,63,63,63	0
57	MG	1A	3766	1/1	0.94	0.06	26,26,26,26	0
57	MG	1A	3768	1/1	0.94	0.07	29,29,29,29	0
57	MG	2a	1794	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3770	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3209	1/1	0.94	0.23	61,61,61,61	0
57	MG	1A	3667	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3458	1/1	0.94	0.18	44,44,44,44	0
57	MG	1A	3671	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3672	1/1	0.94	0.13	67,67,67,67	0
57	MG	2A	3630	1/1	0.94	0.15	58,58,58,58	0
57	MG	1E	301	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3082	1/1	0.94	0.08	67,67,67,67	0
57	MG	2A	3221	1/1	0.94	0.28	51,51,51,51	0
57	MG	2A	3391	1/1	0.94	0.37	67,67,67,67	0
57	MG	1A	3998	1/1	0.94	0.13	52,52,52,52	0
57	MG	2a	1808	1/1	0.94	0.21	54,54,54,54	0
57	MG	1a	1667	1/1	0.94	0.14	68,68,68,68	0
57	MG	1A	3386	1/1	0.94	0.13	62,62,62,62	0
57	MG	2d	301	1/1	0.94	0.32	57,57,57,57	0
57	MG	2A	3395	1/1	0.94	0.31	62,62,62,62	0
57	MG	2A	3227	1/1	0.94	0.25	52,52,52,52	0
57	MG	1A	4001	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3321	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3889	1/1	0.94	0.11	62,62,62,62	0
57	MG	1A	3467	1/1	0.94	0.24	34,34,34,34	0
57	MG	1F	310	1/1	0.94	0.12	54,54,54,54	0
57	MG	1A	4007	1/1	0.94	0.09	41,41,41,41	0
57	MG	1A	3681	1/1	0.94	0.14	52,52,52,52	0
57	MG	2q	201	1/1	0.94	0.09	65,65,65,65	0
57	MG	2R	201	1/1	0.94	0.14	61,61,61,61	0
57	MG	2T	201	1/1	0.94	0.09	61,61,61,61	0
57	MG	2T	202	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3408	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3358	1/1	0.94	0.11	46,46,46,46	0
57	MG	2W	201	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3537	1/1	0.94	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3653	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3412	1/1	0.94	0.15	50,50,50,50	0
57	MG	1I	201	1/1	0.94	0.07	52,52,52,52	0
57	MG	21	101	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3265	1/1	0.94	0.09	58,58,58,58	0
57	MG	25	102	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3608	1/1	0.94	0.06	23,23,23,23	0
57	MG	25	104	1/1	0.94	0.07	50,50,50,50	0
57	MG	1a	1683	1/1	0.94	0.24	55,55,55,55	0
57	MG	2A	3016	1/1	0.94	0.14	49,49,49,49	0
57	MG	2x	107	1/1	0.94	0.17	53,53,53,53	0
57	MG	27	102	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3244	1/1	0.94	0.13	58,58,58,58	0
57	MG	1A	3539	1/1	0.94	0.25	41,41,41,41	0
57	MG	28	103	1/1	0.94	0.29	59,59,59,59	0
57	MG	29	101	1/1	0.94	0.21	65,65,65,65	0
58	K	2A	3423	1/1	0.94	0.07	52,52,52,52	0
57	MG	2A	3422	1/1	0.94	0.27	60,60,60,60	0
57	MG	1A	3690	1/1	0.94	0.09	27,27,27,27	0
60	ZN	24	501	1/1	0.94	0.13	118,118,118,118	0
57	MG	1l	3201	1/1	0.95	0.14	54,54,54,54	0
57	MG	1m	3001	1/1	0.95	0.13	56,56,56,56	0
57	MG	2A	3213	1/1	0.95	0.31	61,61,61,61	0
57	MG	2a	1601	1/1	0.95	0.08	55,55,55,55	0
57	MG	1a	1635	1/1	0.95	0.28	62,62,62,62	0
57	MG	1n	102	1/1	0.95	0.08	45,45,45,45	0
57	MG	1r	101	1/1	0.95	0.21	58,58,58,58	0
57	MG	2A	3219	1/1	0.95	0.21	57,57,57,57	0
57	MG	2A	3220	1/1	0.95	0.25	43,43,43,43	0
57	MG	1A	3839	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3620	1/1	0.95	0.06	20,20,20,20	0
57	MG	1w	102	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3963	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3621	1/1	0.95	0.07	19,19,19,19	0
57	MG	2A	3677	1/1	0.95	0.09	47,47,47,47	0
57	MG	1B	216	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3431	1/1	0.95	0.09	47,47,47,47	0
57	MG	1a	1642	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3842	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3360	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3235	1/1	0.95	0.06	37,37,37,37	0
57	MG	1a	1648	1/1	0.95	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	103	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3122	1/1	0.95	0.09	41,41,41,41	0
57	MG	2A	3237	1/1	0.95	0.26	65,65,65,65	0
57	MG	1A	3301	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3737	1/1	0.95	0.14	58,58,58,58	0
57	MG	1A	3050	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3740	1/1	0.95	0.04	23,23,23,23	0
57	MG	1A	3077	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3027	1/1	0.95	0.20	34,34,34,34	0
57	MG	1A	3136	1/1	0.95	0.12	41,41,41,41	0
57	MG	2a	1631	1/1	0.95	0.21	43,43,43,43	0
57	MG	2A	3698	1/1	0.95	0.20	61,61,61,61	0
57	MG	1B	232	1/1	0.95	0.06	44,44,44,44	0
57	MG	2A	3700	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3979	1/1	0.95	0.09	59,59,59,59	0
57	MG	1x	114	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3455	1/1	0.95	0.28	57,57,57,57	0
57	MG	1A	3530	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3002	1/1	0.95	0.21	49,49,49,49	0
57	MG	2A	3458	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	3057	1/1	0.95	0.05	45,45,45,45	0
57	MG	2A	3460	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3641	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3252	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3464	1/1	0.95	0.42	72,72,72,72	0
57	MG	2a	1646	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3186	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3006	1/1	0.95	0.12	45,45,45,45	0
57	MG	1D	312	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3433	1/1	0.95	0.11	51,51,51,51	0
57	MG	2A	3471	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3040	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3474	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3249	1/1	0.95	0.07	47,47,47,47	0
57	MG	2A	3721	1/1	0.95	0.12	62,62,62,62	0
57	MG	1A	3865	1/1	0.95	0.07	69,69,69,69	0
57	MG	1A	3992	1/1	0.95	0.10	53,53,53,53	0
57	MG	2a	1659	1/1	0.95	0.48	68,68,68,68	0
57	MG	1A	3541	1/1	0.95	0.20	44,44,44,44	0
57	MG	2A	3262	1/1	0.95	0.16	50,50,50,50	0
57	MG	1E	316	1/1	0.95	0.05	37,37,37,37	0
57	MG	2a	1664	1/1	0.95	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3995	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3484	1/1	0.95	0.10	62,62,62,62	0
57	MG	2A	3265	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3757	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3732	1/1	0.95	0.08	57,57,57,57	0
57	MG	1A	3260	1/1	0.95	0.11	50,50,50,50	0
57	MG	2a	1672	1/1	0.95	0.10	53,53,53,53	0
57	MG	1a	1677	1/1	0.95	0.24	59,59,59,59	0
57	MG	1F	312	1/1	0.95	0.12	30,30,30,30	0
57	MG	1A	3440	1/1	0.95	0.17	46,46,46,46	0
57	MG	2A	3036	1/1	0.95	0.12	43,43,43,43	0
57	MG	1F	314	1/1	0.95	0.16	42,42,42,42	0
57	MG	2A	3039	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3744	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3041	1/1	0.95	0.19	54,54,54,54	0
