



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 04:16 AM UTC

PDB ID : 7RQ8 / pdb_00007rq8
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNAs, and aminoacylated P-site tRNA at 2.50Å resolution
Authors : Mitcheltree, M.J.; Pisipati, A.; Syroegin, E.A.; Silvestre, K.J.; Klepacki, D.; Mason, J.D.; Terwilliger, D.W.; Testolin, G.; Pote, A.R.; Wu, K.J.Y.; Ladley, R.P.; Chatman, K.; Mankin, A.S.; Polikanov, Y.S.; Myers, A.G.
Deposited on : 2021-08-06
Resolution : 2.50 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	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

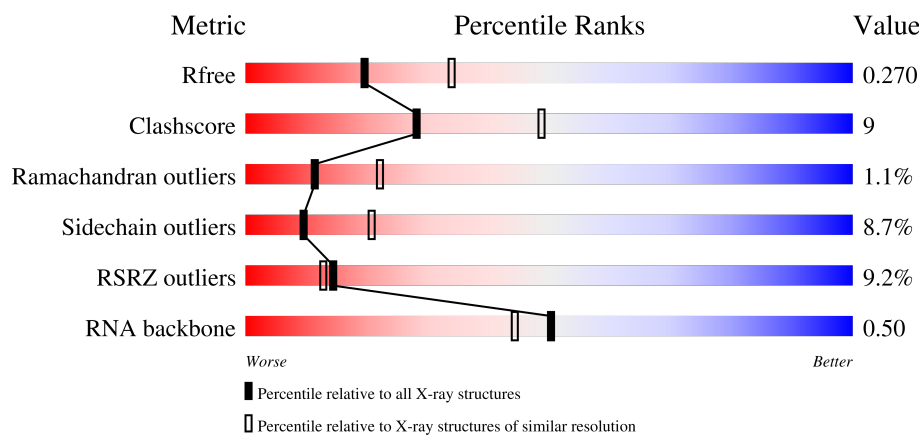
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

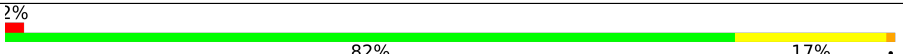
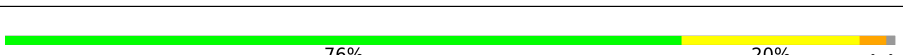
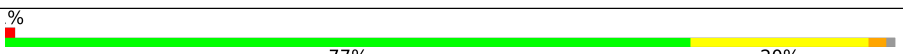
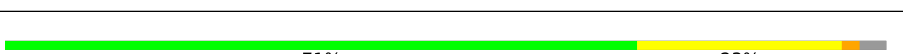
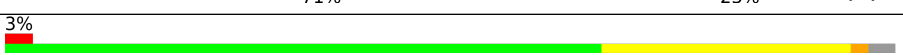
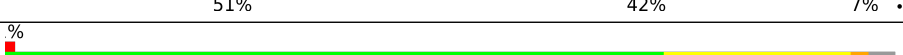
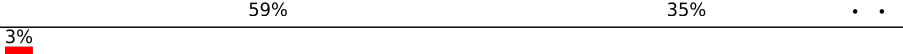
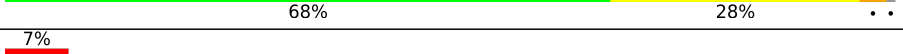
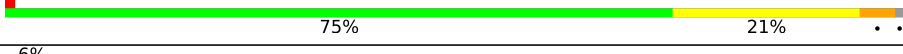
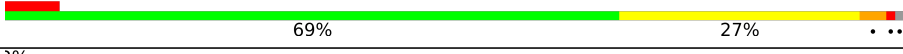
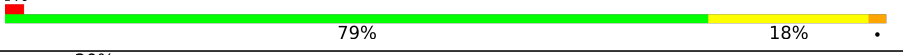
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 4% 67% 25% 6% •
1	2A	2915	 4% 59% 31% 7% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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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
56	PSU	2y	55	-	-	X	-
57	MG	1A	3436	-	-	-	X
57	MG	2a	1646	-	-	-	X
57	MG	2a	1739	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 299504 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0
			1530	685	274	498	71	2		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1108	Total	Mg	0	0
			1108	1108		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	12	Total	Mg	0	0
			12	12		

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	1	Total 1	Mg 1	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	229	Total 229	Mg 229	0	0
57	1b	2	Total 2	Mg 2	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	1l	3	Total 3	Mg 3	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	5	Total 5	Mg 5	0	0
57	1x	15	Total 15	Mg 15	0	0
57	1y	4	Total 4	Mg 4	0	0
57	2A	729	Total 729	Mg 729	0	0
57	2B	18	Total 18	Mg 18	0	0
57	2D	6	Total 6	Mg 6	0	0

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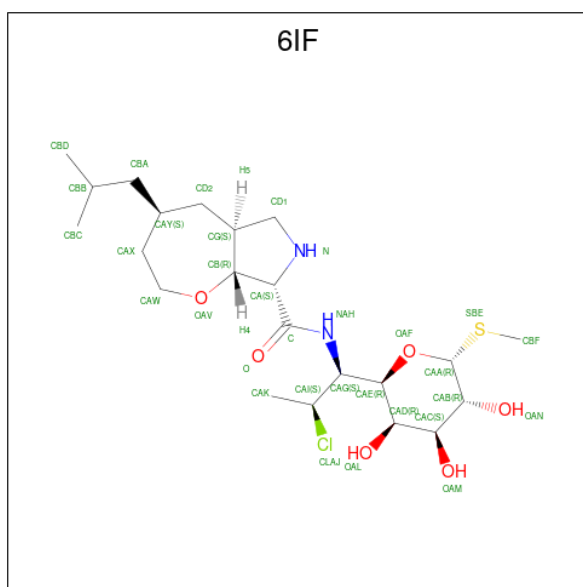
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2Q	1	Total 1	Mg 1	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	3	Total 3	Mg 3	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	3	Total 3	Mg 3	0	0
57	26	1	Total 1	Mg 1	0	0
57	27	3	Total 3	Mg 3	0	0
57	28	3	Total 3	Mg 3	0	0
57	2a	186	Total 186	Mg 186	0	0
57	2d	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2e	1	Total	Mg	0	0
			1	1		
57	2f	2	Total	Mg	0	0
			2	2		
57	2l	3	Total	Mg	0	0
			3	3		
57	2q	3	Total	Mg	0	0
			3	3		
57	2r	1	Total	Mg	0	0
			1	1		
57	2t	1	Total	Mg	0	0
			1	1		
57	2v	1	Total	Mg	0	0
			1	1		
57	2w	1	Total	Mg	0	0
			1	1		
57	2x	5	Total	Mg	0	0
			5	5		
57	2y	3	Total	Mg	0	0
			3	3		

- Molecule 58 is methyl 7-chloro-6,7,8-trideoxy-6-{[(4S,5aS,8S,8aR)-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carbonyl]amino}-1-thio-L-threo- α -D-galacto-octopyranoside (CCD ID: 6IF) (formula: $C_{22}H_{39}ClN_2O_6S$).

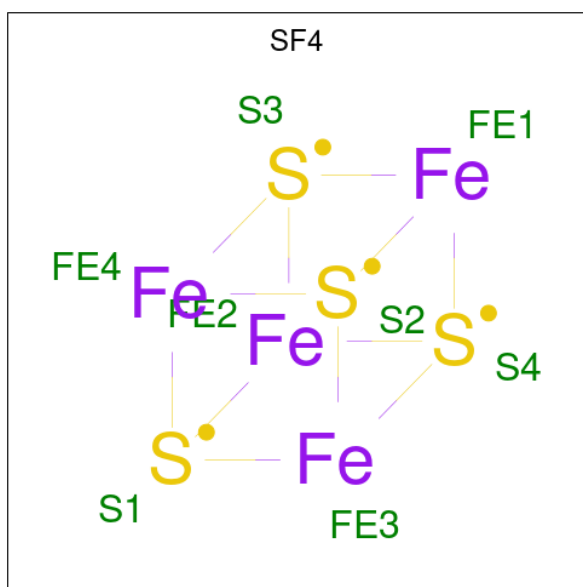


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
58	1A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		
58	2A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total	K	0	0
			1	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	2122	Total	O	0	0
			2122	2122		
62	1B	69	Total	O	0	0
			69	69		
62	1D	24	Total	O	0	0
			24	24		
62	1E	27	Total	O	0	0
			27	27		
62	1F	18	Total	O	0	0
			18	18		
62	1G	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1H	2	Total	O	0	0
			2	2		
62	1N	4	Total	O	0	0
			4	4		
62	1O	7	Total	O	0	0
			7	7		
62	1P	20	Total	O	0	0
			20	20		
62	1Q	8	Total	O	0	0
			8	8		
62	1R	10	Total	O	0	0
			10	10		
62	1S	4	Total	O	0	0
			4	4		
62	1T	8	Total	O	0	0
			8	8		
62	1U	10	Total	O	0	0
			10	10		
62	1V	9	Total	O	0	0
			9	9		
62	1W	7	Total	O	0	0
			7	7		
62	1X	7	Total	O	0	0
			7	7		
62	1Y	3	Total	O	0	0
			3	3		
62	1Z	1	Total	O	0	0
			1	1		
62	10	10	Total	O	0	0
			10	10		
62	11	12	Total	O	0	0
			12	12		
62	12	4	Total	O	0	0
			4	4		
62	13	5	Total	O	0	0
			5	5		
62	15	7	Total	O	0	0
			7	7		
62	16	1	Total	O	0	0
			1	1		
62	17	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	18	10	Total O 10 10	0	0
62	1a	361	Total O 361 361	0	0
62	1b	1	Total O 1 1	0	0
62	1d	1	Total O 1 1	0	0
62	1e	1	Total O 1 1	0	0
62	1g	1	Total O 1 1	0	0
62	1l	4	Total O 4 4	0	0
62	1m	2	Total O 2 2	0	0
62	1q	4	Total O 4 4	0	0
62	1u	1	Total O 1 1	0	0
62	1v	5	Total O 5 5	0	0
62	1w	6	Total O 6 6	0	0
62	1x	16	Total O 16 16	0	0
62	1y	2	Total O 2 2	0	0
62	2A	968	Total O 968 968	0	0
62	2B	15	Total O 15 15	0	0
62	2D	16	Total O 16 16	0	0
62	2E	9	Total O 9 9	0	0
62	2F	9	Total O 9 9	0	0
62	2I	1	Total O 1 1	0	0
62	2N	1	Total O 1 1	0	0

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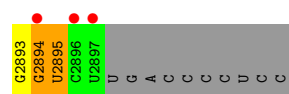
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2O	2	Total	O	0	0
			2	2		
62	2P	10	Total	O	0	0
			10	10		
62	2Q	1	Total	O	0	0
			1	1		
62	2R	3	Total	O	0	0
			3	3		
62	2T	2	Total	O	0	0
			2	2		
62	2W	1	Total	O	0	0
			1	1		
62	2X	3	Total	O	0	0
			3	3		
62	2Y	1	Total	O	0	0
			1	1		
62	20	2	Total	O	0	0
			2	2		
62	21	3	Total	O	0	0
			3	3		
62	23	2	Total	O	0	0
			2	2		
62	25	2	Total	O	0	0
			2	2		
62	26	1	Total	O	0	0
			1	1		
62	27	2	Total	O	0	0
			2	2		
62	28	6	Total	O	0	0
			6	6		
62	29	1	Total	O	0	0
			1	1		
62	2a	51	Total	O	0	0
			51	51		
62	2d	1	Total	O	0	0
			1	1		
62	2i	1	Total	O	0	0
			1	1		
62	2j	1	Total	O	0	0
			1	1		
62	2l	3	Total	O	0	0
			3	3		

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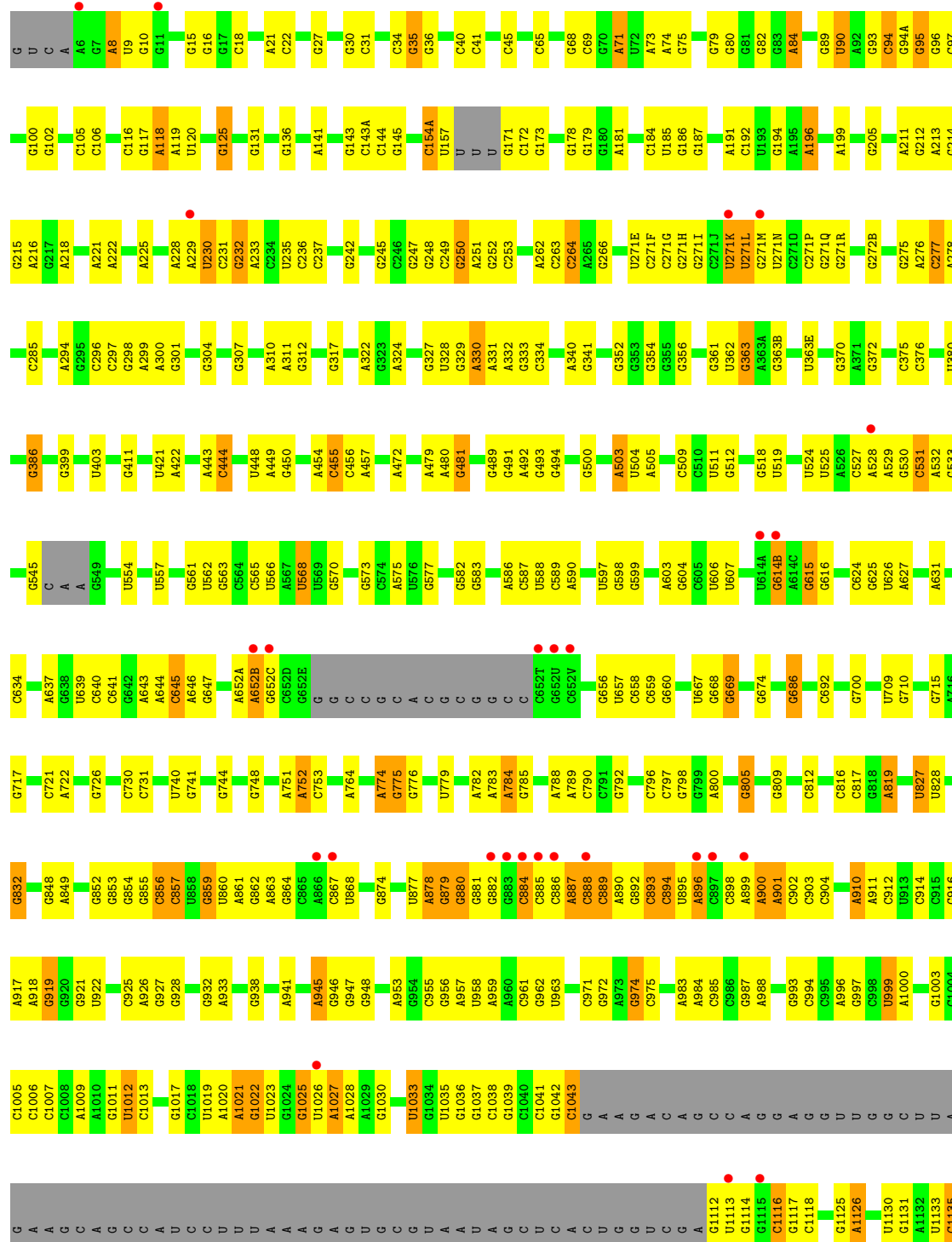
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2p	1	Total	O	0	0
			1	1		
62	2t	2	Total	O	0	0
			2	2		
62	2x	3	Total	O	0	0
			3	3		
62	2y	8	Total	O	0	0
			8	8		

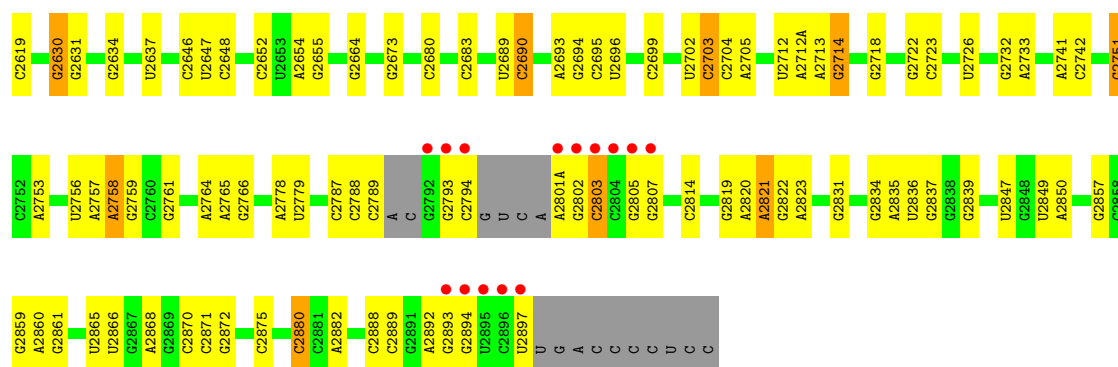
A2778	G2631	A2478	C2359	U2244	G2153	U2086	U1955	A1810	G1674	G1519	C1407	G1286	G1110
U2779	C2646	C2483	A2360	U2245	G2154	G2087	U1956	G1811	G1674	C1532	G1416	G1266	A1111
A2780	C2647	C2484	A2361	G2251	G2155	G2093	C1958	G1814	C1686	G	C1417	G1267	G1112
G2781	C2648	C2499	A2362	G2252	G2156	G2094	C1959	A1815	C1687	U	C1418	U1268	U1113
C2782	C2649	G2502	C2367	C2264	A2157	U2096	C1962	G1816	U1688	C	U1420	A1269	G1114
G2783	C2650	A2503	C2368	A2268	G2159	C2097	U1963	G1823	U1689	G1537	G1421	C1270	C1115
U2784	C2651	G2504	A2369	A2269	G2160	U2098	C1967	G1824	A1700	U1540	G1422	G1271	C1116
C2785	C2652	G2505	U2272	U2272	G2161	U2099	C1968	C1827	A1701	U1541	A1427	G1272	G1125
U2786	C2653	G2506	A2273	A2273	G2162	G2100	A1970	G1828	G1702	C1542	C1428	U1273	U1128
C2787	C2654	A2518	G2277	G2277	G2163	U2102	A1971	G1829	G1703	C1543	C1429	A1278	A1129
G2788	C2655	U2528	G2278	G2278	G2164	G2106	A1972	G1830	G1704	U1544	C1430	U1279	U1130
C2789	C2656	G2529	G2279	G2279	G2165	C2107	U1991	A1847	U1709	C1547	G1432	U1280	G1135
A2790	C2657	G2530	G2280	G2280	G2166	C2108	G1992	C1851	C1710	C1548	C1433	C1293	C1136
G2791	C2658	G2531	C2281	C2281	G2167	U2109	U1993	U1851	C1711	U1554	G1442	G1297	G1137
C2792	C2659	G2532	C2282	C2282	G2168	G2110	C1996	C1852	U1712	U1558	A1445	U1300	G1138
G2793	C2660	G2533	G2283	G2283	G2169	C2111	G1997	G1861	G1721	U1566	G1450	A1301	A1142A
C2794	C2661	G2534	C2284	C2284	G2170	U2112	G2001	C1866	A1722	A1567	G1451	A1302	A1143
U2795	C2662	G2535	C2285	C2285	G2171	G2113	G2002	A1876	U1739	G1568	U1453	G1303	A1156
G2796	C2663	G2536	C2286	C2286	G2172	U2114	G2003	A1877	G1746	A1569	G1455	C1315	G1164
C2797	C2664	G2537	A2287	A2287	G2173	G2115	G2004	A1878	G1750	A1570	G1461	G1332	U1165
U2798	C2665	G2538	C2288	C2288	G2174	G2116	G2005	A1879	G1756	A1571	G1467	A1342	C1166
G2799	C2666	G2539	C2289	C2289	G2175	G2117	G2006	A1880	A1762	U1578	C1468	C1345	G1171
C2800	C2667	G2540	C2290	C2290	G2176	G2118	G2007	A1881	G1763	A1580	A1469	G1346	G1172
A2801	C2668	G2541	C2291	C2291	G2177	U2119	G2008	A1882	G1764	C1581	G1473	U1352	A1173
G2802	C2669	G2542	C2292	C2292	G2178	U2120	G2009	A1883	G1779	C1582	U1477	G1356	U1175
C2803	C2670	G2543	C2293	C2293	G2179	G2121	G2010	A1884	A1780	U1586	A1477	U1357	G1176
G2804	C2671	G2544	C2294	C2294	G2180	G2122	G2011	A1885	C1774	A1587	G1482	G1358	A1177
U2805	C2672	G2545	C2295	C2295	G2181	G2123	G2012	A1886	U1778	C1588	G1484	A1359	C1178
C2806	C2673	G2546	C2296	C2296	G2182	G2124	G2013	A1887	U1779	U1589	U1484	A1360	G1179
G2807	C2674	G2547	C2297	C2297	G2183	G2125	G2014	A1888	A1780	G1594	U1489	G1364	U1187
A2808	C2675	G2548	C2298	C2298	G2184	G2126	G2015	A1889	C1781	G1595	A1490	A1365	U1188
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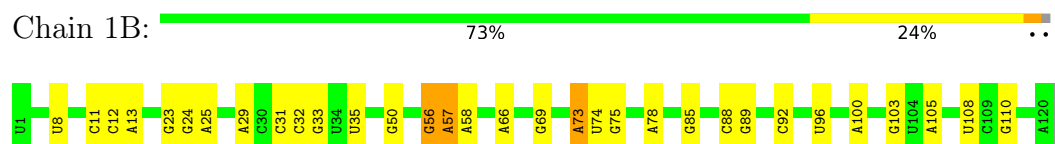
• Molecule 1: 23S Ribosomal RNA