57	MG	1A	3651	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3499	1/1	0.95	0.10	64,64,64,64	0
57	MG	1A	3442	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3654	1/1	0.95	0.15	40,40,40,40	0
57	MG	1H	201	1/1	0.95	0.24	48,48,48,48	0
57	MG	1A	3144	1/1	0.95	0.34	34,34,34,34	0
57	MG	2A	3281	1/1	0.95	0.23	62,62,62,62	0
57	MG	2A	3754	1/1	0.95	0.16	59,59,59,59	0
57	MG	1A	3021	1/1	0.95	0.14	51,51,51,51	0
57	MG	1N	202	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3378	1/1	0.95	0.10	49,49,49,49	0
57	MG	2a	1692	1/1	0.95	0.09	56,56,56,56	0
57	MG	1N	206	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3055	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3056	1/1	0.95	0.15	64,64,64,64	0
57	MG	1A	3148	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3552	1/1	0.95	0.07	24,24,24,24	0
57	MG	2A	3518	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3764	1/1	0.95	0.06	63,63,63,63	0
57	MG	1O	202	1/1	0.95	0.20	54,54,54,54	0
57	MG	1A	3771	1/1	0.95	0.07	33,33,33,33	0
57	MG	2A	3768	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3381	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	4016	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	4018	1/1	0.95	0.09	48,48,48,48	0
57	MG	1a	1701	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	3450	1/1	0.95	0.30	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1703	1/1	0.95	0.15	59,59,59,59	0
57	MG	1A	3775	1/1	0.95	0.20	47,47,47,47	0
57	MG	1Q	208	1/1	0.95	0.08	37,37,37,37	0
57	MG	1A	3193	1/1	0.95	0.25	56,56,56,56	0
57	MG	2A	3534	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3149	1/1	0.95	0.06	34,34,34,34	0
57	MG	2A	3080	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3778	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3199	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3559	1/1	0.95	0.14	50,50,50,50	0
57	MG	1U	203	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3200	1/1	0.95	0.08	47,47,47,47	0
57	MG	1U	205	1/1	0.95	0.10	30,30,30,30	0
57	MG	1U	207	1/1	0.95	0.19	46,46,46,46	0
57	MG	2a	1725	1/1	0.95	0.12	61,61,61,61	0
57	MG	2a	1727	1/1	0.95	0.08	60,60,60,60	0
57	MG	1A	3010	1/1	0.95	0.14	52,52,52,52	0
57	MG	2A	3801	1/1	0.95	0.07	23,23,23,23	0
57	MG	1A	3323	1/1	0.95	0.25	36,36,36,36	0
57	MG	1V	206	1/1	0.95	0.13	57,57,57,57	0
57	MG	1V	207	1/1	0.95	0.07	34,34,34,34	0
57	MG	2a	1733	1/1	0.95	0.12	69,69,69,69	0
57	MG	1A	3461	1/1	0.95	0.11	25,25,25,25	0
57	MG	2A	3551	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3676	1/1	0.95	0.08	52,52,52,52	0
57	MG	1A	3389	1/1	0.95	0.10	42,42,42,42	0
57	MG	2A	3321	1/1	0.95	0.09	62,62,62,62	0
57	MG	1X	103	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3813	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3273	1/1	0.95	0.18	54,54,54,54	0
57	MG	1a	1736	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3109	1/1	0.95	0.07	41,41,41,41	0
57	MG	2a	1747	1/1	0.95	0.13	50,50,50,50	0
57	MG	1X	106	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3906	1/1	0.95	0.10	67,67,67,67	0
57	MG	2a	1751	1/1	0.95	0.12	65,65,65,65	0
57	MG	1A	3578	1/1	0.95	0.06	28,28,28,28	0
57	MG	1A	3087	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3909	1/1	0.95	0.12	26,26,26,26	0
57	MG	1Z	303	1/1	0.95	0.16	53,53,53,53	0
57	MG	2a	1756	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3682	1/1	0.95	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3117	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3794	1/1	0.95	0.09	53,53,53,53	0
57	MG	10	104	1/1	0.95	0.18	49,49,49,49	0
57	MG	1A	3094	1/1	0.95	0.21	36,36,36,36	0
57	MG	10	107	1/1	0.95	0.06	41,41,41,41	0
57	MG	2A	3576	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	3913	1/1	0.95	0.09	59,59,59,59	0
57	MG	2A	3836	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3125	1/1	0.95	0.29	62,62,62,62	0
57	MG	1A	3154	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3278	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3474	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3917	1/1	0.95	0.08	68,68,68,68	0
57	MG	1A	4053	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3397	1/1	0.95	0.20	40,40,40,40	0
57	MG	12	101	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3689	1/1	0.95	0.10	32,32,32,32	0
57	MG	2A	3589	1/1	0.95	0.12	49,49,49,49	0
57	MG	2A	3350	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3802	1/1	0.95	0.06	34,34,34,34	0
57	MG	2A	3145	1/1	0.95	0.28	55,55,55,55	0
57	MG	1A	3155	1/1	0.95	0.07	28,28,28,28	0
57	MG	1A	3213	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3150	1/1	0.95	0.16	35,35,35,35	0
57	MG	2A	3152	1/1	0.95	0.11	66,66,66,66	0
57	MG	15	102	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3215	1/1	0.95	0.12	56,56,56,56	0
57	MG	1a	1773	1/1	0.95	0.07	64,64,64,64	0
57	MG	1a	1775	1/1	0.95	0.07	77,77,77,77	0
57	MG	2A	3160	1/1	0.95	0.10	37,37,37,37	0
57	MG	2A	3161	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3363	1/1	0.95	0.18	53,53,53,53	0
57	MG	1A	3222	1/1	0.95	0.10	40,40,40,40	0
57	MG	2B	211	1/1	0.95	0.24	68,68,68,68	0
57	MG	1A	3594	1/1	0.95	0.06	30,30,30,30	0
57	MG	16	101	1/1	0.95	0.07	59,59,59,59	0
57	MG	2a	1796	1/1	0.95	0.16	68,68,68,68	0
57	MG	1A	3927	1/1	0.95	0.17	48,48,48,48	0
57	MG	1a	1781	1/1	0.95	0.08	58,58,58,58	0
57	MG	1a	1782	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	4064	1/1	0.95	0.12	39,39,39,39	0
57	MG	1a	1784	1/1	0.95	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2D	303	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3283	1/1	0.95	0.23	60,60,60,60	0
57	MG	18	104	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3174	1/1	0.95	0.12	52,52,52,52	0
57	MG	2E	301	1/1	0.95	0.15	59,59,59,59	0
57	MG	1A	3338	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3284	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3342	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3223	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3604	1/1	0.95	0.05	31,31,31,31	0
57	MG	2E	308	1/1	0.95	0.12	74,74,74,74	0
57	MG	1A	4078	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3017	1/1	0.95	0.11	49,49,49,49	0
57	MG	2E	311	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	4081	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3104	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3711	1/1	0.95	0.06	36,36,36,36	0
57	MG	2G	201	1/1	0.95	0.09	57,57,57,57	0
57	MG	2A	3187	1/1	0.95	0.09	70,70,70,70	0
57	MG	1A	4084	1/1	0.95	0.11	57,57,57,57	0
57	MG	2A	3387	1/1	0.95	0.21	58,58,58,58	0
57	MG	1A	3292	1/1	0.95	0.26	54,54,54,54	0
57	MG	1A	3293	1/1	0.95	0.11	50,50,50,50	0
57	MG	1a	1614	1/1	0.95	0.20	61,61,61,61	0
57	MG	2R	202	1/1	0.95	0.06	41,41,41,41	0
57	MG	1a	1615	1/1	0.95	0.12	41,41,41,41	0
57	MG	1a	1618	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3112	1/1	0.95	0.17	49,49,49,49	0
57	MG	2U	201	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3945	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	4091	1/1	0.95	0.08	47,47,47,47	0
57	MG	2X	101	1/1	0.95	0.12	57,57,57,57	0
57	MG	1A	3049	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3296	1/1	0.95	0.14	55,55,55,55	0
57	MG	2x	102	1/1	0.95	0.20	63,63,63,63	0
57	MG	1A	4095	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3165	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3831	1/1	0.95	0.11	32,32,32,32	0
57	MG	23	101	1/1	0.95	0.15	64,64,64,64	0
57	MG	1A	3512	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3833	1/1	0.95	0.08	31,31,31,31	0
57	MG	2A	3405	1/1	0.95	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3617	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3727	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3837	1/1	0.95	0.08	27,27,27,27	0
57	MG	1a	1634	1/1	0.95	0.08	60,60,60,60	0
57	MG	27	103	1/1	0.95	0.10	55,55,55,55	0
60	ZN	14	102	1/1	0.95	0.11	107,107,107,107	0
57	MG	2A	3411	1/1	0.95	0.34	60,60,60,60	0
57	MG	1A	3781	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3491	1/1	0.96	0.08	40,40,40,40	0
57	MG	2A	3075	1/1	0.96	0.15	50,50,50,50	0
57	MG	2A	3076	1/1	0.96	0.21	41,41,41,41	0
57	MG	2a	1626	1/1	0.96	0.23	68,68,68,68	0
57	MG	2A	3078	1/1	0.96	0.14	30,30,30,30	0
57	MG	1W	206	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3444	1/1	0.96	0.23	41,41,41,41	0
57	MG	1a	1729	1/1	0.96	0.10	49,49,49,49	0
57	MG	2A	3725	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3038	1/1	0.96	0.17	30,30,30,30	0
57	MG	2A	3083	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3266	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3447	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3089	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3060	1/1	0.96	0.04	24,24,24,24	0
57	MG	1a	1735	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3298	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3268	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3789	1/1	0.96	0.08	61,61,61,61	0
57	MG	2A	3738	1/1	0.96	0.09	71,71,71,71	0
57	MG	1A	3001	1/1	0.96	0.06	42,42,42,42	0
57	MG	10	101	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3270	1/1	0.96	0.12	40,40,40,40	0
57	MG	2A	3513	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3099	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3670	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3454	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3205	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3098	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3007	1/1	0.96	0.09	22,22,22,22	0
57	MG	10	109	1/1	0.96	0.20	64,64,64,64	0
57	MG	2A	3108	1/1	0.96	0.27	58,58,58,58	0
57	MG	2A	3313	1/1	0.96	0.15	55,55,55,55	0
57	MG	1A	3562	1/1	0.96	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3563	1/1	0.96	0.09	12,12,12,12	0
57	MG	1A	3327	1/1	0.96	0.13	46,46,46,46	0
57	MG	1a	1751	1/1	0.96	0.06	76,76,76,76	0
57	MG	1A	3568	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	4066	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3043	1/1	0.96	0.06	31,31,31,31	0
57	MG	1l	106	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3105	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3573	1/1	0.96	0.07	52,52,52,52	0
57	MG	1a	1760	1/1	0.96	0.06	65,65,65,65	0
57	MG	13	102	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3542	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3214	1/1	0.96	0.26	47,47,47,47	0
57	MG	1A	3106	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	4076	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3771	1/1	0.96	0.11	74,74,74,74	0
57	MG	1A	3396	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3331	1/1	0.96	0.10	63,63,63,63	0
57	MG	15	104	1/1	0.96	0.13	32,32,32,32	0
57	MG	2A	3776	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3216	1/1	0.96	0.27	37,37,37,37	0
57	MG	2A	3334	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3581	1/1	0.96	0.07	24,24,24,24	0
57	MG	2A	3130	1/1	0.96	0.08	67,67,67,67	0
57	MG	2A	3133	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3691	1/1	0.96	0.04	14,14,14,14	0
57	MG	2A	3137	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3788	1/1	0.96	0.10	62,62,62,62	0
57	MG	1A	3219	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3335	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3939	1/1	0.96	0.06	52,52,52,52	0
57	MG	2A	3793	1/1	0.96	0.05	56,56,56,56	0
57	MG	2A	3142	1/1	0.96	0.18	40,40,40,40	0
57	MG	1A	4086	1/1	0.96	0.11	53,53,53,53	0
57	MG	1A	3221	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3402	1/1	0.96	0.27	35,35,35,35	0
57	MG	1A	3110	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3943	1/1	0.96	0.14	25,25,25,25	0
57	MG	2A	3151	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3820	1/1	0.96	0.14	41,41,41,41	0
57	MG	2a	1700	1/1	0.96	0.20	64,64,64,64	0
57	MG	1A	3026	1/1	0.96	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3823	1/1	0.96	0.09	28,28,28,28	0
57	MG	1A	3947	1/1	0.96	0.09	69,69,69,69	0
57	MG	2A	3158	1/1	0.96	0.08	42,42,42,42	0
57	MG	1B	201	1/1	0.96	0.21	52,52,52,52	0
57	MG	2A	3809	1/1	0.96	0.13	37,37,37,37	0
57	MG	1A	3824	1/1	0.96	0.11	31,31,31,31	0
57	MG	2A	3811	1/1	0.96	0.14	57,57,57,57	0
57	MG	1a	1607	1/1	0.96	0.29	66,66,66,66	0
57	MG	1a	1795	1/1	0.96	0.12	71,71,71,71	0
57	MG	2A	3163	1/1	0.96	0.06	60,60,60,60	0
57	MG	2a	1712	1/1	0.96	0.11	53,53,53,53	0
57	MG	2A	3816	1/1	0.96	0.07	56,56,56,56	0
57	MG	2a	1714	1/1	0.96	0.18	46,46,46,46	0
57	MG	1B	203	1/1	0.96	0.09	46,46,46,46	0
57	MG	1a	1610	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3585	1/1	0.96	0.11	62,62,62,62	0
57	MG	1A	3113	1/1	0.96	0.09	43,43,43,43	0
57	MG	1B	205	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3951	1/1	0.96	0.06	28,28,28,28	0
57	MG	2A	3825	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3952	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3591	1/1	0.96	0.05	31,31,31,31	0
57	MG	1a	1616	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3703	1/1	0.96	0.05	42,42,42,42	0