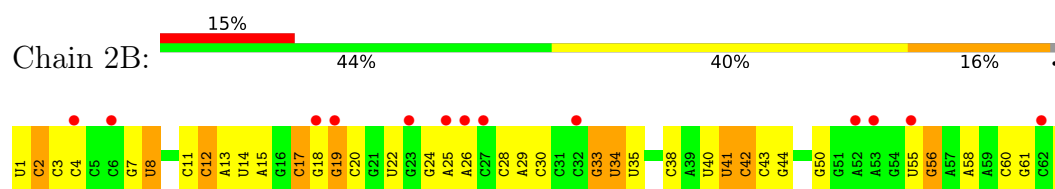




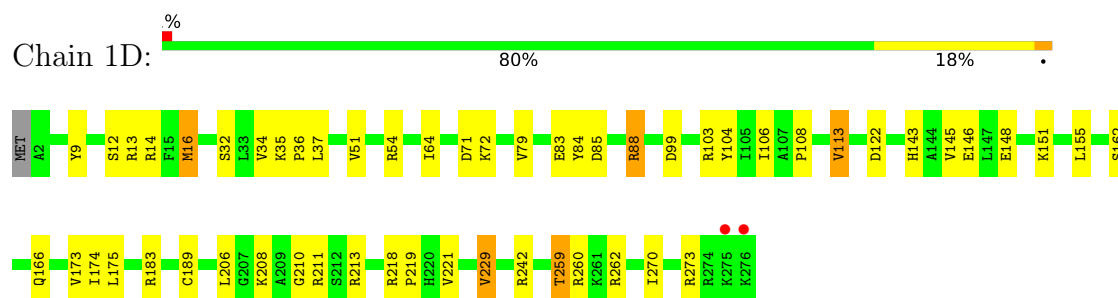
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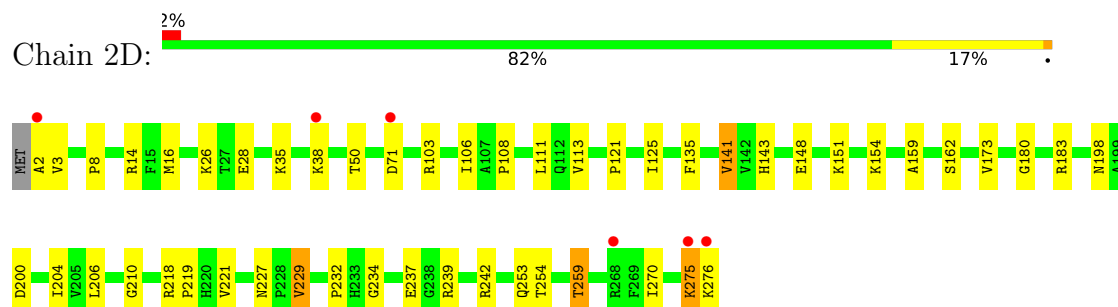
• Molecule 2: 5S Ribosomal RNA



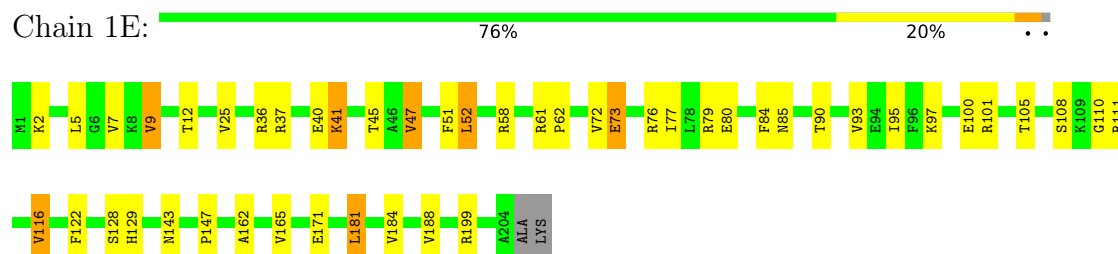
• Molecule 3: 50S ribosomal protein L2



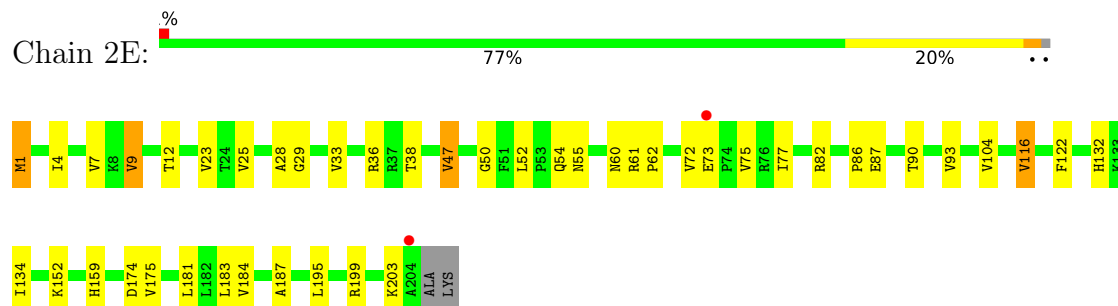
• Molecule 3: 50S ribosomal protein L2



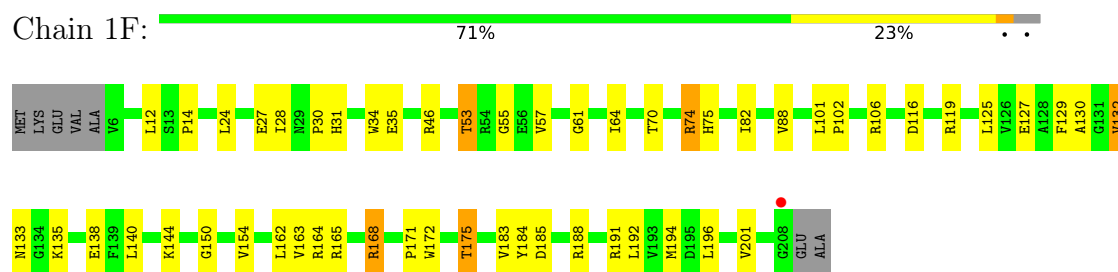
- Molecule 4: 50S ribosomal protein L3



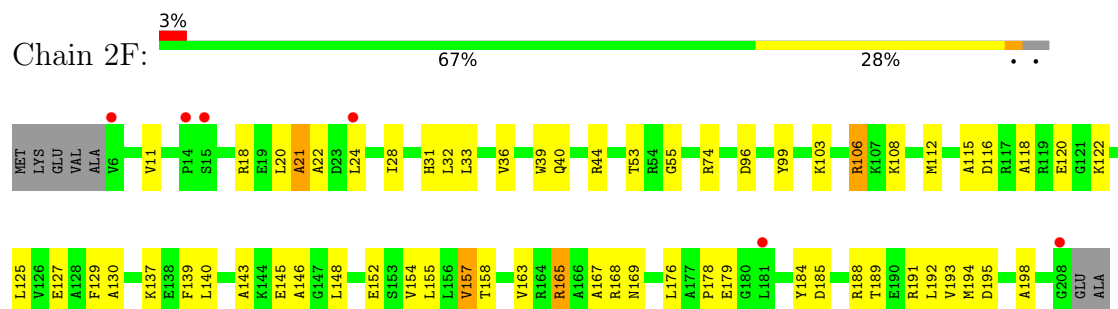
- Molecule 4: 50S ribosomal protein L3



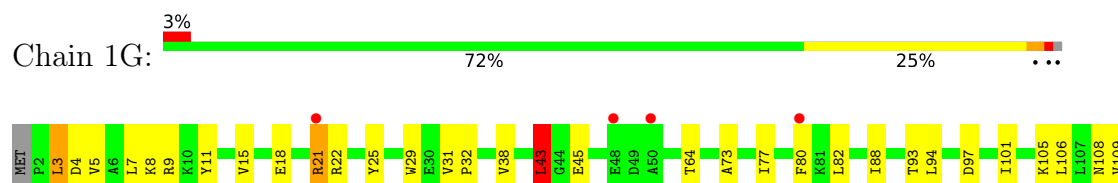
- Molecule 5: 50S ribosomal protein L4

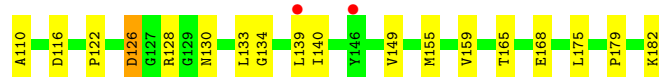


- Molecule 5: 50S ribosomal protein L4

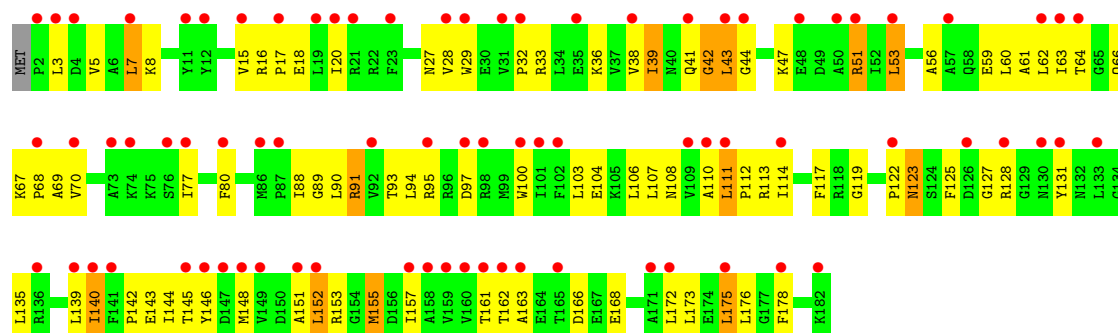
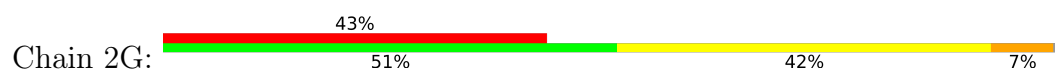


- Molecule 6: 50S ribosomal protein L5

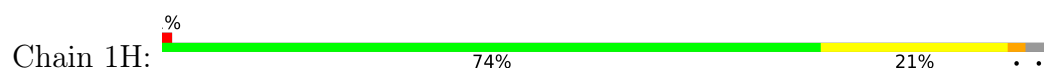




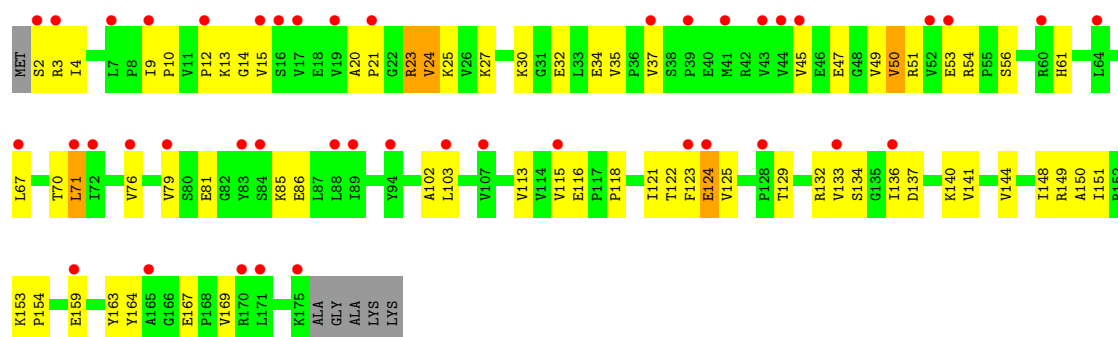
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

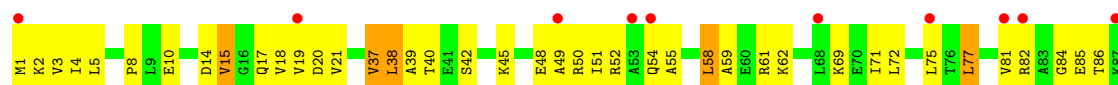


• Molecule 8: 50S ribosomal protein L9

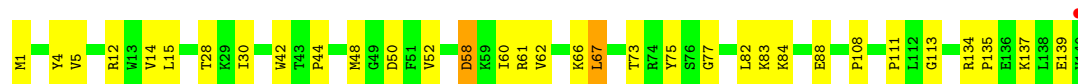
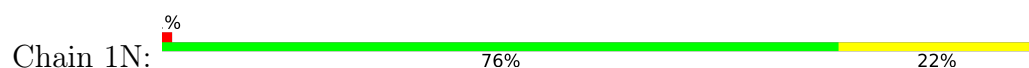




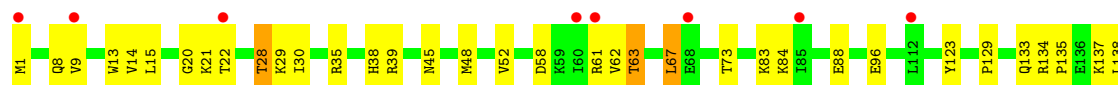
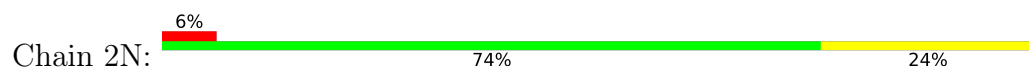
- Molecule 8: 50S ribosomal protein L9



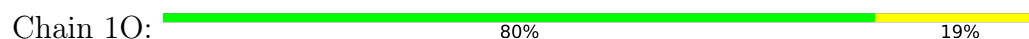
- Molecule 9: 50S ribosomal protein L13



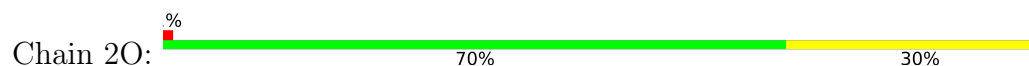
- Molecule 9: 50S ribosomal protein L13



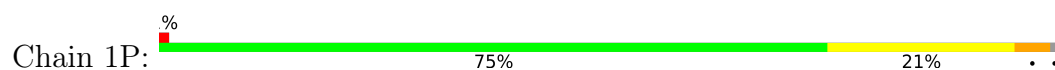
- Molecule 10: 50S ribosomal protein L14



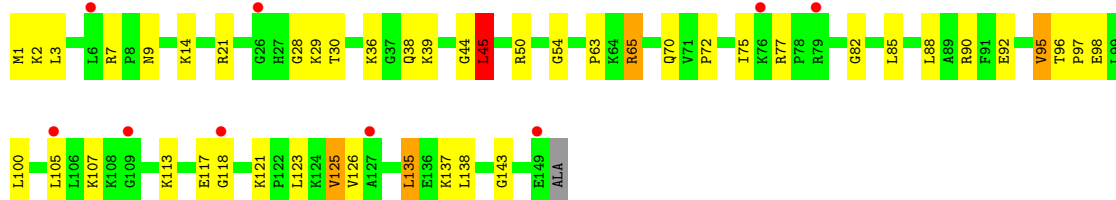
- Molecule 10: 50S ribosomal protein L14



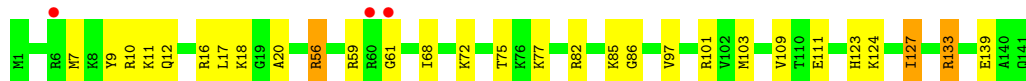
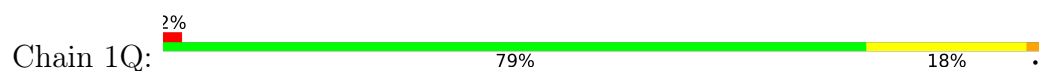
- Molecule 11: 50S ribosomal protein L15



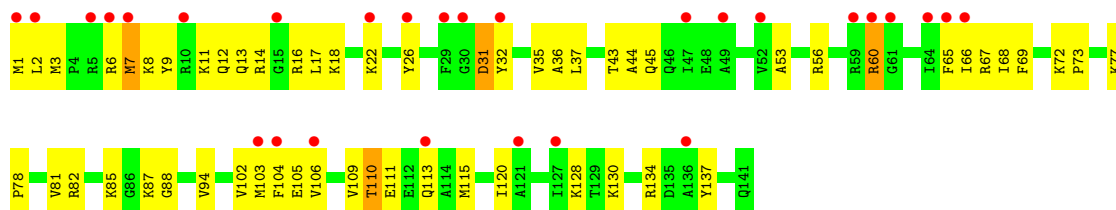
- Molecule 11: 50S ribosomal protein L15



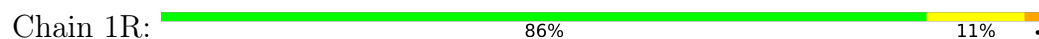
- Molecule 12: 50S ribosomal protein L16



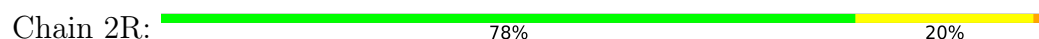
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



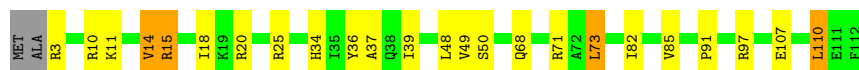
- Molecule 13: 50S ribosomal protein L17





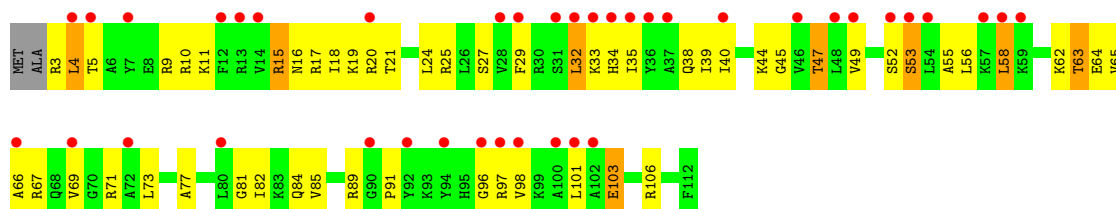
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 77% 18% . .