57	MG	2A	3594	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3595	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3596	1/1	0.96	0.16	58,58,58,58	0
57	MG	2A	3597	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3116	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3287	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3958	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3483	1/1	0.96	0.13	35,35,35,35	0
57	MG	1A	3117	1/1	0.96	0.05	38,38,38,38	0
57	MG	2A	3179	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3290	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3412	1/1	0.96	0.08	54,54,54,54	0
57	MG	1a	1813	1/1	0.96	0.12	57,57,57,57	0
57	MG	1B	218	1/1	0.96	0.19	47,47,47,47	0
57	MG	2a	1741	1/1	0.96	0.21	57,57,57,57	0
57	MG	1A	3008	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3489	1/1	0.96	0.07	22,22,22,22	0
57	MG	1A	3602	1/1	0.96	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1e	202	1/1	0.96	0.13	53,53,53,53	0
57	MG	2a	1748	1/1	0.96	0.09	70,70,70,70	0
57	MG	1A	3838	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3603	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3490	1/1	0.96	0.12	50,50,50,50	0
57	MG	1B	226	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3605	1/1	0.96	0.05	30,30,30,30	0
57	MG	1A	3723	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3169	1/1	0.96	0.16	41,41,41,41	0
57	MG	1A	3073	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3493	1/1	0.96	0.09	48,48,48,48	0
57	MG	1t	201	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3237	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3031	1/1	0.96	0.32	31,31,31,31	0
57	MG	1A	3733	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3611	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3033	1/1	0.96	0.08	39,39,39,39	0
57	MG	1D	311	1/1	0.96	0.17	28,28,28,28	0
57	MG	1A	3500	1/1	0.96	0.08	49,49,49,49	0
57	MG	1D	313	1/1	0.96	0.11	38,38,38,38	0
57	MG	1D	314	1/1	0.96	0.19	37,37,37,37	0
57	MG	1A	3503	1/1	0.96	0.11	38,38,38,38	0
57	MG	1E	307	1/1	0.96	0.17	29,29,29,29	0
57	MG	1A	3504	1/1	0.96	0.21	38,38,38,38	0
57	MG	2D	302	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3407	1/1	0.96	0.20	50,50,50,50	0
57	MG	2D	305	1/1	0.96	0.26	45,45,45,45	0
57	MG	1A	3421	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	3619	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3184	1/1	0.96	0.07	33,33,33,33	0
57	MG	1E	314	1/1	0.96	0.11	40,40,40,40	0
57	MG	1A	3990	1/1	0.96	0.07	44,44,44,44	0
57	MG	1a	1661	1/1	0.96	0.38	69,69,69,69	0
57	MG	1A	3127	1/1	0.96	0.08	52,52,52,52	0
57	MG	1a	1663	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3625	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3626	1/1	0.96	0.09	61,61,61,61	0
57	MG	1F	306	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3229	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3299	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3242	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3751	1/1	0.96	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3128	1/1	0.96	0.06	39,39,39,39	0
57	MG	2F	3304	1/1	0.96	0.13	42,42,42,42	0
57	MG	1G	201	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	3515	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	4002	1/1	0.96	0.05	39,39,39,39	0
57	MG	1A	4003	1/1	0.96	0.05	20,20,20,20	0
57	MG	1a	1675	1/1	0.96	0.16	37,37,37,37	0
57	MG	2Q	201	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3633	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3871	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3872	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3079	1/1	0.96	0.10	42,42,42,42	0
57	MG	1N	204	1/1	0.96	0.22	55,55,55,55	0
57	MG	1A	3246	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3025	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3052	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3444	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3673	1/1	0.96	0.10	56,56,56,56	0
57	MG	2Y	201	1/1	0.96	0.20	60,60,60,60	0
57	MG	2Z	301	1/1	0.96	0.13	67,67,67,67	0
57	MG	1A	3368	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3189	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3526	1/1	0.96	0.10	37,37,37,37	0
57	MG	2f	201	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3527	1/1	0.96	0.18	50,50,50,50	0
57	MG	2A	3035	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3528	1/1	0.96	0.19	47,47,47,47	0
57	MG	23	103	1/1	0.96	0.10	49,49,49,49	0
57	MG	2l	202	1/1	0.96	0.10	65,65,65,65	0
57	MG	1A	3037	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3251	1/1	0.96	0.07	43,43,43,43	0
57	MG	1Q	202	1/1	0.96	0.21	44,44,44,44	0
57	MG	1A	4022	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3532	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3435	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3045	1/1	0.96	0.13	56,56,56,56	0
57	MG	1A	3436	1/1	0.96	0.18	43,43,43,43	0
57	MG	2A	3691	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3461	1/1	0.96	0.09	51,51,51,51	0
57	MG	1S	3602	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3893	1/1	0.96	0.07	62,62,62,62	0
57	MG	1A	3772	1/1	0.96	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3895	1/1	0.96	0.12	43,43,43,43	0
57	MG	2A	3053	1/1	0.96	0.16	60,60,60,60	0
57	MG	1T	203	1/1	0.96	0.16	63,63,63,63	0
57	MG	1a	1704	1/1	0.96	0.24	58,58,58,58	0
57	MG	1A	3252	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3472	1/1	0.96	0.11	60,60,60,60	0
57	MG	1A	3374	1/1	0.96	0.19	51,51,51,51	0
57	MG	1A	3055	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	3899	1/1	0.96	0.05	46,46,46,46	0
57	MG	1U	206	1/1	0.96	0.35	39,39,39,39	0
57	MG	1A	3540	1/1	0.96	0.29	44,44,44,44	0
57	MG	2A	3063	1/1	0.96	0.07	69,69,69,69	0
57	MG	1A	3056	1/1	0.96	0.09	35,35,35,35	0
57	MG	1V	202	1/1	0.96	0.21	41,41,41,41	0
57	MG	1A	4036	1/1	0.96	0.33	41,41,41,41	0
58	K	1A	3508	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	4037	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3441	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3145	1/1	0.96	0.20	56,56,56,56	0
57	MG	2A	3071	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3084	1/1	0.96	0.05	28,28,28,28	0
62	PHE	2w	108	11/12	0.96	0.12	35,38,45,45	0
63	FME	2x	108	10/11	0.96	0.11	34,43,46,53	0
57	MG	1A	3883	1/1	0.97	0.04	53,53,53,53	0
57	MG	1A	4012	1/1	0.97	0.06	15,15,15,15	0
57	MG	1A	3208	1/1	0.97	0.19	27,27,27,27	0