- Molecule 14: 50S ribosomal protein L18

Chain 2S: 35% 49% 42% 7% .



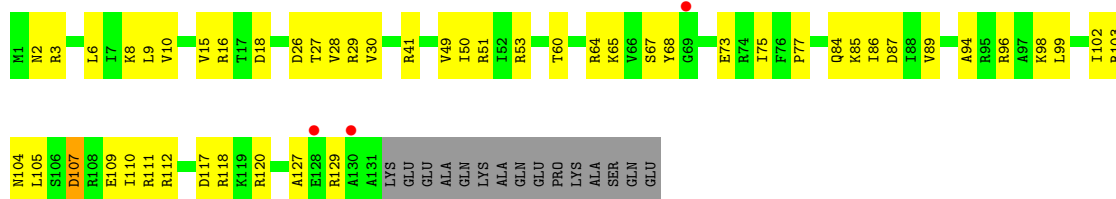
- Molecule 15: 50S ribosomal protein L19

Chain 1T: 2% 74% 16% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T: 2% 55% 34% 10%



- Molecule 16: 50S ribosomal protein L20

Chain 1U: 2% 79% 17% . .

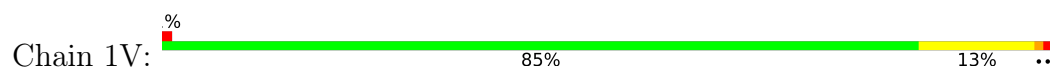


- Molecule 16: 50S ribosomal protein L20

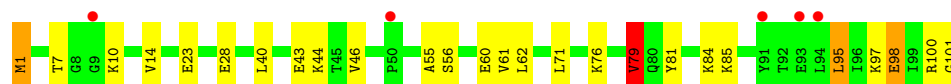
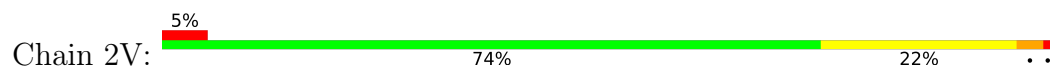
Chain 2U: 2% 75% 23% .



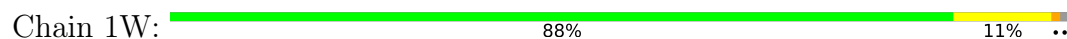
- Molecule 17: 50S ribosomal protein L21



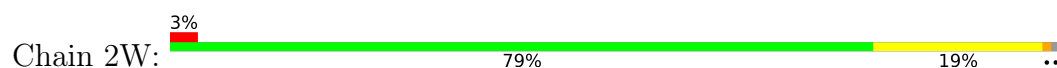
- Molecule 17: 50S ribosomal protein L21



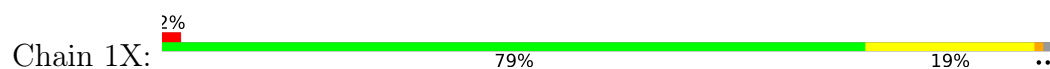
- Molecule 18: 50S ribosomal protein L22



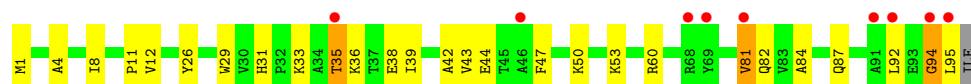
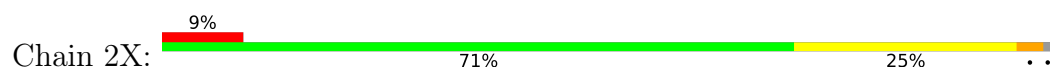
- Molecule 18: 50S ribosomal protein L22



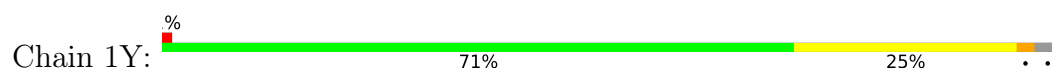
- Molecule 19: 50S ribosomal protein L23



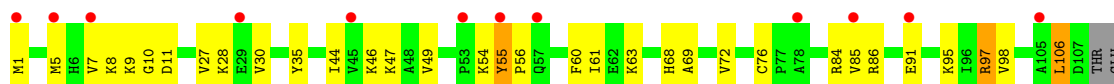
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

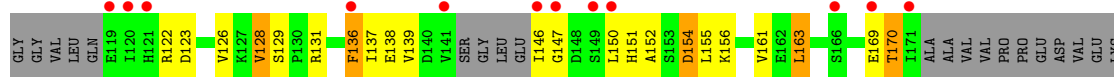
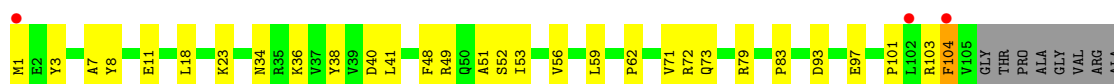


• Molecule 20: 50S ribosomal protein L24



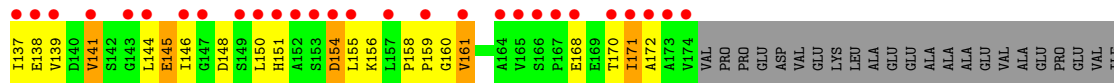
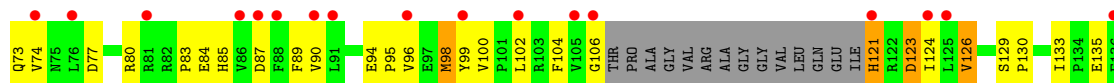
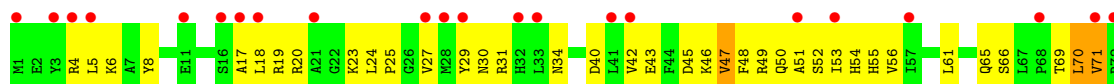
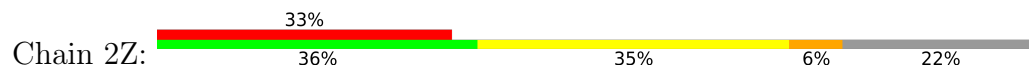
GLU

• Molecule 21: 50S ribosomal protein L25



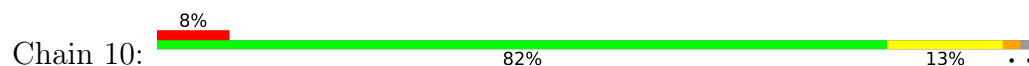
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• Molecule 21: 50S ribosomal protein L25



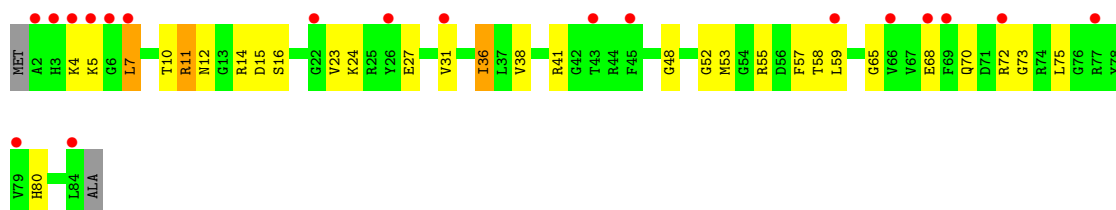
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GLU
GLU

• Molecule 22: 50S ribosomal protein L27

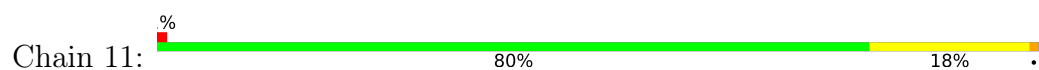




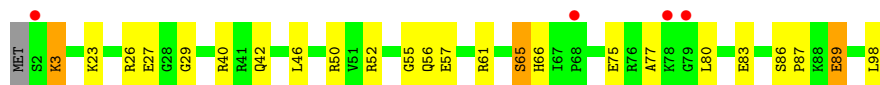
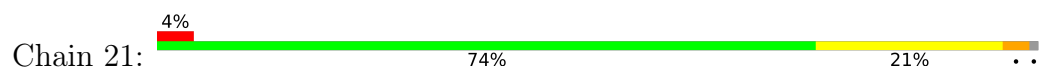
- Molecule 22: 50S ribosomal protein L27



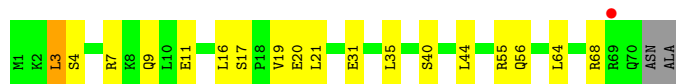
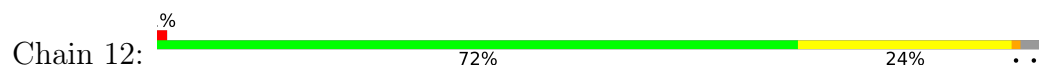
- Molecule 23: 50S ribosomal protein L28



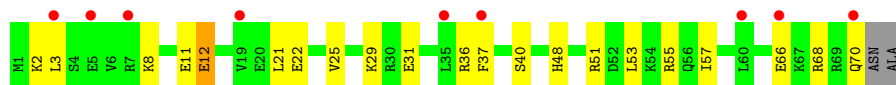
- Molecule 23: 50S ribosomal protein L28



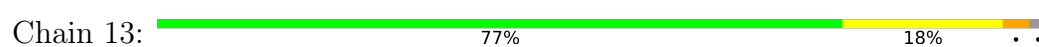
- Molecule 24: 50S ribosomal protein L29



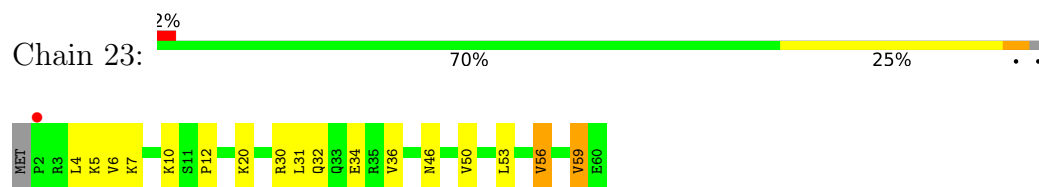
- Molecule 24: 50S ribosomal protein L29



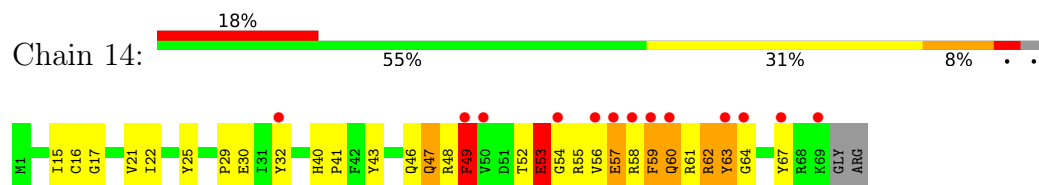
- Molecule 25: 50S ribosomal protein L30



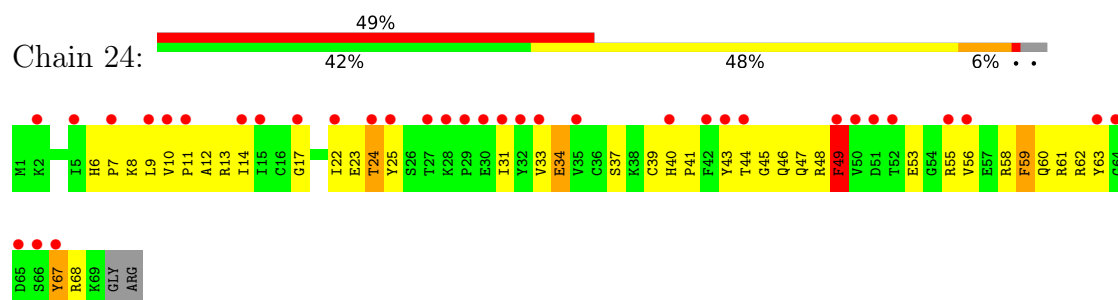
- Molecule 25: 50S ribosomal protein L30



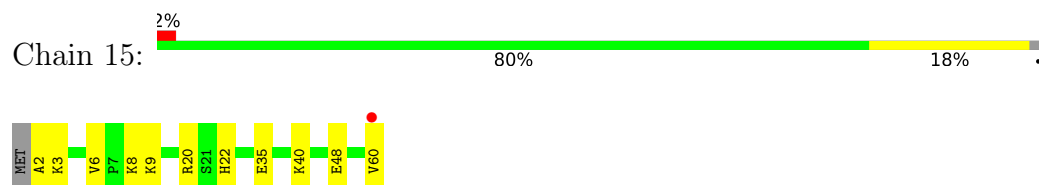
- Molecule 26: 50S ribosomal protein L31



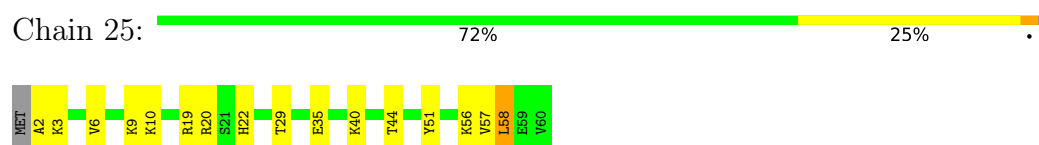
- Molecule 26: 50S ribosomal protein L31



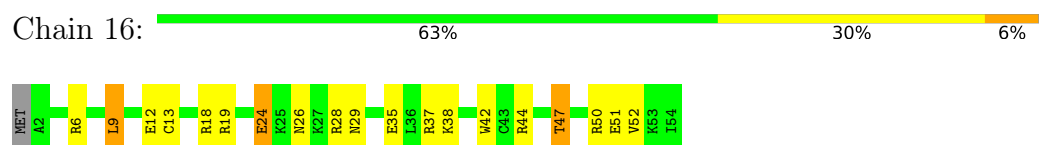
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

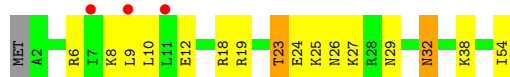


- Molecule 28: 50S ribosomal protein L33

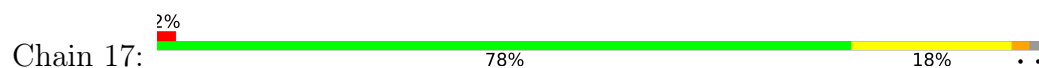


- Molecule 28: 50S ribosomal protein L33

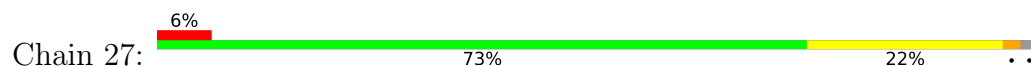




- Molecule 29: 50S ribosomal protein L34



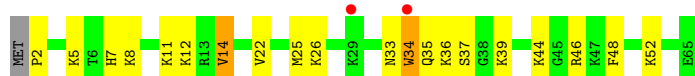
- Molecule 29: 50S ribosomal protein L34



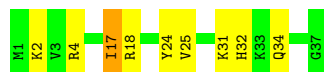
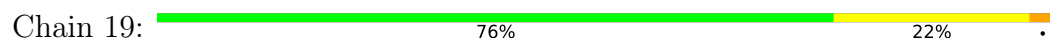
- Molecule 30: 50S ribosomal protein L35



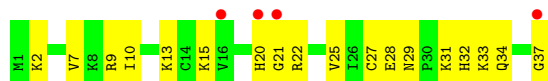
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



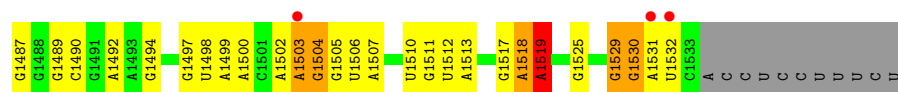
- Molecule 31: 50S ribosomal protein L36



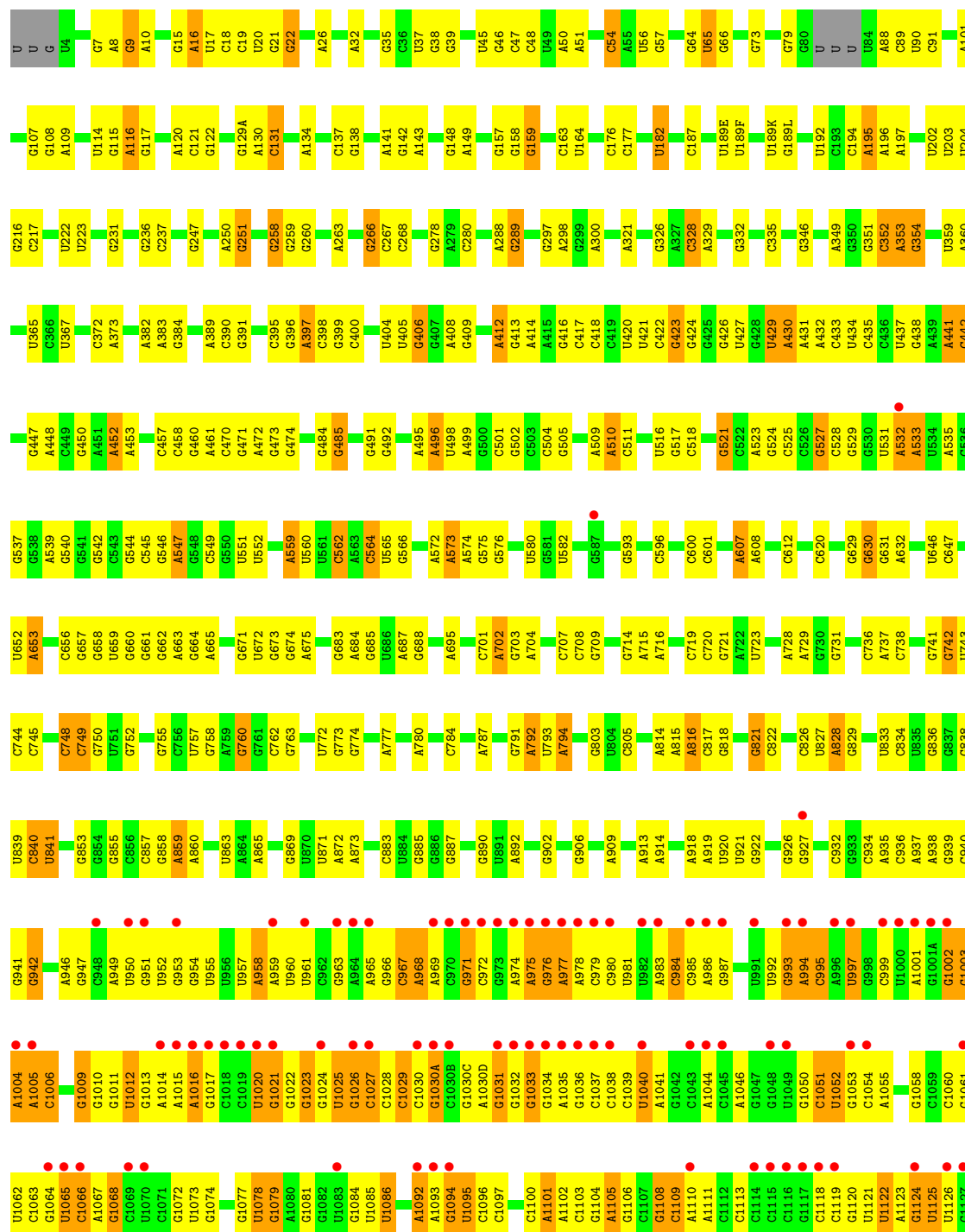
- Molecule 32: 16S Ribosomal RNA

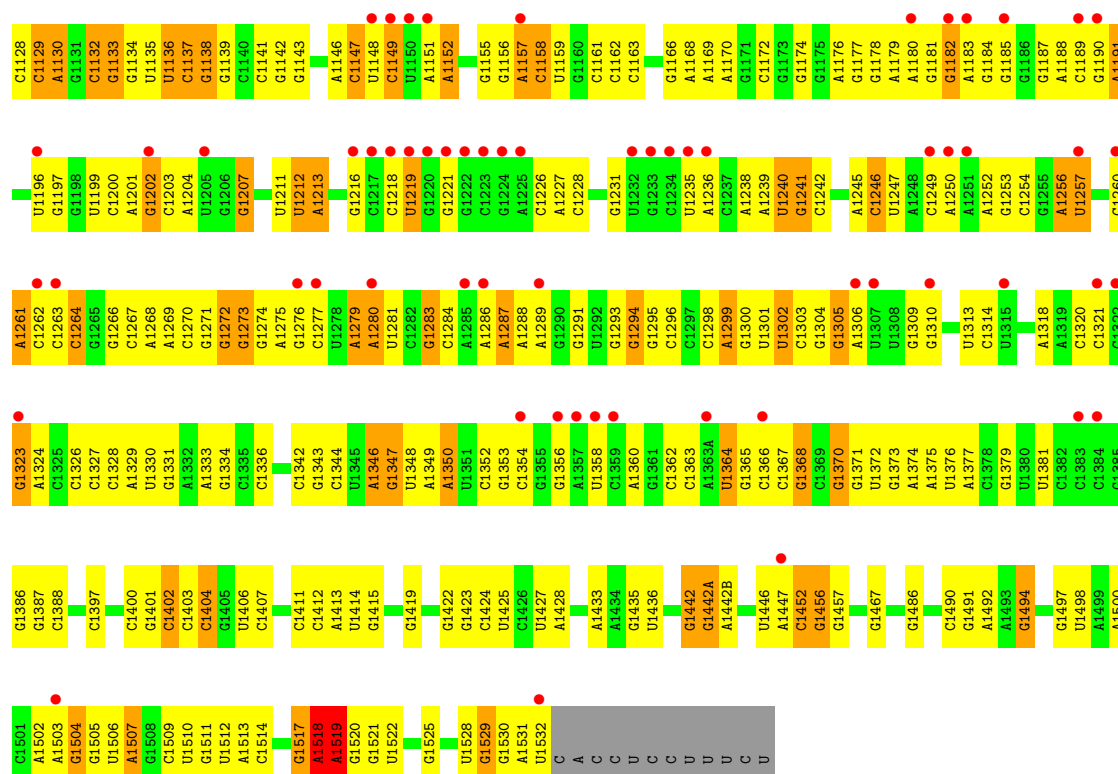


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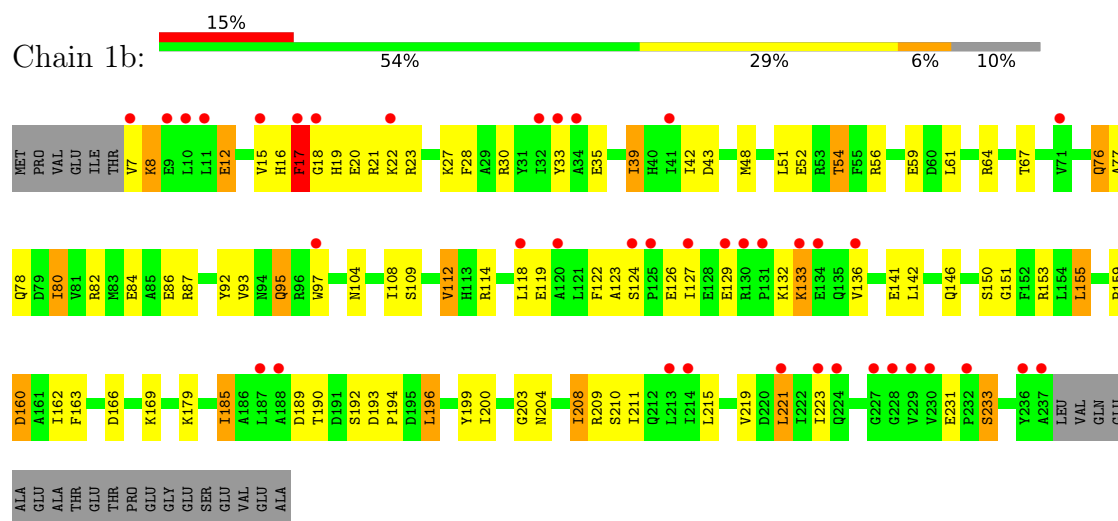


• Molecule 32: 16S Ribosomal RNA

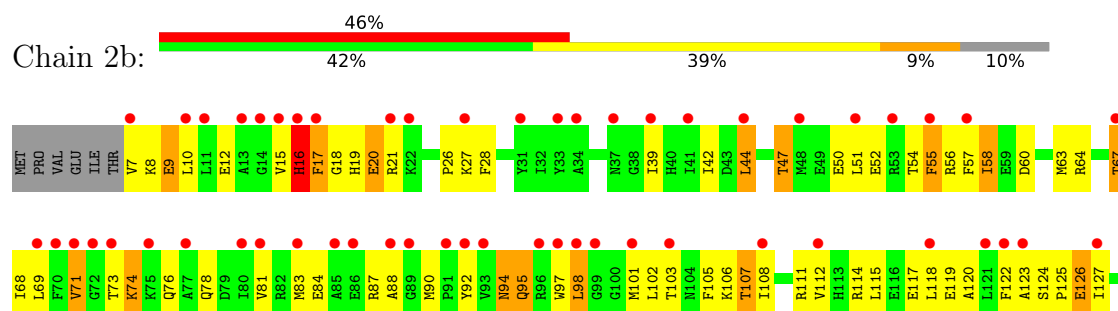


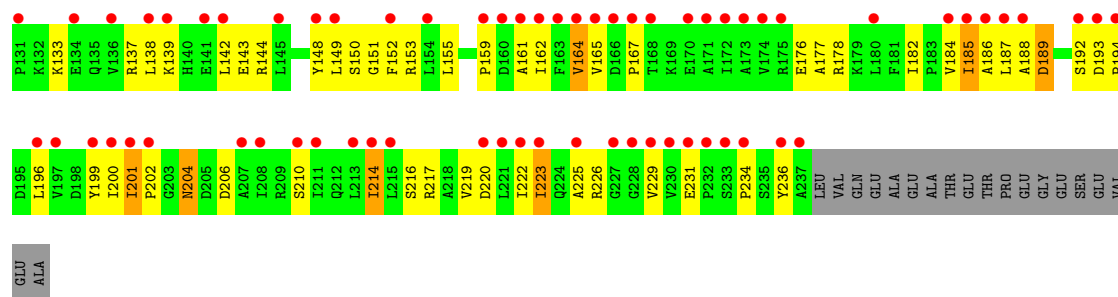


• Molecule 33: 30S ribosomal protein S2

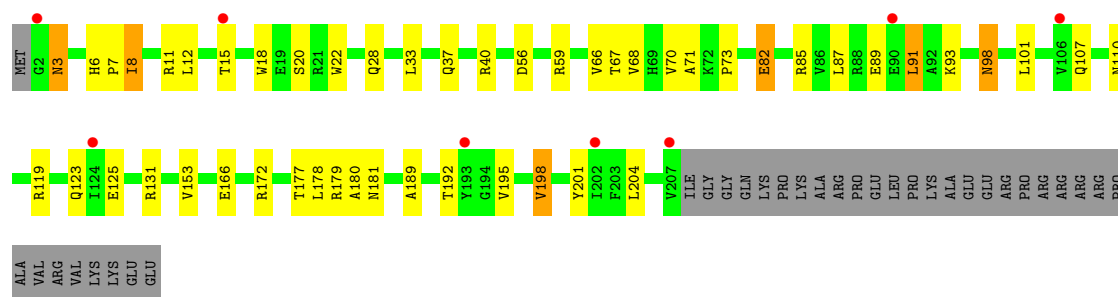


• Molecule 33: 30S ribosomal protein S2

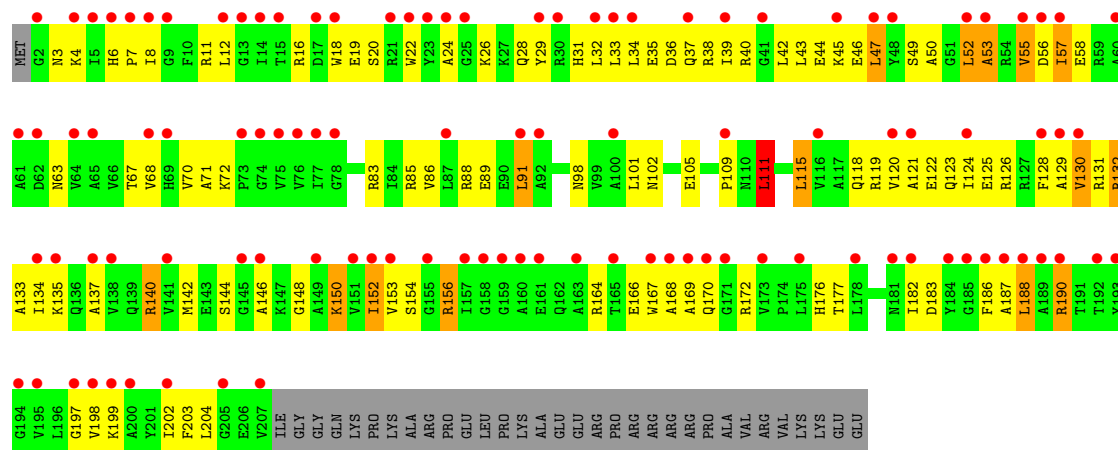




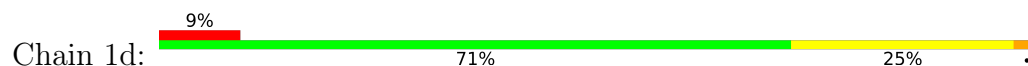
• Molecule 34: 30S ribosomal protein S3

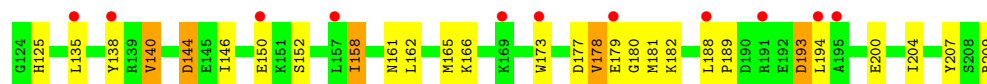


• Molecule 34: 30S ribosomal protein S3

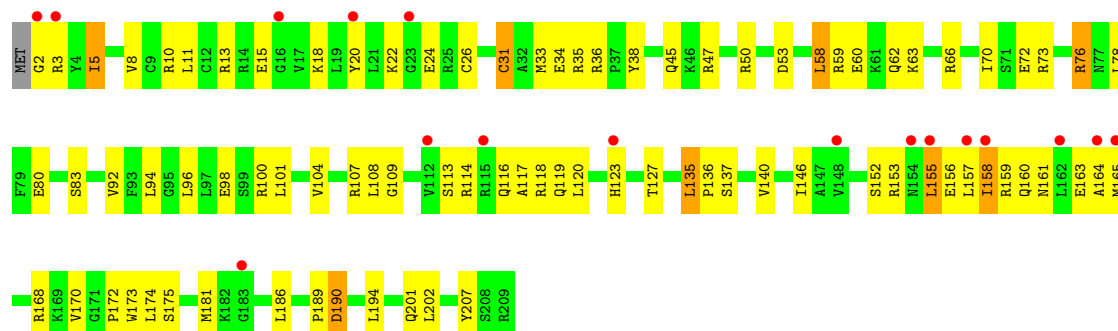


• Molecule 35: 30S ribosomal protein S4

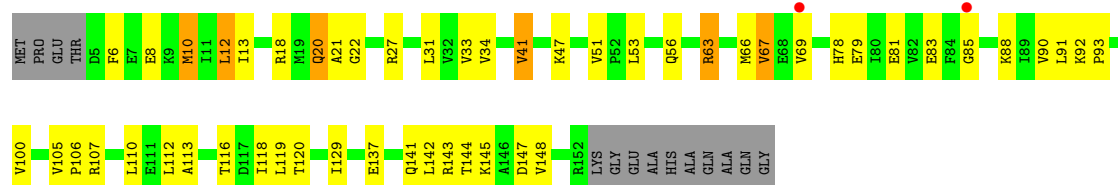




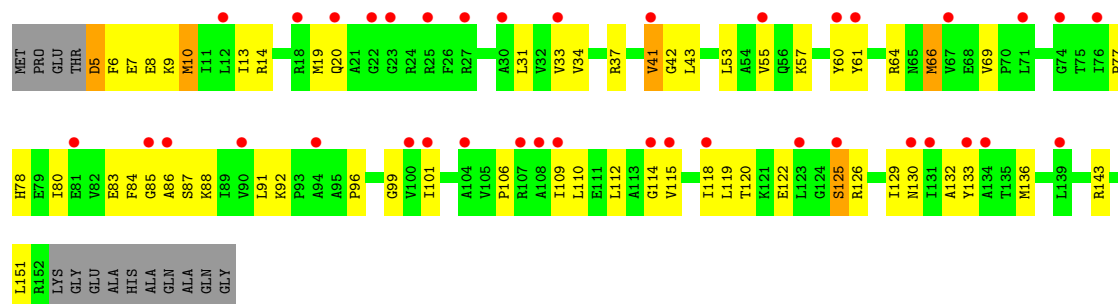
- Molecule 35: 30S ribosomal protein S4



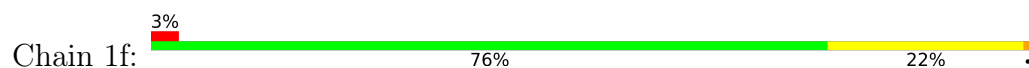
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



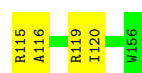
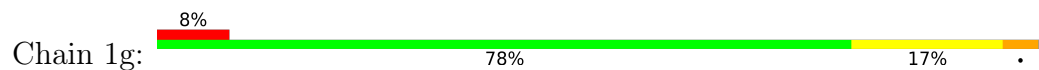
- Molecule 37: 30S ribosomal protein S6



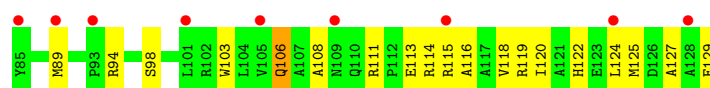
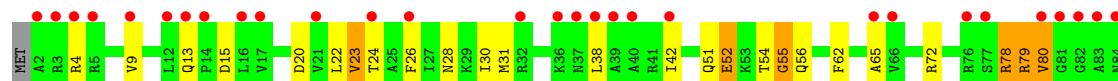
- Molecule 37: 30S ribosomal protein S6



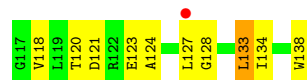
- Molecule 38: 30S ribosomal protein S7



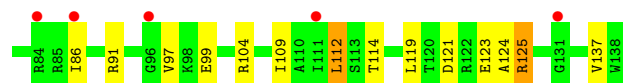
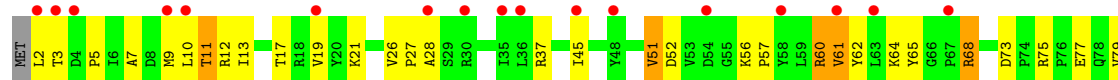
- Molecule 38: 30S ribosomal protein S7



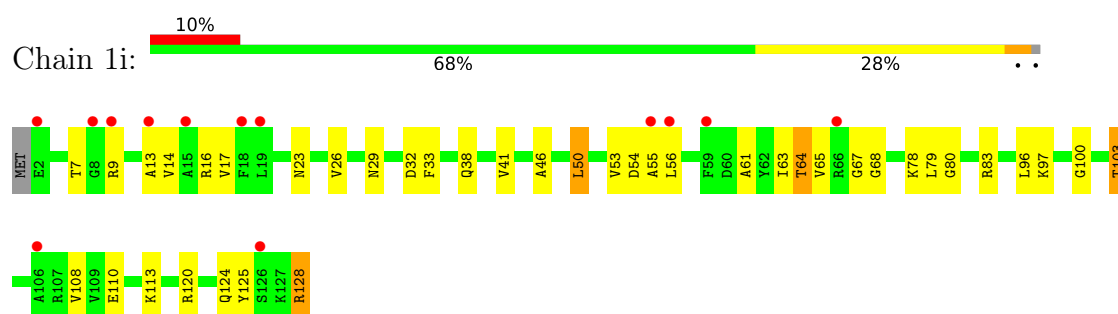
- Molecule 39: 30S ribosomal protein S8



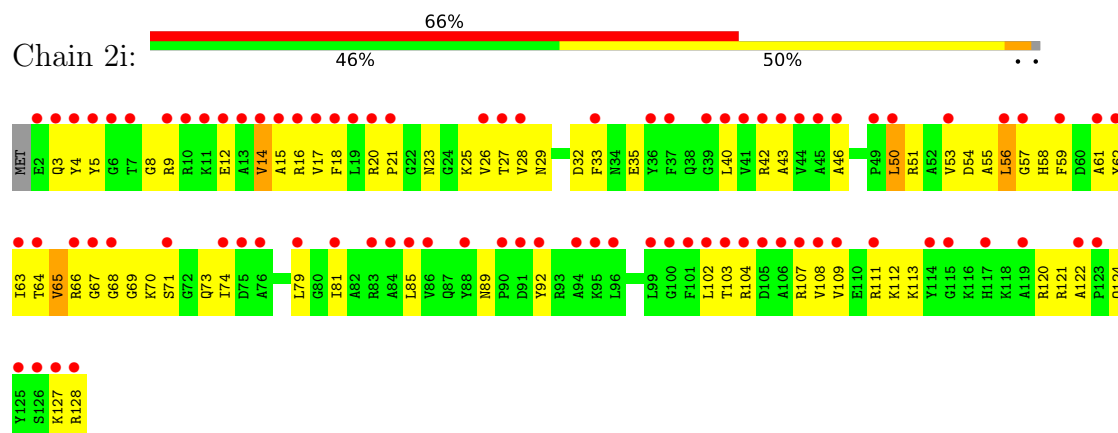
- Molecule 39: 30S ribosomal protein S8



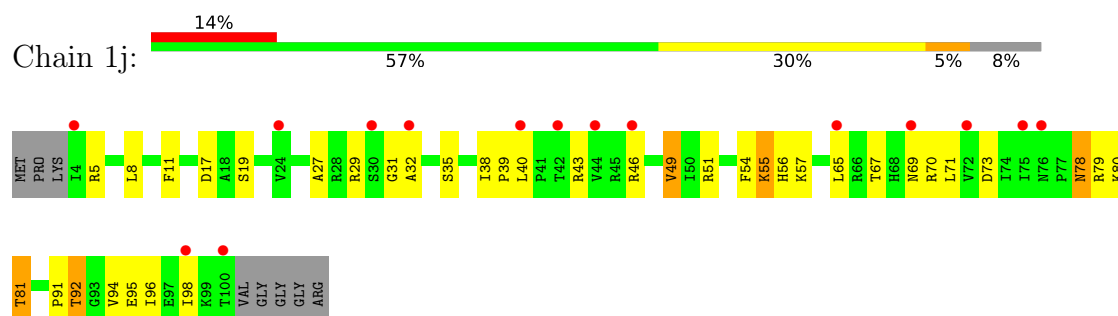
- Molecule 40: 30S ribosomal protein S9



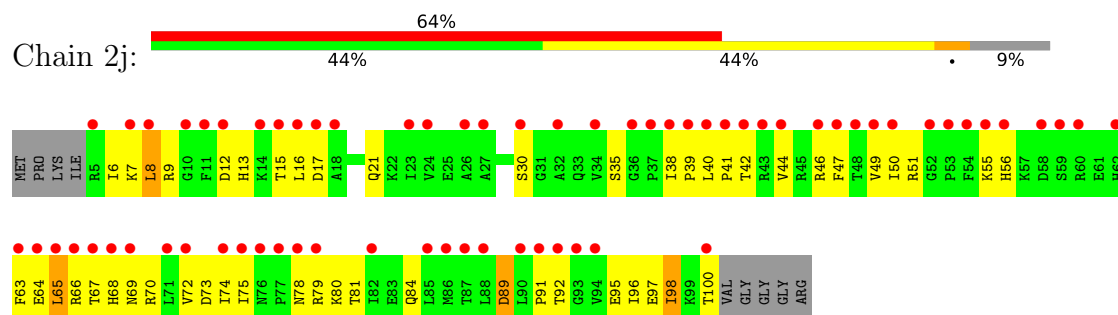
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