57	MG	2A	3225	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3459	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	4015	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3550	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	4017	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3108	1/1	0.97	0.17	35,35,35,35	0
57	MG	1A	3109	1/1	0.97	0.16	36,36,36,36	0
57	MG	1A	3767	1/1	0.97	0.08	30,30,30,30	0
57	MG	2A	3012	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3014	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3462	1/1	0.97	0.08	47,47,47,47	0
57	MG	2A	3454	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3891	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3769	1/1	0.97	0.04	30,30,30,30	0
57	MG	2A	3019	1/1	0.97	0.18	59,59,59,59	0
57	MG	1A	3014	1/1	0.97	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3111	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	3466	1/1	0.97	0.14	33,33,33,33	0
57	MG	2A	3707	1/1	0.97	0.17	43,43,43,43	0
57	MG	1A	4027	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3026	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3022	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3468	1/1	0.97	0.24	36,36,36,36	0
57	MG	2A	3029	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3159	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3661	1/1	0.97	0.04	13,13,13,13	0
57	MG	2A	3032	1/1	0.97	0.11	43,43,43,43	0
57	MG	2A	3033	1/1	0.97	0.07	50,50,50,50	0
57	MG	1P	206	1/1	0.97	0.10	41,41,41,41	0
57	MG	1Q	201	1/1	0.97	0.19	35,35,35,35	0
57	MG	1A	3561	1/1	0.97	0.08	24,24,24,24	0
57	MG	2A	3037	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3663	1/1	0.97	0.08	34,34,34,34	0
57	MG	1Q	206	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3218	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3039	1/1	0.97	0.17	32,32,32,32	0
57	MG	1R	201	1/1	0.97	0.14	37,37,37,37	0
57	MG	1R	203	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3482	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3565	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3114	1/1	0.97	0.14	60,60,60,60	0
57	MG	1a	1694	1/1	0.97	0.12	47,47,47,47	0
57	MG	2A	3487	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3567	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3028	1/1	0.97	0.15	35,35,35,35	0
57	MG	2A	3734	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3006	1/1	0.97	0.07	34,34,34,34	0
57	MG	1a	1700	1/1	0.97	0.14	59,59,59,59	0
57	MG	2A	3737	1/1	0.97	0.10	49,49,49,49	0
57	MG	1A	3786	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3739	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3269	1/1	0.97	0.16	55,55,55,55	0
57	MG	2A	3494	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3570	1/1	0.97	0.10	56,56,56,56	0
57	MG	2a	1663	1/1	0.97	0.13	45,45,45,45	0
57	MG	1U	202	1/1	0.97	0.11	41,41,41,41	0
57	MG	2a	1665	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3072	1/1	0.97	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3675	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3225	1/1	0.97	0.17	47,47,47,47	0
57	MG	1a	1707	1/1	0.97	0.11	51,51,51,51	0
57	MG	2A	3061	1/1	0.97	0.11	43,43,43,43	0
57	MG	1a	1708	1/1	0.97	0.07	58,58,58,58	0
57	MG	1A	3479	1/1	0.97	0.05	49,49,49,49	0
57	MG	1a	1710	1/1	0.97	0.05	36,36,36,36	0
57	MG	2A	3752	1/1	0.97	0.11	72,72,72,72	0
57	MG	1A	4049	1/1	0.97	0.05	35,35,35,35	0
57	MG	1a	1713	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3121	1/1	0.97	0.29	31,31,31,31	0
57	MG	1A	3577	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3167	1/1	0.97	0.15	41,41,41,41	0
57	MG	1V	205	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3072	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	4054	1/1	0.97	0.06	61,61,61,61	0
57	MG	2A	3514	1/1	0.97	0.08	34,34,34,34	0
57	MG	1a	1719	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3795	1/1	0.97	0.12	44,44,44,44	0
57	MG	1A	3482	1/1	0.97	0.10	39,39,39,39	0
57	MG	2A	3077	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3351	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3484	1/1	0.97	0.18	44,44,44,44	0
57	MG	2A	3524	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3414	1/1	0.97	0.28	56,56,56,56	0
57	MG	1A	3289	1/1	0.97	0.09	41,41,41,41	0
57	MG	1X	104	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3032	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3084	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3530	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3531	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3088	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3086	1/1	0.97	0.06	56,56,56,56	0
57	MG	2A	3087	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3587	1/1	0.97	0.05	14,14,14,14	0
57	MG	2A	3303	1/1	0.97	0.25	66,66,66,66	0
57	MG	2A	3786	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3804	1/1	0.97	0.25	41,41,41,41	0
57	MG	1Y	202	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3357	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3234	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3931	1/1	0.97	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3792	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3693	1/1	0.97	0.10	62,62,62,62	0
57	MG	1A	4070	1/1	0.97	0.07	61,61,61,61	0
57	MG	2A	3097	1/1	0.97	0.12	61,61,61,61	0
57	MG	1A	3809	1/1	0.97	0.09	46,46,46,46	0
57	MG	2A	3546	1/1	0.97	0.08	26,26,26,26	0
57	MG	1A	3935	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	4074	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	4075	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3316	1/1	0.97	0.11	56,56,56,56	0
57	MG	1A	3420	1/1	0.97	0.20	42,42,42,42	0
57	MG	1A	3170	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3236	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3174	1/1	0.97	0.14	29,29,29,29	0
57	MG	2A	3107	1/1	0.97	0.13	50,50,50,50	0
57	MG	11	101	1/1	0.97	0.34	42,42,42,42	0
57	MG	1A	4080	1/1	0.97	0.19	48,48,48,48	0
57	MG	2a	1726	1/1	0.97	0.09	76,76,76,76	0
57	MG	2A	3561	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3698	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3175	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3596	1/1	0.97	0.06	46,46,46,46	0
57	MG	1a	1754	1/1	0.97	0.07	58,58,58,58	0
57	MG	2A	3817	1/1	0.97	0.13	56,56,56,56	0
57	MG	1A	3124	1/1	0.97	0.11	32,32,32,32	0
57	MG	1A	4085	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3598	1/1	0.97	0.08	41,41,41,41	0
57	MG	13	101	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3118	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3497	1/1	0.97	0.10	57,57,57,57	0