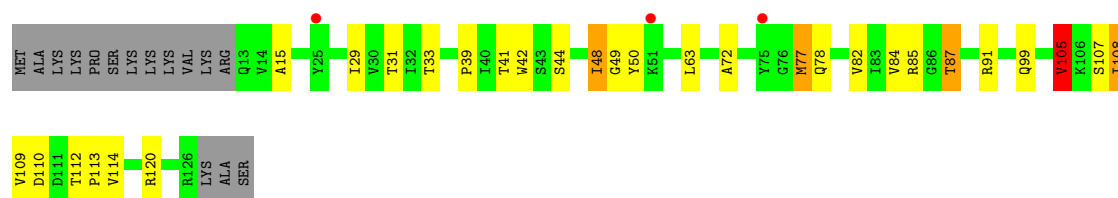


- Molecule 41: 30S ribosomal protein S10

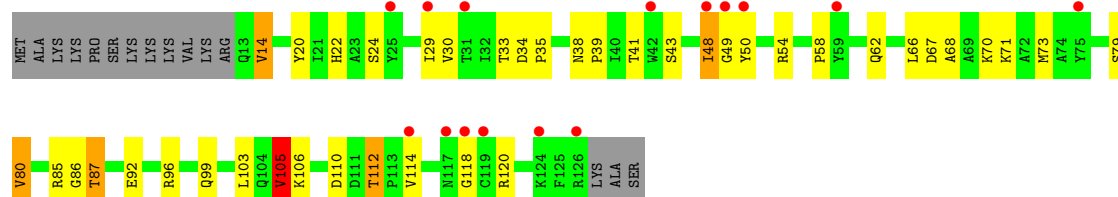


- Molecule 42: 30S ribosomal protein S11

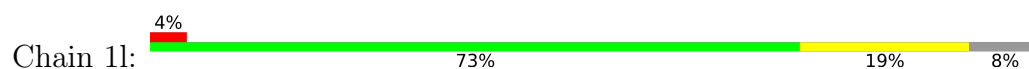




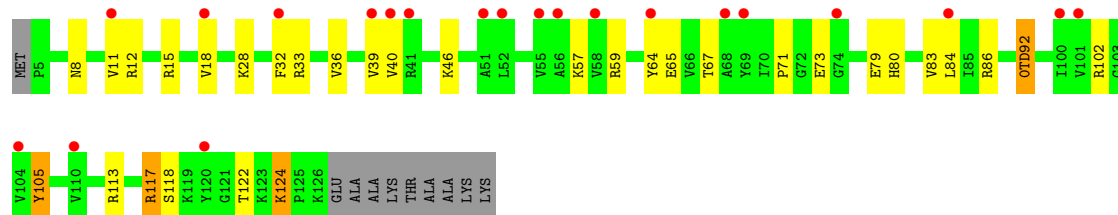
- Molecule 42: 30S ribosomal protein S11



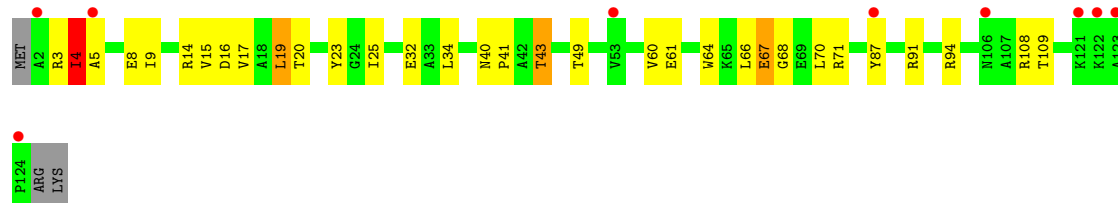
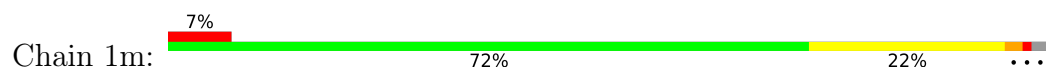
- Molecule 43: 30S ribosomal protein S12



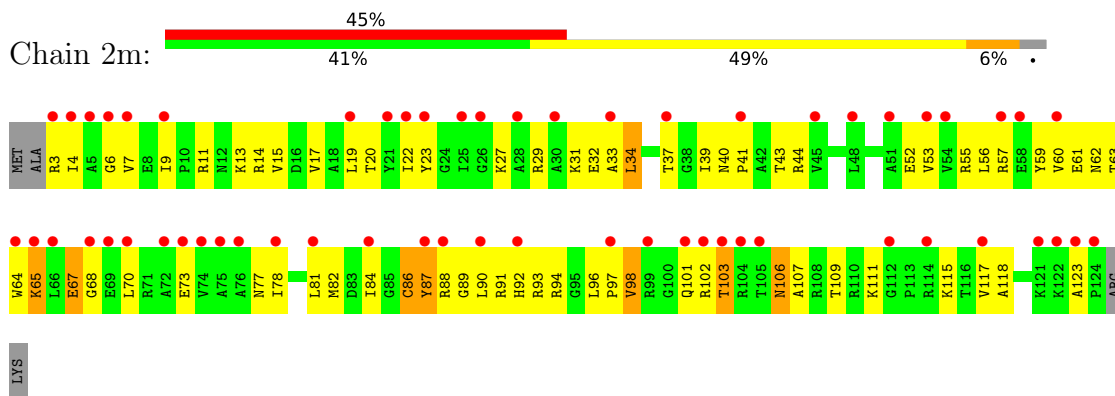
- Molecule 43: 30S ribosomal protein S12



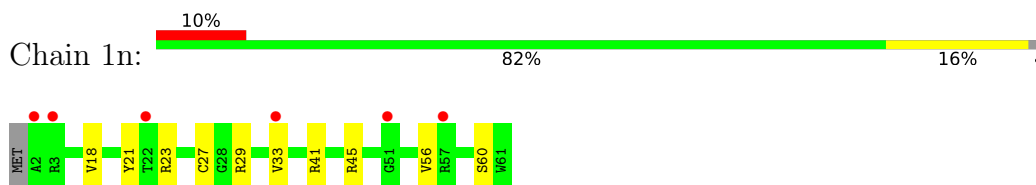
- Molecule 44: 30S ribosomal protein S13



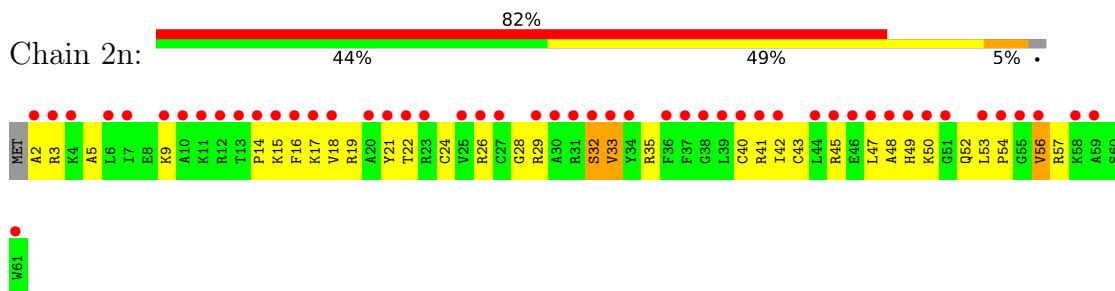
- Molecule 44: 30S ribosomal protein S13



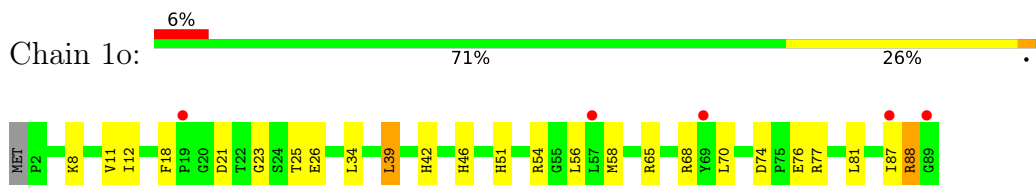
- Molecule 45: 30S ribosomal protein S14 type Z



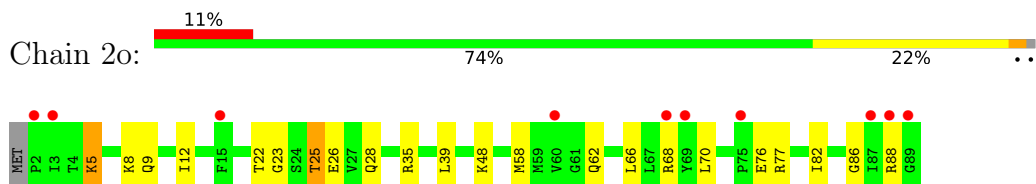
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

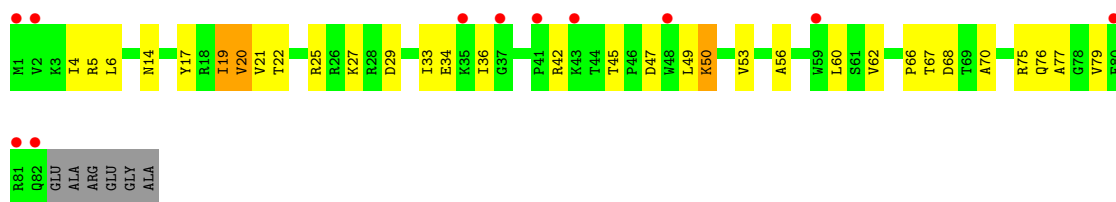


- Molecule 46: 30S ribosomal protein S15

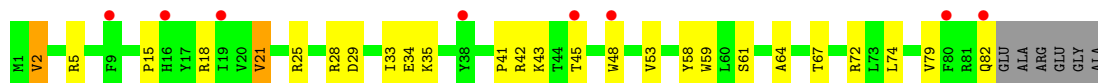


- Molecule 47: 30S ribosomal protein S16





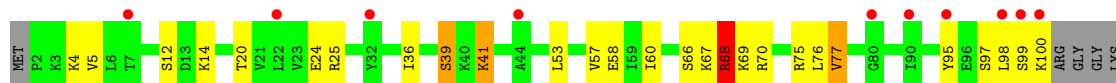
- Molecule 47: 30S ribosomal protein S16



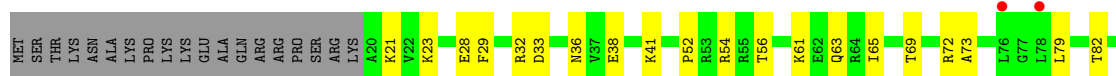
- Molecule 48: 30S ribosomal protein S17



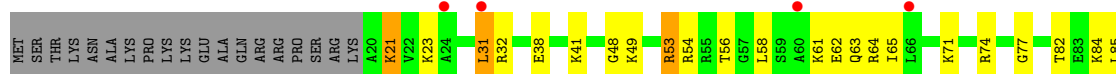
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

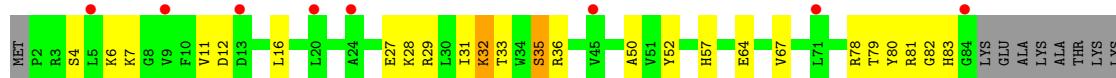


- Molecule 49: 30S ribosomal protein S18

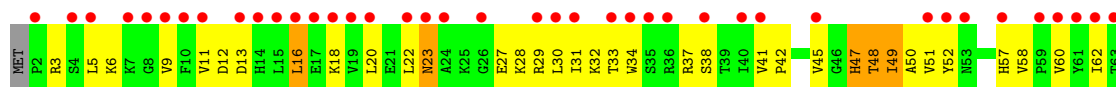




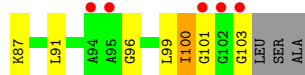
- Molecule 50: 30S ribosomal protein S19



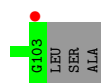
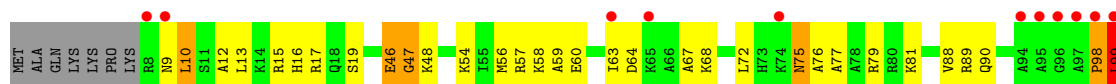
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

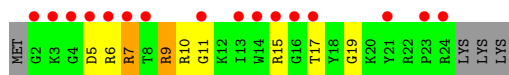


- Molecule 52: 30S ribosomal protein Thx





- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



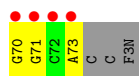
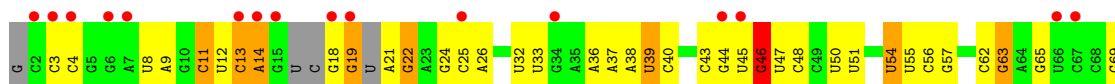
- Molecule 53: mRNA



- Molecule 54: A-site tRNA



- Molecule 54: A-site tRNA



- Molecule 55: P-site tRNA





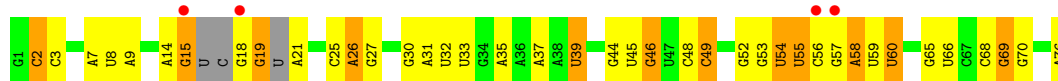
• Molecule 55: P-site tRNA



• Molecule 56: E-site tRNA



• Molecule 56: E-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.86Å 449.80Å 621.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	198.84 – 2.50 198.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (198.84-2.50) 99.8 (198.84-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.224 , 0.268 0.226 , 0.270	Depositor DCC
R_{free} test set	100061 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299504	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 7MG, 31H, OMC, 4OC, 6IF, K, MG, OMU, 4SU, M2G, 5MC, UR3, 0TD, ZN, SF4, 2MA, MIA, MA6, 2MG, 5MU, OMG, PSU

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	0.28	0/69011	0.48	1/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.40	2/105042 (0.0%)
2	1B	0.22	0/2882	0.42	0/4494
2	2B	0.21	0/2879	0.39	0/4487
3	1D	0.27	0/2186	0.52	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.27	0/1592	0.49	0/2149
4	2E	0.23	0/1592	0.45	0/2149
5	1F	0.26	0/1619	0.47	0/2193
5	2F	0.20	0/1615	0.45	2/2188 (0.1%)
6	1G	0.21	0/1448	0.44	0/1957
6	2G	0.20	0/1453	0.43	0/1963
7	1H	0.21	0/1356	0.41	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.18	0/1112	0.40	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.46	0/1543
9	2N	0.19	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.45	0/1269
10	2O	0.18	0/943	0.40	0/1269
11	1P	0.26	0/1152	0.52	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.27	0/1143	0.49	0/1527
12	2Q	0.21	0/1143	0.45	0/1527
13	1R	0.29	0/982	0.49	0/1312
13	2R	0.20	0/982	0.47	0/1312
14	1S	0.21	0/883	0.45	0/1176
14	2S	0.22	0/880	0.51	0/1172
15	1T	0.25	0/1105	0.49	0/1477
15	2T	0.21	0/1097	0.44	0/1468
16	1U	0.30	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.41	0/1301
17	1V	0.26	0/782	0.50	0/1049
17	2V	0.17	0/782	0.39	0/1049
18	1W	0.29	0/897	0.45	0/1205
18	2W	0.21	0/897	0.39	0/1205
19	1X	0.26	0/764	0.52	0/1025
19	2X	0.21	0/764	0.50	0/1025
20	1Y	0.23	0/819	0.50	0/1095
20	2Y	0.19	0/819	0.48	0/1095
21	1Z	0.23	0/1267	0.49	1/1717 (0.1%)
21	2Z	0.22	0/1299	0.44	0/1763
22	10	0.26	0/662	0.51	0/881
22	20	0.21	0/662	0.45	0/881
23	11	0.24	0/762	0.43	0/1014
23	21	0.21	0/762	0.44	0/1014
24	12	0.23	0/590	0.43	0/781
24	22	0.19	0/590	0.38	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.20	0/469	0.41	0/630
26	14	0.26	0/565	0.53	0/761
26	24	0.25	0/545	0.54	0/737
27	15	0.27	0/469	0.51	0/635
27	25	0.22	0/469	0.46	0/635
28	16	0.26	0/460	0.46	0/613
28	26	0.21	0/456	0.48	0/608
29	17	0.29	0/426	0.52	0/561
29	27	0.22	0/426	0.48	0/561
30	18	0.26	0/525	0.48	0/691
30	28	0.18	0/525	0.39	0/691
31	19	0.26	0/310	0.48	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.39	1/55864 (0.0%)
32	2a	0.20	0/35886	0.39	0/56005
33	1b	0.21	0/1881	0.49	0/2542
33	2b	0.24	0/1860	0.52	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.23	0/1566	0.46	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.20	0/1704	0.45	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.19	0/823	0.39	0/1115
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.41	0/1679
38	2g	0.20	0/1254	0.39	0/1683
39	1h	0.19	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.19	0/722	0.42	0/982
41	2j	0.24	0/727	0.48	0/988
42	1k	0.20	0/844	0.40	0/1145
42	2k	0.16	0/848	0.36	0/1149
43	1l	0.21	0/937	0.42	0/1260
43	2l	0.19	0/937	0.43	0/1260
44	1m	0.22	0/969	0.47	0/1302
44	2m	0.22	0/961	0.48	0/1291
45	1n	0.20	0/501	0.42	0/664
45	2n	0.22	0/501	0.44	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.16	0/739	0.39	0/985
47	1p	0.19	0/697	0.45	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.19	0/836	0.44	0/1117
49	1r	0.21	0/560	0.43	0/746
49	2r	0.18	0/560	0.42	0/746
50	1s	0.19	0/667	0.51	0/900
50	2s	0.26	0/661	0.60	0/893
51	1t	0.19	0/730	0.47	0/965
51	2t	0.20	0/729	0.44	0/965
52	1u	0.17	0/203	0.40	0/266
52	2u	0.19	0/203	0.43	0/266
53	1v	0.22	0/310	0.35	0/480
53	2v	0.18	0/310	0.32	0/480
54	1w	0.27	1/1537 (0.1%)	0.40	0/2390
54	2w	0.29	1/1487 (0.1%)	0.43	0/2311
55	1x	0.27	0/1700	0.42	0/2650
55	2x	0.25	0/1700	0.38	0/2650
56	1y	0.25	1/1606 (0.1%)	0.42	0/2497
56	2y	0.25	0/1583	0.40	0/2459
All	All	0.23	4/316502 (0.0%)	0.43	7/473837 (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
51	1t	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	8	4SU	O3'-P	5.15	1.61	1.56
1	2A	2552	OMU	O3'-P	5.14	1.61	1.56
54	1w	8	4SU	O3'-P	5.13	1.61	1.56
54	2w	8	4SU	O3'-P	5.04	1.61	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1Z	53	ILE	N-CA-C	-8.15	104.65	111.91
1	1A	1992	G	C2'-C3'-O3'	6.74	119.61	109.50
1	2A	1992	G	C2'-C3'-O3'	5.43	117.65	109.50
32	1a	266	G	C2'-C3'-O3'	5.28	117.42	109.50
5	2F	21	ALA	CA-C-N	5.18	131.03	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide

5.2 Too-close contacts [i](#)

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	61852	0	31197	568	0
1	2A	60322	0	30426	677	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	52	0
3	1D	2136	0	2218	35	0
3	2D	2136	0	2218	35	0
4	1E	1559	0	1618	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	25	0
5	1F	1584	0	1625	31	0
5	2F	1580	0	1619	43	0
6	1G	1423	0	1436	32	0
6	2G	1428	0	1438	74	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	35	0
8	1I	1097	0	1140	23	0
8	2I	1064	0	1082	44	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	15	0
10	2O	933	0	996	21	0
11	1P	1135	0	1212	28	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	38	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	15	0
14	2S	870	0	923	46	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	33	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	14	0
17	1V	771	0	830	9	0
17	2V	771	0	830	19	0
18	1W	886	0	940	6	0
18	2W	886	0	940	13	0
19	1X	750	0	814	12	0
19	2X	750	0	814	24	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	21	0
21	1Z	1240	0	1240	32	0
21	2Z	1271	0	1273	58	0
22	10	653	0	674	14	0
22	20	653	0	674	20	0
23	11	755	0	826	14	0
23	21	755	0	826	15	0
24	12	588	0	643	10	0
24	22	588	0	643	15	0
25	13	469	0	518	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	8	0
26	14	552	0	533	21	0
26	24	532	0	503	31	0
27	15	455	0	465	5	0
27	25	455	0	465	11	0
28	16	453	0	473	12	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	11	0
30	18	517	0	582	14	0
30	28	517	0	582	17	0
31	19	307	0	335	7	0
31	29	307	0	335	12	0
32	1a	32246	0	16295	378	0
32	2a	32327	0	16339	575	0
33	1b	1846	0	1867	55	0
33	2b	1825	0	1828	93	0
34	1c	1548	0	1535	29	0
34	2c	1542	0	1517	83	0
35	1d	1655	0	1672	32	0
35	2d	1674	0	1714	67	0
36	1e	1129	0	1185	36	0
36	2e	1133	0	1191	37	0
37	1f	810	0	804	16	0
37	2f	816	0	808	22	0
38	1g	1231	0	1238	18	0
38	2g	1235	0	1249	41	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	24	0
40	2i	978	0	966	52	0
41	1j	709	0	650	29	0
41	2j	714	0	672	33	0
42	1k	829	0	825	15	0
42	2k	833	0	836	25	0
43	1l	932	0	981	13	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	19	0
44	2m	950	0	988	57	0
45	1n	492	0	529	7	0
45	2n	492	0	529	27	0
46	1o	728	0	760	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	14	0
47	1p	681	0	697	23	0
47	2p	677	0	686	19	0
48	1q	823	0	891	19	0
48	2q	823	0	891	19	0
49	1r	555	0	618	14	0
49	2r	555	0	618	19	0
50	1s	652	0	662	16	0
50	2s	646	0	644	45	0
51	1t	728	0	798	26	0
51	2t	727	0	796	28	0
52	1u	199	0	208	7	0
52	2u	199	0	208	8	0
53	1v	277	0	140	1	0
53	2v	277	0	140	3	0
54	1w	1530	0	786	17	0
54	2w	1482	0	755	21	0
55	1x	1635	0	839	7	0
55	2x	1635	0	839	12	0
56	1y	1585	0	804	21	0
56	2y	1565	0	795	27	0
57	10	8	0	0	0	0
57	11	5	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	9	0	0	0	0
57	16	1	0	0	0	0
57	17	6	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1108	0	0	0	0
57	1B	36	0	0	0	0
57	1D	12	0	0	0	0
57	1E	16	0	0	0	0
57	1F	12	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	6	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1R	4	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	9	0	0	0	0
57	1V	6	0	0	0	0
57	1W	6	0	0	0	0
57	1X	5	0	0	0	0
57	1Y	4	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	229	0	0	0	0
57	1b	2	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	1l	3	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	5	0	0	0	0
57	1x	15	0	0	0	0
57	1y	4	0	0	0	0
57	20	3	0	0	0	0
57	21	1	0	0	0	0
57	23	2	0	0	0	0
57	25	3	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	2A	729	0	0	0	0
57	2B	18	0	0	0	0
57	2D	6	0	0	0	0
57	2E	7	0	0	0	0
57	2F	6	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	2Q	1	0	0	0	0
57	2R	1	0	0	0	0
57	2T	3	0	0	0	0
57	2W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	186	0	0	0	0
57	2d	1	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2l	3	0	0	0	0
57	2q	3	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	1	0	0	0	0
57	2w	1	0	0	0	0
57	2x	5	0	0	0	0
57	2y	3	0	0	0	0
58	1A	32	0	0	2	0
58	2A	32	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	1	0
61	2A	1	0	0	0	0
62	10	10	0	0	0	0
62	11	12	0	0	1	0
62	12	4	0	0	0	0
62	13	5	0	0	1	0
62	15	7	0	0	0	0
62	16	1	0	0	0	0
62	17	8	0	0	1	0
62	18	10	0	0	0	0
62	1A	2122	0	0	77	0
62	1B	69	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1D	24	0	0	0	0
62	1E	27	0	0	0	0
62	1F	18	0	0	1	0
62	1G	7	0	0	0	0
62	1H	2	0	0	0	0
62	1N	4	0	0	1	0
62	1O	7	0	0	1	0
62	1P	20	0	0	2	0
62	1Q	8	0	0	0	0
62	1R	10	0	0	2	0
62	1S	4	0	0	0	0
62	1T	8	0	0	0	0
62	1U	10	0	0	1	0
62	1V	9	0	0	0	0
62	1W	7	0	0	0	0
62	1X	7	0	0	1	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	361	0	0	25	0
62	1b	1	0	0	0	0
62	1d	1	0	0	0	0
62	1e	1	0	0	0	0
62	1g	1	0	0	0	0
62	1l	4	0	0	0	0
62	1m	2	0	0	0	0
62	1q	4	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	6	0	0	0	0
62	1x	16	0	0	1	0
62	1y	2	0	0	0	0
62	20	2	0	0	0	0
62	21	3	0	0	0	0
62	23	2	0	0	0	0
62	25	2	0	0	1	0
62	26	1	0	0	0	0
62	27	2	0	0	0	0
62	28	6	0	0	0	0
62	29	1	0	0	0	0
62	2A	968	0	0	65	0
62	2B	15	0	0	0	0
62	2D	16	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2E	9	0	0	0	0
62	2F	9	0	0	0	0
62	2I	1	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	3	0	0	0	0
62	2T	2	0	0	0	0
62	2W	1	0	0	0	0
62	2X	3	0	0	1	0
62	2Y	1	0	0	0	0
62	2a	51	0	0	6	0
62	2d	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	1	0	0	0	0
62	2l	3	0	0	0	0
62	2p	1	0	0	0	0
62	2t	2	0	0	0	0
62	2x	3	0	0	0	0
62	2y	8	0	0	1	0
All	All	299504	0	196651	4204	0

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 9.

The worst 5 of 4204 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	1.32	1.26
6:1G:21:ARG:HA	6:1G:21:ARG:HH11	1.20	1.02
1:1A:1082:U:O4	1:1A:1086:A:N1	1.93	1.01
1:2A:2138:C:N4	1:2A:2153:G:H1	1.61	0.98
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.45	0.97

There are no symmetry-related clashes.

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%)	258 (94%)	14 (5%)	1 (0%)	30	49
3	2D	273/276 (99%)	253 (93%)	20 (7%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43
4	2E	202/206 (98%)	186 (92%)	15 (7%)	1 (0%)	24	43
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	43
5	2F	201/210 (96%)	187 (93%)	12 (6%)	2 (1%)	12	24
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	38
6	2G	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	7	13
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	21	38
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	17
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	34
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	6	10
11	2P	147/150 (98%)	127 (86%)	15 (10%)	5 (3%)	3	4
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	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%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	96 (89%)	8 (7%)	4 (4%)	2	3
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	24
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	24
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5	9
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	22
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	24
20	2Y	105/110 (96%)	99 (94%)	3 (3%)	3 (3%)	3	5
21	1Z	148/206 (72%)	125 (84%)	21 (14%)	2 (1%)	9	17
21	2Z	156/206 (76%)	122 (78%)	33 (21%)	1 (1%)	21	38
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	10	20
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	22
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	22
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	12
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	0
26	24	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3	5
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	4
33	2b	229/256 (90%)	180 (79%)	40 (18%)	9 (4%)	2	3
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24	43
34	2c	204/239 (85%)	169 (83%)	31 (15%)	4 (2%)	6	10
35	1d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	24	43
35	2d	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	12	24
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18	34
36	2e	146/162 (90%)	125 (86%)	17 (12%)	4 (3%)	4	6
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	18
38	2g	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	18
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	18	34
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	31
40	2i	125/128 (98%)	101 (81%)	23 (18%)	1 (1%)	16	31
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	4
41	2j	94/105 (90%)	76 (81%)	14 (15%)	4 (4%)	2	2
42	1k	112/129 (87%)	99 (88%)	10 (9%)	3 (3%)	4	6
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	12
43	1l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	16	31
44	1m	121/126 (96%)	109 (90%)	10 (8%)	2 (2%)	7	13
44	2m	120/126 (95%)	97 (81%)	21 (18%)	2 (2%)	7	13
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	13
46	1o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	8
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	20
47	1p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	12	24
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	7
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	4	7
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3	4
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	2
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	13 (62%)	8 (38%)	0	100	100
All	All	11370/12128 (94%)	10356 (91%)	891 (8%)	123 (1%)	11	22

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	38	GLN
21	1Z	52	SER
21	1Z	163	LEU
23	11	3	LYS

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%)	199 (93%)	16 (7%)	13	27
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	43
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	24
4	2E	164/166 (99%)	151 (92%)	13 (8%)	11	24
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	152 (96%)	7 (4%)	25	50
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7	16
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	9
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	26
7	2H	144/148 (97%)	125 (87%)	19 (13%)	4	8
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	2
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	9
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	31
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	26
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	54
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	54
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	29
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	17
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	41
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	23
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	64
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	44
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	14
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	3
15	1T	115/127 (91%)	112 (97%)	3 (3%)	40	68
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	42
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	21
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	21
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	44
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	12
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	50
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	55
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	29
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8	17
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	3	5
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	62
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	34
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	82
23	21	80/83 (96%)	75 (94%)	5 (6%)	16	34
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	34
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	36
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	8
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	3
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	54
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	16
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	54
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	16
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	39
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	37
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	192/220 (87%)	166 (86%)	26 (14%)	4	8
33	2b	187/220 (85%)	158 (84%)	29 (16%)	2	5
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8	19
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2	4
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	12
35	2d	173/181 (96%)	156 (90%)	17 (10%)	7	16
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	20
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	17
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	29
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	15
38	2g	120/127 (94%)	105 (88%)	15 (12%)	4	9
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	20
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4	8
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	15
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9	19
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	6
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	13
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	17
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	62
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	27
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	13
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	8
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	35
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	15
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	68
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	43
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	27
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	27
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	27
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	78
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	15
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	38
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	4
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13	29
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	51
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	39
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9303/10064 (92%)	8489 (91%)	814 (9%)	9 21

5 of 814 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	2N	134	ARG
23	21	65	SER
50	2s	16	LEU
11	2P	117	GLU
9	2N	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	125	HIS
44	2m	62	ASN
36	2e	73	ASN
38	2g	148	ASN
50	2s	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	25 (0%)
1	2A	2791/2915 (95%)	463 (16%)	25 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1497/1521 (98%)	235 (15%)	0
32	2a	1501/1521 (98%)	302 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	69/76 (90%)	20 (28%)	0
54	2w	66/76 (86%)	16 (24%)	0
55	1x	74/77 (96%)	8 (10%)	0
55	2x	74/77 (96%)	9 (12%)	0
56	1y	72/76 (94%)	24 (33%)	0
56	2y	70/76 (92%)	17 (24%)	0
All	All	9339/9620 (97%)	1567 (16%)	50 (0%)

5 of 1567 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	271(M)	G
1	2A	900	A
1	2A	2756	U
1	2A	277	C
1	2A	774	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.16	4 (19%)
54	4SU	2w	8	54	18,21,22	1.66	3 (16%)	25,30,33	2.15	5 (20%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.89	5 (15%)
56	7MG	1y	46	56	23,26,27	1.33	4 (17%)	27,39,42	2.64	7 (25%)
1	PSU	1A	1917	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	3 (14%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.20	3 (14%)
1	OMG	1A	2251	57,1,55	23,26,27	1.26	3 (13%)	32,38,41	1.95	7 (21%)
56	5MU	2y	54	56	19,22,23	1.51	4 (21%)	27,32,35	1.98	8 (29%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.90	3 (14%)
55	5MU	1x	54	55	19,22,23	1.42	6 (31%)	27,32,35	1.82	6 (22%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.71	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	2605	57,1	18,21,22	1.43	4 (22%)	21,30,33	2.02	4 (19%)
56	4SU	2y	8	56	18,21,22	1.70	4 (22%)	25,30,33	2.17	5 (20%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.26	4 (15%)
1	PSU	2A	2605	1	18,21,22	1.31	3 (16%)	21,30,33	2.02	4 (19%)
54	4SU	1w	8	54	18,21,22	1.82	5 (27%)	25,30,33	2.02	4 (16%)
1	5MC	1A	1962	57,1	19,22,23	1.65	3 (15%)	26,32,35	1.14	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.04	2 (8%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.95	3 (14%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.20	6 (22%)
32	PSU	1a	516	32	18,21,22	1.44	2 (11%)	21,30,33	1.98	4 (19%)
55	5MU	2x	54	55	19,22,23	1.45	5 (26%)	27,32,35	2.15	6 (22%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.05	9 (27%)
32	5MC	2a	1407	32	19,22,23	1.69	3 (15%)	26,32,35	1.22	3 (11%)
1	5MU	2A	1939	57,1	19,22,23	1.42	5 (26%)	27,32,35	2.27	6 (22%)
54	7MG	1w	46	54	23,26,27	1.39	2 (8%)	27,39,42	2.55	7 (25%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.09	5 (23%)
56	PSU	1y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.11	6 (18%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
56	PSU	1y	39	56	18,21,22	1.42	2 (11%)	21,30,33	1.89	3 (14%)
54	7MG	2w	46	54	23,26,27	1.36	2 (8%)	27,39,42	2.51	8 (29%)
1	5MC	2A	1962	1	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
32	4OC	2a	1402	32,57	20,23,24	0.79	0	25,32,35	1.14	3 (12%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.07	2 (8%)
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.84	0
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.18	3 (11%)
55	4SU	2x	8	55	18,21,22	1.99	5 (27%)	25,30,33	1.49	5 (20%)
32	5MC	1a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.08	9 (27%)
54	5MU	2w	54	54	19,22,23	1.44	5 (26%)	27,32,35	1.76	6 (22%)
1	OMU	1A	2552	57,1	19,22,23	1.23	3 (15%)	25,31,34	1.81	5 (20%)
1	OMU	2A	2552	57,1	19,22,23	1.29	3 (15%)	25,31,34	1.99	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.79	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.05	6 (22%)
55	4SU	1x	8	55	18,21,22	2.05	6 (33%)	25,30,33	1.33	3 (12%)
54	MIA	2w	37	54	24,27,32	1.99	5 (20%)	32,39,47	2.50	10 (31%)
1	5MU	1A	1939	1	19,22,23	1.45	5 (26%)	27,32,35	2.12	7 (25%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	2.06	9 (27%)
56	MIA	2y	37	56	21,24,32	1.61	3 (14%)	30,35,47	2.09	10 (33%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
56	PSU	2y	32	56	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
54	PSU	1w	55	54	18,21,22	1.45	2 (11%)	21,30,33	2.03	4 (19%)
1	2MA	1A	2503	57,1	22,25,26	1.54	4 (18%)	32,37,40	2.29	8 (25%)
54	PSU	1w	32	57,54	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
1	2MA	2A	2503	57,1	22,25,26	1.49	4 (18%)	32,37,40	2.34	8 (25%)
43	0TD	2l	92	43	8,9,10	4.57	1 (12%)	6,11,13	5.09	3 (50%)
32	7MG	1a	527	32,57	23,26,27	1.46	4 (17%)	27,39,42	2.54	7 (25%)
1	5MC	2A	1942	1	19,22,23	1.69	3 (15%)	26,32,35	1.18	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.13	3 (11%)
1	5MC	1A	1942	57,1	19,22,23	1.43	3 (15%)	26,32,35	1.20	2 (7%)
54	5MU	1w	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.97	6 (22%)
1	OMG	2A	2251	1,55	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
32	7MG	2a	527	32,57	23,26,27	1.33	4 (17%)	27,39,42	2.62	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.95	3 (14%)
54	PSU	1w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.16	4 (19%)
55	31H	2x	76	57,55	31,34,35	1.18	3 (9%)	35,47,50	2.06	12 (34%)
43	0TD	1l	92	43	8,9,10	4.51	1 (12%)	6,11,13	5.91	2 (33%)
32	M2G	2a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.97	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.80	3 (11%)
56	5MU	1y	54	56	19,22,23	1.46	4 (21%)	27,32,35	1.58	5 (18%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
56	PSU	2y	39	56	18,21,22	1.35	2 (11%)	21,30,33	1.89	4 (19%)
56	4SU	1y	8	56	18,21,22	1.81	5 (27%)	25,30,33	2.11	4 (16%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.31	9 (27%)
56	MIA	1y	37	56	21,24,32	1.61	3 (14%)	30,35,47	2.02	9 (30%)
55	31H	1x	76	57,55	31,34,35	1.15	3 (9%)	35,47,50	2.05	12 (34%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.14	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	2y	55	56	18,21,22	1.34	3 (16%)	21,30,33	2.00	4 (19%)
56	7MG	2y	46	56	23,26,27	1.34	2 (8%)	27,39,42	2.71	7 (25%)
55	5MC	1x	32	55	19,22,23	1.84	3 (15%)	26,32,35	1.24	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.13	3 (11%)

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	1A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
56	7MG	1y	46	56	-	4/7/37/38	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/9/27/28	0/3/3/3
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	2a	1207	32	-	4/9/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	1/7/37/38	0/3/3/3
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	2/9/29/30	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
56	MIA	2y	37	56	-	0/7/25/34	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	2/7/25/26	0/3/3/3
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	4/7/12/14	-
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	31H	2x	76	57,55	-	3/22/40/41	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
56	MIA	1y	37	56	-	0/7/25/34	0/3/3/3
55	31H	1x	76	57,55	-	4/22/40/41	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
56	PSU	2y	55	56	-	4/7/25/26	0/2/2/2
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2

The worst 5 of 247 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.52	1.69	1.82
43	1l	92	0TD	CB-SB	-12.30	1.69	1.82
54	1w	37	MIA	C13-C14	6.88	1.53	1.32
55	1x	32	5MC	C5-C4	6.83	1.49	1.44
54	1w	37	MIA	C2-S10	-6.39	1.70	1.75

The worst 5 of 432 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-13.89	77.39	102.36
43	2l	92	0TD	CSB-SB-CB	-11.47	81.74	102.36
56	2y	46	7MG	N9-C4-N3	9.49	139.37	125.46
56	1y	46	7MG	N9-C4-N3	9.26	139.03	125.46
54	1w	37	MIA	C12-C13-C14	-8.77	111.27	127.01

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	46	7MG	C4'-C5'-O5'-P
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

32 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2251	OMG	1	0
54	2w	39	PSU	2	0
55	2x	32	5MC	1	0
32	1a	1402	4OC	1	0
1	1A	1915	5MU	1	0
32	2a	1518	MA6	3	0
32	2a	967	5MC	2	0
56	1y	39	PSU	1	0
54	2w	46	7MG	1	0
32	2a	1402	4OC	2	0
32	2a	1404	5MC	1	0
55	2x	8	4SU	1	0
32	2a	1519	MA6	3	0
54	2w	54	5MU	1	0
1	2A	2552	OMU	2	0
1	2A	1915	5MU	1	0
55	1x	8	4SU	2	0
1	1A	1939	5MU	1	0
32	1a	1518	MA6	1	0
56	1y	55	PSU	2	0
54	1w	55	PSU	1	0
1	1A	2503	2MA	1	0
1	2A	2503	2MA	2	0
43	2l	92	0TD	1	0
55	2x	76	31H	1	0
56	1y	54	5MU	1	0
32	1a	967	5MC	1	0
56	2y	39	PSU	2	0
56	1y	8	4SU	2	0
32	1a	1519	MA6	1	0
56	2y	55	PSU	9	0
56	2y	46	7MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2586 ligands modelled in this entry, 2582 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	1d	302	35	0,12,12	-	-	-		
58	6IF	1A	4109	-	30,34,34	1.02	1 (3%)	30,49,49	1.18	3 (10%)
58	6IF	2A	3731	-	30,34,34	0.77	0	30,49,49	1.08	3 (10%)
60	SF4	2d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	1d	302	35	-	-	0/6/5/5
58	6IF	1A	4109	-	-	4/22/65/65	0/3/3/3
58	6IF	2A	3731	-	-	2/22/65/65	0/3/3/3
60	SF4	2d	302	35	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4109	6IF	CG-CB	-2.40	1.49	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4109	6IF	CBB-CBA-CAY	-3.07	110.73	116.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4109	6IF	CAK-CAI-CAG	-2.96	110.28	114.17
58	2A	3731	6IF	CBB-CBA-CAY	-2.74	111.37	116.68
58	2A	3731	6IF	CD2-CAY-CAX	-2.51	110.03	113.78
58	2A	3731	6IF	CAK-CAI-CAG	-2.38	111.04	114.17

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

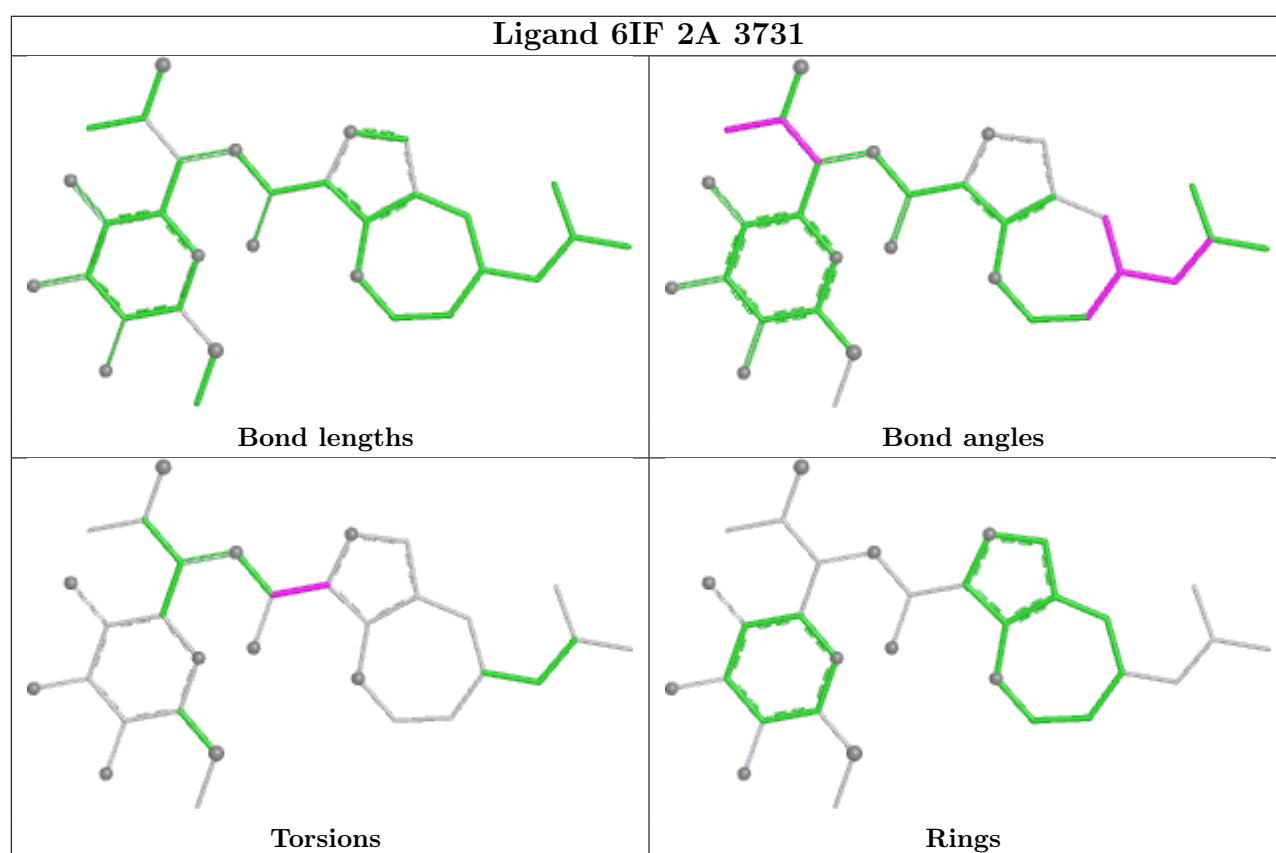
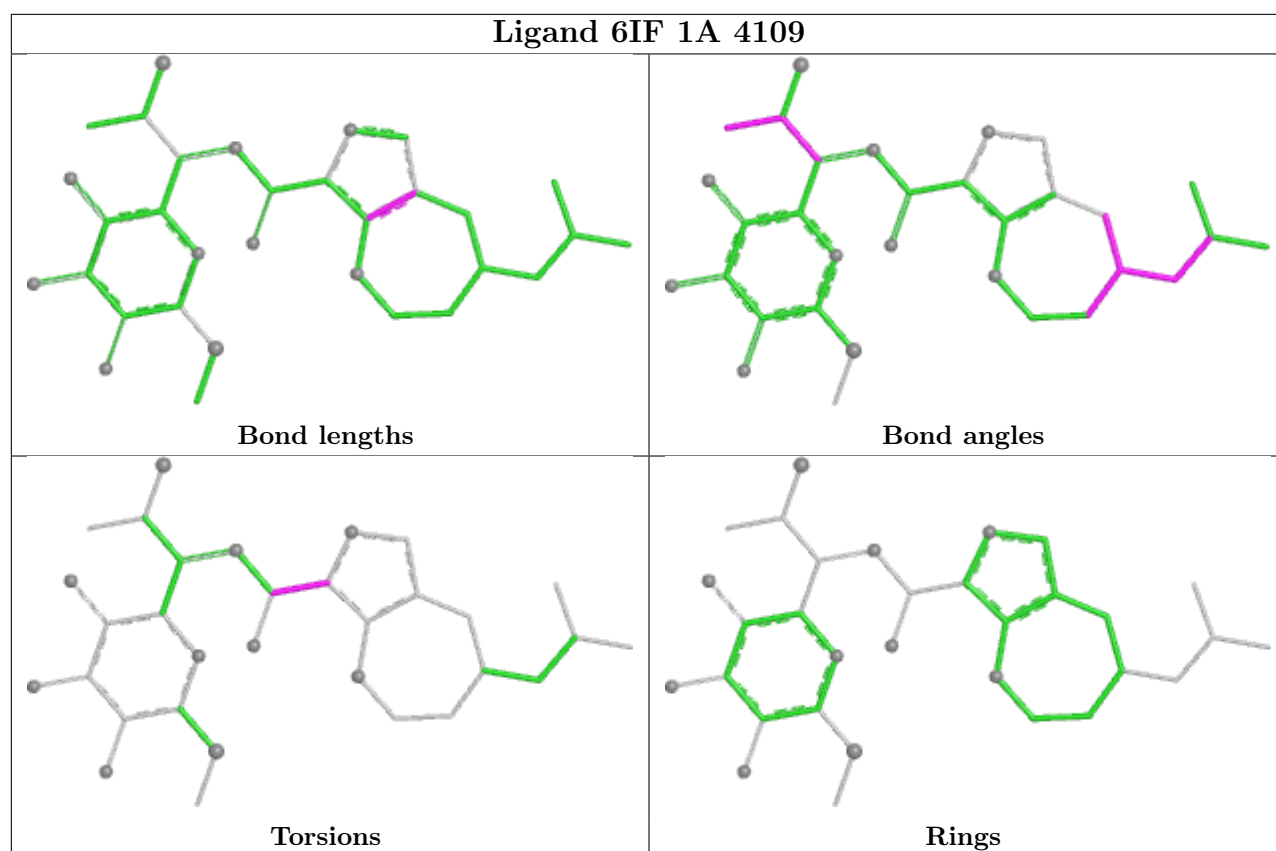
Mol	Chain	Res	Type	Atoms
58	1A	4109	6IF	O-C-CA-CB
58	1A	4109	6IF	NAH-C-CA-CB
58	2A	3731	6IF	NAH-C-CA-CB
58	1A	4109	6IF	NAH-C-CA-N
58	1A	4109	6IF	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4109	6IF	2	0
60	2d	302	SF4	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	2860/2915 (98%)	-0.57	129 (4%)	38	33	19, 36, 89, 102	0
1	2A	2789/2915 (95%)	0.01	109 (3%)	43	38	34, 57, 89, 99	0
2	1B	120/121 (99%)	-0.47	0	100	100	29, 47, 62, 82	0
2	2B	120/121 (99%)	1.29	18 (15%)	5	4	62, 80, 88, 92	0
3	1D	275/276 (99%)	-0.16	2 (0%)	84	81	21, 37, 51, 74	0
3	2D	275/276 (99%)	0.38	6 (2%)	62	58	33, 52, 64, 81	0
4	1E	204/206 (99%)	-0.13	0	100	100	18, 40, 58, 71	0
4	2E	204/206 (99%)	0.41	2 (0%)	79	76	33, 56, 68, 74	0
5	1F	203/210 (96%)	-0.03	1 (0%)	87	85	20, 41, 65, 79	0
5	2F	203/210 (96%)	0.69	6 (2%)	52	48	35, 66, 77, 83	0
6	1G	181/182 (99%)	0.57	6 (3%)	49	45	38, 56, 69, 83	0
6	2G	181/182 (99%)	1.86	79 (43%)	0	0	72, 79, 83, 88	0
7	1H	174/180 (96%)	0.26	2 (1%)	78	75	36, 52, 63, 67	0
7	2H	174/180 (96%)	1.55	43 (24%)	2	1	66, 78, 85, 88	0
8	1I	146/148 (98%)	0.90	4 (2%)	56	51	45, 70, 79, 83	0
8	2I	146/148 (98%)	1.16	11 (7%)	20	18	53, 71, 79, 83	0
9	1N	140/140 (100%)	-0.05	1 (0%)	84	81	24, 39, 56, 71	0
9	2N	140/140 (100%)	0.82	8 (5%)	29	26	45, 63, 75, 79	0
10	1O	122/122 (100%)	-0.10	0	100	100	25, 40, 57, 62	0
10	2O	122/122 (100%)	0.53	1 (0%)	82	80	47, 57, 69, 73	0
11	1P	149/150 (99%)	0.11	2 (1%)	75	71	20, 44, 65, 71	0
11	2P	149/150 (99%)	0.85	9 (6%)	27	24	38, 65, 79, 83	0
12	1Q	141/141 (100%)	0.06	3 (2%)	63	59	28, 41, 56, 70	0
12	2Q	141/141 (100%)	1.30	28 (19%)	3	2	49, 66, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.25	0 100 100	25, 33, 46, 54	0
13	2R	118/118 (100%)	0.27	0 100 100	39, 50, 60, 64	0
14	1S	110/112 (98%)	0.16	0 100 100	37, 48, 58, 64	0
14	2S	110/112 (98%)	1.76	39 (35%) 1 1	65, 74, 79, 81	0
15	1T	131/146 (89%)	0.14	3 (2%) 61 57	33, 44, 65, 70	0
15	2T	131/146 (89%)	0.56	3 (2%) 61 57	50, 59, 71, 78	0
16	1U	116/118 (98%)	-0.36	1 (0%) 81 78	21, 29, 47, 62	0
16	2U	116/118 (98%)	0.72	2 (1%) 69 65	46, 61, 74, 83	0
17	1V	101/101 (100%)	-0.25	1 (0%) 79 76	22, 39, 56, 64	0
17	2V	101/101 (100%)	0.84	5 (4%) 34 30	42, 70, 75, 81	0
18	1W	112/113 (99%)	-0.30	0 100 100	22, 31, 50, 73	0
18	2W	112/113 (99%)	0.30	3 (2%) 56 51	40, 50, 67, 85	0
19	1X	95/96 (98%)	-0.09	2 (2%) 63 59	25, 37, 56, 76	0
19	2X	95/96 (98%)	0.97	9 (9%) 14 12	45, 59, 73, 83	0
20	1Y	107/110 (97%)	0.24	1 (0%) 81 78	34, 47, 64, 71	0
20	2Y	107/110 (97%)	1.12	12 (11%) 10 8	56, 69, 79, 84	0
21	1Z	154/206 (74%)	0.82	15 (9%) 13 11	38, 61, 78, 84	0
21	2Z	160/206 (77%)	1.95	67 (41%) 0 0	65, 78, 87, 89	0
22	10	83/85 (97%)	0.33	7 (8%) 17 15	27, 37, 66, 79	0
22	20	83/85 (97%)	1.48	19 (22%) 2 1	46, 65, 76, 82	0
23	11	97/98 (98%)	0.20	1 (1%) 79 76	27, 43, 66, 71	0
23	21	97/98 (98%)	0.51	4 (4%) 41 37	40, 53, 71, 75	0
24	12	70/72 (97%)	0.27	1 (1%) 73 70	35, 47, 57, 70	0
24	22	70/72 (97%)	1.10	9 (12%) 7 6	59, 69, 76, 78	0
25	13	59/60 (98%)	-0.17	0 100 100	24, 34, 57, 74	0
25	23	59/60 (98%)	0.81	1 (1%) 69 65	54, 64, 74, 82	0
26	14	69/71 (97%)	1.06	13 (18%) 3 2	48, 69, 83, 87	0
26	24	69/71 (97%)	2.18	35 (50%) 0 0	75, 82, 88, 95	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 65	20, 30, 52, 62	0
27	25	59/60 (98%)	0.17	0 100 100	35, 49, 61, 74	0
28	16	53/54 (98%)	-0.12	0 100 100	29, 42, 54, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.85	3 (5%) 29 26	54, 62, 68, 73	0
29	17	48/49 (97%)	-0.26	1 (2%) 63 59	21, 27, 55, 61	0
29	27	48/49 (97%)	0.21	3 (6%) 26 23	32, 42, 64, 67	0
30	18	64/65 (98%)	-0.17	0 100 100	28, 34, 41, 55	0
30	28	64/65 (98%)	0.61	2 (3%) 51 47	46, 56, 62, 68	0
31	19	37/37 (100%)	-0.11	0 100 100	29, 38, 54, 56	0
31	29	37/37 (100%)	1.09	4 (10%) 11 9	59, 67, 75, 76	0
32	1a	1488/1521 (97%)	0.19	37 (2%) 58 54	35, 64, 87, 99	0
32	2a	1491/1521 (98%)	0.82	152 (10%) 12 10	52, 76, 92, 101	0
33	1b	231/256 (90%)	1.22	39 (16%) 4 3	62, 74, 82, 86	0
33	2b	231/256 (90%)	2.09	119 (51%) 0 0	71, 82, 87, 89	0
34	1c	206/239 (86%)	0.88	8 (3%) 43 38	56, 68, 76, 82	0
34	2c	206/239 (86%)	2.11	106 (51%) 0 0	72, 82, 88, 93	0
35	1d	208/209 (99%)	0.94	18 (8%) 16 14	52, 68, 75, 79	0
35	2d	208/209 (99%)	1.06	17 (8%) 17 15	61, 70, 77, 80	0
36	1e	148/162 (91%)	0.49	2 (1%) 73 70	49, 62, 70, 76	0
36	2e	148/162 (91%)	1.57	38 (25%) 1 1	68, 76, 81, 87	0
37	1f	100/101 (99%)	0.69	3 (3%) 52 48	52, 64, 71, 74	0
37	2f	100/101 (99%)	0.87	2 (2%) 65 61	63, 70, 75, 79	0
38	1g	155/156 (99%)	0.92	12 (7%) 19 17	56, 67, 75, 81	0
38	2g	155/156 (99%)	1.60	42 (27%) 1 1	69, 77, 83, 86	0
39	1h	137/138 (99%)	0.69	4 (2%) 53 49	53, 64, 71, 79	0
39	2h	137/138 (99%)	1.37	22 (16%) 4 4	70, 77, 81, 82	0
40	1i	127/128 (99%)	1.20	13 (10%) 12 10	49, 72, 78, 83	0
40	2i	127/128 (99%)	2.40	85 (66%) 0 0	72, 81, 86, 87	0
41	1j	97/105 (92%)	1.24	15 (15%) 5 4	58, 74, 80, 83	0
41	2j	96/105 (91%)	2.58	67 (69%) 0 0	76, 83, 87, 90	0
42	1k	114/129 (88%)	0.66	3 (2%) 57 52	45, 63, 74, 77	0
42	2k	114/129 (88%)	1.24	15 (13%) 7 6	61, 73, 79, 82	0
43	1l	121/132 (91%)	0.49	5 (4%) 41 37	45, 54, 64, 75	0
43	2l	121/132 (91%)	1.28	21 (17%) 4 3	55, 70, 77, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.97	9 (7%) 21 19	54, 66, 74, 84	0
44	2m	122/126 (96%)	2.08	57 (46%) 0 0	72, 80, 85, 88	0
45	1n	60/61 (98%)	1.14	6 (10%) 12 10	55, 65, 70, 74	0
45	2n	60/61 (98%)	3.27	50 (83%) 0 0	76, 83, 87, 89	0
46	1o	88/89 (98%)	0.80	5 (5%) 29 26	50, 61, 71, 74	0
46	2o	88/89 (98%)	1.13	10 (11%) 10 8	63, 72, 80, 83	0
47	1p	82/88 (93%)	1.31	11 (13%) 7 5	56, 68, 74, 82	0
47	2p	82/88 (93%)	1.08	8 (9%) 13 11	57, 67, 74, 78	0
48	1q	99/105 (94%)	0.92	1 (1%) 79 76	52, 64, 72, 76	0
48	2q	99/105 (94%)	0.97	10 (10%) 12 10	61, 71, 78, 81	0
49	1r	68/88 (77%)	0.65	3 (4%) 39 34	54, 64, 75, 77	0
49	2r	68/88 (77%)	0.96	4 (5%) 28 24	65, 72, 78, 83	0
50	1s	83/93 (89%)	1.10	8 (9%) 13 11	61, 69, 78, 81	0
50	2s	83/93 (89%)	2.65	57 (68%) 0 0	76, 84, 88, 91	0
51	1t	96/106 (90%)	1.18	15 (15%) 5 4	58, 67, 74, 79	0
51	2t	96/106 (90%)	0.92	12 (12%) 8 6	58, 69, 76, 78	0
52	1u	23/27 (85%)	1.24	2 (8%) 16 14	57, 63, 67, 71	0
52	2u	23/27 (85%)	2.69	16 (69%) 0 0	76, 79, 83, 84	0
53	1v	13/24 (54%)	0.84	3 (23%) 2 1	49, 65, 82, 92	0
53	2v	13/24 (54%)	1.70	4 (30%) 1 1	75, 83, 93, 97	0
54	1w	64/76 (84%)	1.03	8 (12%) 8 6	64, 85, 97, 101	0
54	2w	62/76 (81%)	1.66	20 (32%) 1 1	84, 92, 98, 103	0
55	1x	71/77 (92%)	0.19	0 100 100	28, 60, 80, 86	0
55	2x	71/77 (92%)	0.75	2 (2%) 55 50	46, 79, 89, 90	0
56	1y	67/76 (88%)	0.86	6 (8%) 15 13	38, 85, 93, 95	0
56	2y	66/76 (86%)	1.09	4 (6%) 27 23	54, 91, 94, 98	0
All	All	20867/21748 (95%)	0.48	1913 (9%) 14 13	18, 63, 86, 103	0