57	MG	2A	3824	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3091	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3181	1/1	0.97	0.11	29,29,29,29	0
57	MG	2a	1743	1/1	0.97	0.10	60,60,60,60	0
57	MG	1A	3093	1/1	0.97	0.14	37,37,37,37	0
57	MG	2A	3575	1/1	0.97	0.09	55,55,55,55	0
57	MG	1a	1767	1/1	0.97	0.05	63,63,63,63	0
57	MG	1A	3709	1/1	0.97	0.06	46,46,46,46	0
57	MG	1a	1769	1/1	0.97	0.07	53,53,53,53	0
57	MG	15	103	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3950	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3710	1/1	0.97	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3582	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3505	1/1	0.97	0.14	34,34,34,34	0
57	MG	2A	3131	1/1	0.97	0.13	48,48,48,48	0
57	MG	2A	3838	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3074	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3045	1/1	0.97	0.04	21,21,21,21	0
57	MG	2A	3135	1/1	0.97	0.18	38,38,38,38	0
57	MG	2A	3842	1/1	0.97	0.06	45,45,45,45	0
57	MG	2A	3843	1/1	0.97	0.06	56,56,56,56	0
57	MG	17	101	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3845	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3133	1/1	0.97	0.21	41,41,41,41	0
57	MG	2A	3139	1/1	0.97	0.11	47,47,47,47	0
57	MG	1a	1780	1/1	0.97	0.06	66,66,66,66	0
57	MG	17	104	1/1	0.97	0.07	34,34,34,34	0
57	MG	17	105	1/1	0.97	0.17	54,54,54,54	0
57	MG	1A	3715	1/1	0.97	0.07	30,30,30,30	0
57	MG	17	107	1/1	0.97	0.14	29,29,29,29	0
57	MG	1a	1785	1/1	0.97	0.04	52,52,52,52	0
57	MG	2A	3147	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3148	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3370	1/1	0.97	0.10	40,40,40,40	0
57	MG	18	102	1/1	0.97	0.20	44,44,44,44	0
57	MG	1A	3135	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	3834	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3434	1/1	0.97	0.07	35,35,35,35	0
57	MG	1B	209	1/1	0.97	0.14	49,49,49,49	0
57	MG	2A	3155	1/1	0.97	0.18	46,46,46,46	0
57	MG	1A	3100	1/1	0.97	0.29	38,38,38,38	0
57	MG	2A	3157	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3720	1/1	0.97	0.04	33,33,33,33	0
57	MG	1A	3722	1/1	0.97	0.06	67,67,67,67	0
57	MG	2A	3613	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3516	1/1	0.97	0.12	33,33,33,33	0
57	MG	1A	3724	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3076	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3250	1/1	0.97	0.11	38,38,38,38	0
57	MG	2a	1790	1/1	0.97	0.27	56,56,56,56	0
57	MG	1a	1608	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3728	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3614	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3520	1/1	0.97	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3521	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3139	1/1	0.97	0.20	37,37,37,37	0
57	MG	2A	3170	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3102	1/1	0.97	0.16	32,32,32,32	0
57	MG	1A	3258	1/1	0.97	0.20	33,33,33,33	0
57	MG	1A	3259	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3628	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3623	1/1	0.97	0.04	20,20,20,20	0
57	MG	1A	3315	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3855	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3739	1/1	0.97	0.08	51,51,51,51	0
57	MG	2A	3634	1/1	0.97	0.21	61,61,61,61	0
57	MG	1A	3380	1/1	0.97	0.11	38,38,38,38	0
57	MG	1B	231	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3141	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3638	1/1	0.97	0.24	35,35,35,35	0
57	MG	2A	3181	1/1	0.97	0.06	54,54,54,54	0
57	MG	1A	3261	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3194	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	3989	1/1	0.97	0.05	39,39,39,39	0
57	MG	1a	1628	1/1	0.97	0.16	59,59,59,59	0
57	MG	1A	3533	1/1	0.97	0.13	54,54,54,54	0
57	MG	2A	3398	1/1	0.97	0.10	55,55,55,55	0
57	MG	1D	303	1/1	0.97	0.15	42,42,42,42	0
57	MG	1D	304	1/1	0.97	0.12	39,39,39,39	0
57	MG	1D	306	1/1	0.97	0.11	38,38,38,38	0
57	MG	1D	309	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3384	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3993	1/1	0.97	0.07	26,26,26,26	0
57	MG	1A	3142	1/1	0.97	0.09	27,27,27,27	0
57	MG	1A	3103	1/1	0.97	0.07	37,37,37,37	0
57	MG	2V	201	1/1	0.97	0.18	44,44,44,44	0
57	MG	1A	3749	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3750	1/1	0.97	0.06	19,19,19,19	0
57	MG	1E	303	1/1	0.97	0.16	47,47,47,47	0
57	MG	2A	3199	1/1	0.97	0.06	56,56,56,56	0
57	MG	1a	1644	1/1	0.97	0.15	47,47,47,47	0
57	MG	1E	304	1/1	0.97	0.12	45,45,45,45	0
57	MG	2A	3202	1/1	0.97	0.13	51,51,51,51	0
57	MG	1A	3018	1/1	0.97	0.09	22,22,22,22	0
57	MG	1A	3451	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	4000	1/1	0.97	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3452	1/1	0.97	0.15	33,33,33,33	0
57	MG	2A	3418	1/1	0.97	0.13	37,37,37,37	0
57	MG	1E	312	1/1	0.97	0.10	28,28,28,28	0
57	MG	2x	104	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3201	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3543	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3078	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3147	1/1	0.97	0.08	41,41,41,41	0
57	MG	1F	301	1/1	0.97	0.14	39,39,39,39	0
57	MG	27	101	1/1	0.97	0.18	60,60,60,60	0
57	MG	1A	3047	1/1	0.97	0.11	29,29,29,29	0
57	MG	2A	3429	1/1	0.97	0.17	43,43,43,43	0
57	MG	1A	3107	1/1	0.97	0.18	37,37,37,37	0
57	MG	2A	3215	1/1	0.97	0.43	40,40,40,40	0
57	MG	1A	4009	1/1	0.97	0.07	32,32,32,32	0
57	MG	1F	307	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3218	1/1	0.97	0.15	45,45,45,45	0
60	ZN	2Y	202	1/1	0.97	0.05	90,90,90,90	0
57	MG	1F	308	1/1	0.97	0.12	27,27,27,27	0
60	ZN	2n	501	1/1	0.97	0.05	81,81,81,81	0
62	PHE	1w	109	11/12	0.97	0.08	19,25,28,30	0
57	MG	1A	3882	1/1	0.97	0.08	37,37,37,37	0
63	FME	1x	115	10/11	0.97	0.12	21,25,29,39	10
57	MG	2A	3438	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3536	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3339	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3463	1/1	0.98	0.13	46,46,46,46	0
57	MG	2A	3468	1/1	0.98	0.05	62,62,62,62	0
57	MG	1A	3285	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3020	1/1	0.98	0.06	17,17,17,17	0
57	MG	1A	3115	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3618	1/1	0.98	0.09	25,25,25,25	0
57	MG	1A	3542	1/1	0.98	0.12	32,32,32,32	0
57	MG	1B	219	1/1	0.98	0.05	36,36,36,36	0
57	MG	1A	3405	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3344	1/1	0.98	0.13	35,35,35,35	0
57	MG	1A	3622	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	4008	1/1	0.98	0.06	12,12,12,12	0
57	MG	1a	1699	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3095	1/1	0.98	0.27	29,29,29,29	0
57	MG	10	106	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3471	1/1	0.98	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3483	1/1	0.98	0.08	43,43,43,43	0
57	MG	2A	3658	1/1	0.98	0.05	61,61,61,61	0
57	MG	1A	3408	1/1	0.98	0.08	40,40,40,40	0
57	MG	1A	3347	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3807	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3096	1/1	0.98	0.05	36,36,36,36	0
57	MG	1A	3629	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3349	1/1	0.98	0.21	36,36,36,36	0
57	MG	2A	3008	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	3118	1/1	0.98	0.05	32,32,32,32	0
57	MG	1B	233	1/1	0.98	0.07	61,61,61,61	0
57	MG	2A	3011	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3721	1/1	0.98	0.09	40,40,40,40	0
57	MG	1a	1712	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3097	1/1	0.98	0.12	33,33,33,33	0
57	MG	1A	3634	1/1	0.98	0.09	30,30,30,30	0
57	MG	1D	301	1/1	0.98	0.10	32,32,32,32	0
57	MG	2A	3018	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3553	1/1	0.98	0.04	39,39,39,39	0
57	MG	2A	3020	1/1	0.98	0.05	23,23,23,23	0
57	MG	2A	3021	1/1	0.98	0.16	45,45,45,45	0
57	MG	1A	3725	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3120	1/1	0.98	0.14	28,28,28,28	0
57	MG	2A	3505	1/1	0.98	0.04	43,43,43,43	0
57	MG	2A	3682	1/1	0.98	0.05	49,49,49,49	0
57	MG	1D	305	1/1	0.98	0.09	21,21,21,21	0
57	MG	1A	3063	1/1	0.98	0.18	30,30,30,30	0
57	MG	15	101	1/1	0.98	0.08	42,42,42,42	0
57	MG	1D	307	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3819	1/1	0.98	0.09	34,34,34,34	0
57	MG	2A	3688	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3354	1/1	0.98	0.06	31,31,31,31	0
57	MG	2D	301	1/1	0.98	0.09	37,37,37,37	0
57	MG	1A	3821	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3099	1/1	0.98	0.04	32,32,32,32	0
57	MG	2D	304	1/1	0.98	0.27	45,45,45,45	0
57	MG	1A	3064	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3731	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3516	1/1	0.98	0.11	32,32,32,32	0
57	MG	2A	3517	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3243	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3195	1/1	0.98	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3194	1/1	0.98	0.12	45,45,45,45	0
57	MG	1A	3196	1/1	0.98	0.04	34,34,34,34	0
57	MG	2E	305	1/1	0.98	0.05	44,44,44,44	0
57	MG	1a	1734	1/1	0.98	0.12	51,51,51,51	0
57	MG	2A	3523	1/1	0.98	0.06	50,50,50,50	0
57	MG	1E	305	1/1	0.98	0.07	34,34,34,34	0
57	MG	1E	306	1/1	0.98	0.10	27,27,27,27	0
57	MG	2A	3040	1/1	0.98	0.13	57,57,57,57	0
57	MG	1A	3016	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3198	1/1	0.98	0.14	37,37,37,37	0
57	MG	1E	309	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3564	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3932	1/1	0.98	0.06	29,29,29,29	0
57	MG	2F	3305	1/1	0.98	0.19	43,43,43,43	0
57	MG	1A	3647	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3156	1/1	0.98	0.15	35,35,35,35	0
57	MG	2A	3048	1/1	0.98	0.09	23,23,23,23	0
57	MG	2A	3049	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3158	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3741	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3066	1/1	0.98	0.24	45,45,45,45	0
57	MG	1A	3202	1/1	0.98	0.18	39,39,39,39	0
57	MG	1A	4044	1/1	0.98	0.20	39,39,39,39	0
57	MG	1A	3653	1/1	0.98	0.04	33,33,33,33	0
57	MG	1F	305	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3067	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	4047	1/1	0.98	0.16	26,26,26,26	0
57	MG	1A	3253	1/1	0.98	0.13	23,23,23,23	0
57	MG	1a	1755	1/1	0.98	0.07	47,47,47,47	0
57	MG	1F	309	1/1	0.98	0.12	31,31,31,31	0
57	MG	1A	3068	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3222	1/1	0.98	0.20	37,37,37,37	0
57	MG	1F	311	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3572	1/1	0.98	0.07	23,23,23,23	0
57	MG	2A	3552	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3308	1/1	0.98	0.20	33,33,33,33	0
57	MG	1A	3309	1/1	0.98	0.16	32,32,32,32	0
57	MG	1a	1617	1/1	0.98	0.08	53,53,53,53	0
57	MG	1A	3310	1/1	0.98	0.15	36,36,36,36	0
57	MG	23	102	1/1	0.98	0.07	47,47,47,47	0
57	MG	2a	1774	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3498	1/1	0.98	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3558	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3129	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3130	1/1	0.98	0.21	35,35,35,35	0
57	MG	1A	3580	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3849	1/1	0.98	0.04	35,35,35,35	0
57	MG	1A	3011	1/1	0.98	0.04	25,25,25,25	0
57	MG	1a	1774	1/1	0.98	0.05	58,58,58,58	0
57	MG	1A	3209	1/1	0.98	0.12	29,29,29,29	0
57	MG	1N	203	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3954	1/1	0.98	0.06	26,26,26,26	0
57	MG	2A	3396	1/1	0.98	0.27	54,54,54,54	0
57	MG	1A	3132	1/1	0.98	0.15	28,28,28,28	0
57	MG	1A	3668	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	4065	1/1	0.98	0.07	46,46,46,46	0
57	MG	1A	3854	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3211	1/1	0.98	0.13	44,44,44,44	0
57	MG	1A	3044	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3763	1/1	0.98	0.17	25,25,25,25	0
57	MG	1a	1636	1/1	0.98	0.14	55,55,55,55	0
57	MG	1A	3858	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	4071	1/1	0.98	0.04	49,49,49,49	0
57	MG	1P	202	1/1	0.98	0.18	30,30,30,30	0
57	MG	1P	203	1/1	0.98	0.12	33,33,33,33	0
57	MG	2A	3092	1/1	0.98	0.13	37,37,37,37	0
57	MG	1P	205	1/1	0.98	0.09	58,58,58,58	0
57	MG	1A	3511	1/1	0.98	0.06	24,24,24,24	0
57	MG	1a	1643	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3134	1/1	0.98	0.14	33,33,33,33	0
57	MG	1a	1794	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3036	1/1	0.98	0.20	29,29,29,29	0
57	MG	1Q	203	1/1	0.98	0.07	28,28,28,28	0
57	MG	2A	3590	1/1	0.98	0.04	40,40,40,40	0
57	MG	1a	1797	1/1	0.98	0.12	57,57,57,57	0
57	MG	1Q	204	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3674	1/1	0.98	0.14	53,53,53,53	0
57	MG	1A	3015	1/1	0.98	0.08	47,47,47,47	0
57	MG	2A	3421	1/1	0.98	0.08	48,48,48,48	0
57	MG	1A	3590	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3171	1/1	0.98	0.21	39,39,39,39	0
57	MG	1A	3173	1/1	0.98	0.26	38,38,38,38	0
57	MG	2A	3599	1/1	0.98	0.10	43,43,43,43	0
57	MG	2A	3600	1/1	0.98	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1R	202	1/1	0.98	0.24	40,40,40,40	0
57	MG	1A	3517	1/1	0.98	0.44	45,45,45,45	0
57	MG	2A	3782	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3971	1/1	0.98	0.06	39,39,39,39	0
57	MG	2A	3785	1/1	0.98	0.04	53,53,53,53	0
57	MG	1A	3137	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3029	1/1	0.98	0.13	22,22,22,22	0
57	MG	1A	3975	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3176	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3274	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3089	1/1	0.98	0.29	39,39,39,39	0
57	MG	2A	3436	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3390	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3687	1/1	0.98	0.07	47,47,47,47	0
57	MG	2A	3119	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3878	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3879	1/1	0.98	0.06	29,29,29,29	0
57	MG	2A	3799	1/1	0.98	0.06	64,64,64,64	0
57	MG	1A	3090	1/1	0.98	0.09	48,48,48,48	0
57	MG	1A	3525	1/1	0.98	0.07	49,49,49,49	0
57	MG	1A	3180	1/1	0.98	0.05	42,42,42,42	0
57	MG	1V	201	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3986	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3226	1/1	0.98	0.06	34,34,34,34	0
57	MG	1V	204	1/1	0.98	0.25	32,32,32,32	0
57	MG	1A	3059	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3228	1/1	0.98	0.09	49,49,49,49	0
57	MG	1A	3030	1/1	0.98	0.26	34,34,34,34	0
57	MG	2a	1658	1/1	0.98	0.05	59,59,59,59	0
57	MG	2A	3132	1/1	0.98	0.10	40,40,40,40	0
57	MG	2A	3453	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3531	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3230	1/1	0.98	0.16	47,47,47,47	0
57	MG	2A	3814	1/1	0.98	0.06	62,62,62,62	0
57	MG	1W	202	1/1	0.98	0.12	36,36,36,36	0
57	MG	1W	203	1/1	0.98	0.14	45,45,45,45	0
60	ZN	1n	103	1/1	0.98	0.04	57,57,57,57	0
57	MG	1W	204	1/1	0.98	0.08	32,32,32,32	0
57	MG	2A	3633	1/1	0.98	0.05	42,42,42,42	0
60	ZN	25	106	1/1	0.98	0.04	57,57,57,57	0
57	MG	1A	3231	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3183	1/1	0.98	0.09	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1X	102	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3400	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3143	1/1	0.98	0.08	35,35,35,35	0
57	MG	18	103	1/1	0.99	0.11	44,44,44,44	0
57	MG	1A	3859	1/1	0.99	0.06	34,34,34,34	0
57	MG	1a	1728	1/1	0.99	0.19	40,40,40,40	0
57	MG	1A	3257	1/1	0.99	0.19	31,31,31,31	0
57	MG	1A	3677	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3345	1/1	0.99	0.15	29,29,29,29	0
57	MG	1A	3051	1/1	0.99	0.08	35,35,35,35	0
57	MG	1A	3207	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3035	1/1	0.99	0.12	28,28,28,28	0
57	MG	1A	3053	1/1	0.99	0.04	21,21,21,21	0
57	MG	2A	3795	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3012	1/1	0.99	0.07	15,15,15,15	0
57	MG	2A	3103	1/1	0.99	0.06	28,28,28,28	0
57	MG	2A	3559	1/1	0.99	0.04	38,38,38,38	0
57	MG	1X	101	1/1	0.99	0.22	33,33,33,33	0
57	MG	1A	3092	1/1	0.99	0.04	21,21,21,21	0
57	MG	1A	3152	1/1	0.99	0.08	12,12,12,12	0
57	MG	1A	3191	1/1	0.99	0.15	30,30,30,30	0
57	MG	1A	3025	1/1	0.99	0.14	31,31,31,31	0
57	MG	1A	3355	1/1	0.99	0.13	36,36,36,36	0
57	MG	1a	1743	1/1	0.99	0.04	47,47,47,47	0
57	MG	1A	3922	1/1	0.99	0.06	42,42,42,42	0
57	MG	1A	3873	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3974	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3172	1/1	0.99	0.21	31,31,31,31	0
57	MG	1A	3875	1/1	0.99	0.04	15,15,15,15	0
57	MG	1A	3003	1/1	0.99	0.05	27,27,27,27	0
57	MG	1A	3217	1/1	0.99	0.13	30,30,30,30	0
57	MG	1A	3649	1/1	0.99	0.02	14,14,14,14	0
57	MG	1P	201	1/1	0.99	0.17	36,36,36,36	0
57	MG	1D	308	1/1	0.99	0.10	36,36,36,36	0
57	MG	1A	3326	1/1	0.99	0.12	36,36,36,36	0
57	MG	1P	204	1/1	0.99	0.21	30,30,30,30	0
57	MG	2A	3424	1/1	0.99	0.07	21,21,21,21	0
57	MG	1A	3009	1/1	0.99	0.08	25,25,25,25	0
57	MG	1A	3328	1/1	0.99	0.11	39,39,39,39	0
57	MG	1A	3058	1/1	0.99	0.11	35,35,35,35	0
57	MG	1A	3220	1/1	0.99	0.17	31,31,31,31	0
57	MG	1A	3157	1/1	0.99	0.06	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3125	1/1	0.99	0.05	14,14,14,14	0
57	MG	1E	302	1/1	0.99	0.13	29,29,29,29	0
57	MG	1a	1631	1/1	0.99	0.10	24,24,24,24	0
57	MG	1a	1764	1/1	0.99	0.05	61,61,61,61	0
57	MG	1a	1765	1/1	0.99	0.06	51,51,51,51	0
57	MG	1a	1766	1/1	0.99	0.05	51,51,51,51	0
57	MG	1A	3700	1/1	0.99	0.10	28,28,28,28	0
57	MG	1A	3576	1/1	0.99	0.08	24,24,24,24	0
57	MG	2a	1742	1/1	0.99	0.05	59,59,59,59	0
57	MG	2A	3136	1/1	0.99	0.05	40,40,40,40	0
57	MG	2X	102	1/1	0.99	0.12	51,51,51,51	0
57	MG	1a	1698	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3499	1/1	0.99	0.07	28,28,28,28	0
57	MG	1A	3019	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3991	1/1	0.99	0.06	54,54,54,54	0
57	MG	1A	3501	1/1	0.99	0.16	30,30,30,30	0
57	MG	1A	3502	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3179	1/1	0.99	0.11	23,23,23,23	0
57	MG	2A	3069	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3752	1/1	0.99	0.05	23,23,23,23	0
57	MG	1A	3707	1/1	0.99	0.11	35,35,35,35	0
57	MG	1A	3160	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	4050	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3041	1/1	0.99	0.04	32,32,32,32	0
57	MG	1U	201	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3469	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3624	1/1	0.99	0.03	30,30,30,30	0
57	MG	2A	3767	1/1	0.99	0.04	48,48,48,48	0
57	MG	1F	302	1/1	0.99	0.10	33,33,33,33	0
57	MG	1A	3085	1/1	0.99	0.10	19,19,19,19	0
57	MG	1A	3034	1/1	0.99	0.08	22,22,22,22	0
57	MG	1A	3510	1/1	0.99	0.06	35,35,35,35	0
57	MG	17	102	1/1	0.99	0.09	29,29,29,29	0
57	MG	1U	208	1/1	0.99	0.18	31,31,31,31	0
57	MG	1A	3062	1/1	0.99	0.06	15,15,15,15	0
60	ZN	1Y	203	1/1	0.99	0.03	66,66,66,66	0
57	MG	2A	3775	1/1	0.99	0.11	43,43,43,43	0
60	ZN	15	108	1/1	0.99	0.02	41,41,41,41	0
57	MG	1A	3340	1/1	0.99	0.10	23,23,23,23	0
57	MG	2A	3013	1/1	0.99	0.06	44,44,44,44	0
57	MG	1A	3254	1/1	0.99	0.14	30,30,30,30	0
57	MG	1A	3631	1/1	0.99	0.02	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	29	102	1/1	0.99	0.03	61,61,61,61	0
57	MG	2A	3466	1/1	0.99	0.04	69,69,69,69	0
61	SF4	1d	302	8/8	0.99	0.04	54,57,62,67	0
61	SF4	2d	303	8/8	0.99	0.05	62,68,72,74	0
57	MG	1A	3255	1/1	0.99	0.12	35,35,35,35	0
57	MG	1a	1724	1/1	0.99	0.05	50,50,50,50	0
57	MG	2A	3783	1/1	0.99	0.06	39,39,39,39	0
57	MG	1A	3256	1/1	0.99	0.10	31,31,31,31	0
60	ZN	19	102	1/1	1.00	0.03	40,40,40,40	0
57	MG	2A	3674	1/1	1.00	0.06	35,35,35,35	0
57	MG	1A	3013	1/1	1.00	0.04	28,28,28,28	0
57	MG	1a	1772	1/1	1.00	0.02	53,53,53,53	0
57	MG	1A	3143	1/1	1.00	0.12	25,25,25,25	0
60	ZN	26	102	1/1	1.00	0.02	51,51,51,51	0
60	ZN	16	102	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.