The worst 5 of 1913 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	1n	2	ALA	8.2
41	2j	47	PHE	7.7

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Mol	Chain	Res	Type	RSRZ
21	1Z	141	VAL	7.7
44	1m	2	ALA	6.9
44	2m	124	PRO	6.7

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
54	7MG	2w	46	24/25	0.55	0.16	80,91,98,112	0
56	7MG	2y	46	24/25	0.61	0.18	86,94,100,112	0
54	7MG	1w	46	24/25	0.63	0.16	77,86,96,115	0
56	PSU	2y	55	20/21	0.64	0.17	87,95,102,109	0
56	7MG	1y	46	24/25	0.65	0.17	80,89,98,108	0
54	4SU	2w	8	20/21	0.65	0.15	87,95,103,113	0
56	4SU	2y	8	20/21	0.70	0.15	88,92,98,104	0
56	5MU	2y	54	21/22	0.72	0.17	88,92,99,117	0
56	PSU	1y	55	20/21	0.76	0.15	83,88,100,106	0
56	5MU	1y	54	21/22	0.76	0.15	78,83,92,101	0
32	2MG	2a	1207	24/25	0.77	0.16	79,87,95,98	0
56	MIA	2y	37	22/30	0.77	0.13	76,84,93,104	0
56	4SU	1y	8	20/21	0.79	0.13	83,87,95,95	0
54	PSU	2w	55	20/21	0.79	0.13	81,87,92,98	0
54	5MU	2w	54	21/22	0.80	0.14	78,82,90,92	0
56	PSU	2y	32	20/21	0.80	0.14	71,82,95,95	0
56	MIA	1y	37	22/30	0.82	0.13	65,74,81,86	0
32	PSU	2a	516	20/21	0.83	0.14	79,81,87,89	0
54	PSU	2w	32	20/21	0.83	0.14	82,88,94,98	0
1	5MU	2A	1915	21/22	0.83	0.14	71,75,81,92	0
56	PSU	2y	39	20/21	0.84	0.11	78,81,93,96	0
55	5MU	2x	54	21/22	0.85	0.13	77,81,89,99	0
54	PSU	1w	55	20/21	0.86	0.11	63,81,85,87	0
54	PSU	2w	39	20/21	0.86	0.11	79,84,88,89	0
54	4SU	1w	8	20/21	0.86	0.12	78,82,90,94	0
54	MIA	2w	37	25/30	0.87	0.14	78,85,89,102	0
55	4SU	2x	8	20/21	0.87	0.14	74,79,83,91	0
32	M2G	2a	966	25/26	0.87	0.18	60,70,84,89	0
55	PSU	2x	55	20/21	0.87	0.11	75,81,83,89	0
56	PSU	1y	39	20/21	0.88	0.12	70,76,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
43	0TD	2l	92	10/11	0.88	0.13	67,69,75,87	0
54	PSU	1w	32	20/21	0.89	0.12	68,73,86,90	0
32	5MC	2a	967	21/22	0.89	0.15	68,73,80,84	0
1	PSU	2A	1917	20/21	0.89	0.10	62,70,76,83	0
32	4OC	2a	1402	22/23	0.90	0.12	58,66,73,76	0
32	5MC	2a	1404	21/22	0.90	0.12	59,64,67,71	0
56	PSU	1y	32	20/21	0.90	0.10	73,76,81,82	0
43	0TD	1l	92	10/11	0.90	0.11	44,53,57,69	0
55	PSU	1x	55	20/21	0.91	0.11	46,61,70,71	0
55	5MC	2x	32	21/22	0.91	0.14	68,74,78,81	0
54	MIA	1w	37	29/30	0.92	0.12	55,64,74,79	0
1	PSU	2A	1911	20/21	0.92	0.11	54,63,72,74	0
55	5MU	1x	54	21/22	0.92	0.10	59,65,71,77	0
54	5MU	1w	54	21/22	0.93	0.10	61,72,78,81	0
54	PSU	1w	39	20/21	0.93	0.09	63,74,77,81	0
32	7MG	2a	527	24/25	0.93	0.11	60,67,73,83	0
32	5MC	2a	1400	21/22	0.93	0.13	71,74,78,82	0
32	UR3	2a	1498	21/22	0.93	0.12	60,63,70,74	0
32	5MC	2a	1407	21/22	0.94	0.11	55,59,64,65	0
1	5MU	1A	1915	21/22	0.94	0.09	40,55,60,62	0
32	MA6	2a	1518	24/25	0.94	0.12	52,67,72,73	0
32	MA6	2a	1519	24/25	0.94	0.13	51,66,71,73	0
1	OMC	2A	1920	21/22	0.95	0.09	59,64,68,69	0
1	5MC	2A	1962	21/22	0.95	0.10	42,50,58,66	0
32	M2G	1a	966	25/26	0.95	0.10	47,54,60,64	0
55	4SU	1x	8	20/21	0.95	0.09	55,61,65,65	0
32	PSU	1a	516	20/21	0.95	0.09	58,62,67,69	0
1	5MC	2A	1942	21/22	0.96	0.09	50,56,64,64	0
32	5MC	1a	967	21/22	0.96	0.10	50,56,63,64	0
55	5MC	1x	32	21/22	0.96	0.10	48,53,59,68	0
32	7MG	1a	527	24/25	0.96	0.09	40,48,52,57	0
32	2MG	1a	1207	24/25	0.96	0.09	56,65,68,72	0
1	5MU	2A	1939	21/22	0.96	0.08	35,39,47,48	0
32	MA6	1a	1519	24/25	0.96	0.09	35,41,45,52	0
1	5MC	1A	1942	21/22	0.96	0.08	33,40,46,48	0
1	PSU	1A	1917	20/21	0.97	0.07	39,48,54,59	0
1	PSU	1A	1911	20/21	0.97	0.08	36,45,52,52	0
1	OMG	2A	2251	24/25	0.97	0.09	39,42,46,48	0
32	5MC	1a	1400	21/22	0.97	0.09	43,51,56,63	0
1	2MA	2A	2503	23/24	0.97	0.09	29,37,42,45	0
32	4OC	1a	1402	22/23	0.97	0.08	39,48,54,54	0
1	PSU	2A	2605	20/21	0.97	0.07	33,40,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	1404	21/22	0.97	0.08	38,42,46,50	0
1	OMC	1A	1920	21/22	0.97	0.09	38,45,50,52	0
55	31H	2x	76	32/33	0.97	0.09	40,48,54,68	0
32	MA6	1a	1518	24/25	0.98	0.08	31,42,46,48	0
1	2MA	1A	2503	23/24	0.98	0.06	14,20,24,26	0
1	5MU	1A	1939	21/22	0.98	0.07	22,28,33,34	0
1	OMU	1A	2552	21/22	0.98	0.07	23,30,35,38	0
1	OMU	2A	2552	21/22	0.98	0.07	39,44,49,59	0
32	5MC	1a	1407	21/22	0.98	0.08	33,40,45,49	0
1	PSU	1A	2605	20/21	0.98	0.06	21,26,30,32	0
32	UR3	1a	1498	21/22	0.98	0.06	38,41,43,47	0
55	31H	1x	76	32/33	0.98	0.07	22,29,37,42	10
1	5MC	1A	1962	21/22	0.98	0.06	27,34,40,50	0
1	OMG	1A	2251	24/25	0.99	0.05	22,26,30,32	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	3525	1/1	0.50	0.23	84,84,84,84	0
57	MG	2A	3556	1/1	0.50	0.32	80,80,80,80	0
57	MG	2A	3552	1/1	0.52	0.27	79,79,79,79	0
57	MG	2A	3560	1/1	0.60	0.23	64,64,64,64	0
57	MG	2a	1616	1/1	0.60	0.32	80,80,80,80	0
57	MG	2A	3555	1/1	0.62	0.23	73,73,73,73	0
57	MG	2A	3601	1/1	0.63	0.27	72,72,72,72	0
57	MG	2A	3617	1/1	0.64	0.22	43,43,43,43	0
57	MG	2A	3550	1/1	0.64	0.23	63,63,63,63	0
57	MG	2A	3533	1/1	0.66	0.21	72,72,72,72	0
57	MG	2a	1658	1/1	0.66	0.23	78,78,78,78	0
57	MG	2a	1739	1/1	0.66	0.44	75,75,75,75	0
57	MG	2A	3582	1/1	0.67	0.20	75,75,75,75	0
57	MG	2A	3543	1/1	0.68	0.26	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	1A	3436	1/1	0.68	0.46	77,77,77,77	0
57	MG	1A	4063	1/1	0.68	0.15	70,70,70,70	0
57	MG	2a	1636	1/1	0.69	0.23	81,81,81,81	0
57	MG	1A	3728	1/1	0.69	0.18	63,63,63,63	0
57	MG	1x	114	1/1	0.69	0.18	70,70,70,70	0
57	MG	1a	1824	1/1	0.70	0.23	79,79,79,79	0
57	MG	1Y	203	1/1	0.71	0.15	84,84,84,84	0
57	MG	1a	1741	1/1	0.71	0.33	79,79,79,79	0
57	MG	2A	3341	1/1	0.71	0.33	63,63,63,63	0
57	MG	2A	3166	1/1	0.72	0.20	59,59,59,59	0
57	MG	2A	3656	1/1	0.72	0.15	64,64,64,64	0
57	MG	2A	3588	1/1	0.73	0.26	71,71,71,71	0
57	MG	1A	3692	1/1	0.73	0.20	63,63,63,63	0
57	MG	2A	3378	1/1	0.73	0.20	63,63,63,63	0
57	MG	2A	3512	1/1	0.73	0.18	42,42,42,42	0
57	MG	1B	234	1/1	0.74	0.17	67,67,67,67	0
57	MG	2A	3544	1/1	0.74	0.23	68,68,68,68	0
57	MG	1A	3716	1/1	0.74	0.17	37,37,37,37	0
57	MG	2A	3356	1/1	0.74	0.23	76,76,76,76	0
57	MG	2A	3681	1/1	0.74	0.19	47,47,47,47	0
57	MG	2G	201	1/1	0.74	0.23	76,76,76,76	0
57	MG	1A	3542	1/1	0.74	0.26	66,66,66,66	0
57	MG	1a	1758	1/1	0.74	0.16	69,69,69,69	0
57	MG	2a	1646	1/1	0.74	0.41	76,76,76,76	0
57	MG	1A	3811	1/1	0.74	0.17	58,58,58,58	0
57	MG	1A	3415	1/1	0.74	0.20	63,63,63,63	0
57	MG	2a	1753	1/1	0.74	0.33	71,71,71,71	0
57	MG	1a	1642	1/1	0.75	0.29	78,78,78,78	0
57	MG	1a	1721	1/1	0.75	0.32	81,81,81,81	0
57	MG	2A	3404	1/1	0.75	0.25	67,67,67,67	0
57	MG	1A	3876	1/1	0.75	0.21	57,57,57,57	0
57	MG	2A	3722	1/1	0.75	0.14	78,78,78,78	0
57	MG	1A	3819	1/1	0.75	0.25	58,58,58,58	0
57	MG	1A	4074	1/1	0.76	0.16	64,64,64,64	0
57	MG	2A	3551	1/1	0.76	0.17	79,79,79,79	0
57	MG	1a	1781	1/1	0.76	0.26	71,71,71,71	0
57	MG	2A	3615	1/1	0.76	0.15	74,74,74,74	0
57	MG	2A	3540	1/1	0.76	0.17	66,66,66,66	0
57	MG	2A	3624	1/1	0.76	0.15	76,76,76,76	0
57	MG	2A	3486	1/1	0.76	0.17	54,54,54,54	0
57	MG	1y	102	1/1	0.76	0.16	88,88,88,88	0
57	MG	2v	101	1/1	0.76	0.30	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3290	1/1	0.77	0.18	54,54,54,54	0
57	MG	20	102	1/1	0.77	0.22	63,63,63,63	0
57	MG	2A	3452	1/1	0.77	0.24	73,73,73,73	0
57	MG	1A	3719	1/1	0.77	0.17	46,46,46,46	0
57	MG	2a	1637	1/1	0.77	0.24	73,73,73,73	0
57	MG	2A	3496	1/1	0.77	0.24	66,66,66,66	0
57	MG	2A	3575	1/1	0.77	0.21	74,74,74,74	0
57	MG	1Z	3702	1/1	0.77	0.10	70,70,70,70	0
57	MG	1a	1637	1/1	0.77	0.32	76,76,76,76	0
57	MG	2B	214	1/1	0.77	0.19	70,70,70,70	0
57	MG	2A	3149	1/1	0.78	0.19	53,53,53,53	0
57	MG	2A	3409	1/1	0.78	0.19	51,51,51,51	0
57	MG	2A	3589	1/1	0.78	0.14	58,58,58,58	0
57	MG	1a	1683	1/1	0.78	0.21	72,72,72,72	0
57	MG	1A	4046	1/1	0.78	0.15	53,53,53,53	0
57	MG	1A	3514	1/1	0.78	0.21	65,65,65,65	0
57	MG	1a	1659	1/1	0.78	0.28	74,74,74,74	0
57	MG	2A	3446	1/1	0.79	0.19	53,53,53,53	0
57	MG	1A	3338	1/1	0.79	0.24	51,51,51,51	0
57	MG	1F	308	1/1	0.79	0.13	49,49,49,49	0
57	MG	2A	3263	1/1	0.79	0.27	72,72,72,72	0
57	MG	1A	3548	1/1	0.79	0.22	52,52,52,52	0
57	MG	1w	104	1/1	0.79	0.13	69,69,69,69	0
57	MG	2a	1640	1/1	0.79	0.17	76,76,76,76	0
57	MG	2A	3638	1/1	0.79	0.14	67,67,67,67	0
57	MG	1A	3756	1/1	0.79	0.26	63,63,63,63	0
57	MG	1A	4095	1/1	0.79	0.17	66,66,66,66	0
57	MG	2A	3687	1/1	0.79	0.11	69,69,69,69	0
57	MG	2A	3028	1/1	0.79	0.13	59,59,59,59	0
57	MG	1A	4058	1/1	0.80	0.14	44,44,44,44	0
57	MG	1y	104	1/1	0.80	0.11	87,87,87,87	0
57	MG	2A	3415	1/1	0.80	0.11	37,37,37,37	0
57	MG	2A	3707	1/1	0.80	0.19	72,72,72,72	0
57	MG	1a	1739	1/1	0.80	0.43	73,73,73,73	0
57	MG	2A	3111	1/1	0.80	0.29	64,64,64,64	0
57	MG	2B	217	1/1	0.80	0.24	76,76,76,76	0
57	MG	1A	3401	1/1	0.80	0.11	77,77,77,77	0
57	MG	2A	3493	1/1	0.80	0.20	70,70,70,70	0
57	MG	1A	3437	1/1	0.80	0.15	47,47,47,47	0
57	MG	2a	1619	1/1	0.80	0.14	64,64,64,64	0
57	MG	2a	1626	1/1	0.80	0.31	71,71,71,71	0
57	MG	2A	3175	1/1	0.80	0.32	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	3562	1/1	0.80	0.21	62,62,62,62	0
57	MG	2A	3532	1/1	0.80	0.13	78,78,78,78	0
57	MG	2a	1644	1/1	0.80	0.12	61,61,61,61	0
57	MG	2A	3606	1/1	0.80	0.26	74,74,74,74	0
57	MG	2A	3299	1/1	0.80	0.33	64,64,64,64	0
57	MG	2a	1663	1/1	0.80	0.18	74,74,74,74	0
57	MG	1A	3892	1/1	0.80	0.15	31,31,31,31	0
57	MG	2a	1742	1/1	0.80	0.30	65,65,65,65	0
57	MG	1A	3365	1/1	0.80	0.14	60,60,60,60	0
57	MG	1a	1720	1/1	0.80	0.21	67,67,67,67	0
57	MG	2x	102	1/1	0.80	0.31	77,77,77,77	0
57	MG	2A	3397	1/1	0.81	0.20	74,74,74,74	0
57	MG	2A	3047	1/1	0.81	0.26	69,69,69,69	0
57	MG	2A	3407	1/1	0.81	0.29	69,69,69,69	0
57	MG	1A	4101	1/1	0.81	0.14	43,43,43,43	0
57	MG	2a	1629	1/1	0.81	0.23	74,74,74,74	0
57	MG	1A	3635	1/1	0.81	0.21	58,58,58,58	0
57	MG	1a	1678	1/1	0.81	0.25	64,64,64,64	0
57	MG	1b	302	1/1	0.81	0.21	80,80,80,80	0
57	MG	2A	3256	1/1	0.81	0.35	75,75,75,75	0
57	MG	1E	314	1/1	0.81	0.12	62,62,62,62	0
57	MG	1A	3553	1/1	0.81	0.17	62,62,62,62	0
57	MG	2A	3719	1/1	0.81	0.23	62,62,62,62	0
57	MG	1A	3531	1/1	0.81	0.14	69,69,69,69	0
57	MG	2A	3723	1/1	0.81	0.17	69,69,69,69	0
57	MG	2A	3514	1/1	0.81	0.23	68,68,68,68	0
57	MG	1A	3761	1/1	0.81	0.12	60,60,60,60	0
57	MG	1A	4044	1/1	0.81	0.13	53,53,53,53	0
57	MG	1y	103	1/1	0.82	0.31	77,77,77,77	0
57	MG	2A	3579	1/1	0.82	0.12	70,70,70,70	0
57	MG	2A	3302	1/1	0.82	0.22	64,64,64,64	0
57	MG	1A	3476	1/1	0.82	0.26	70,70,70,70	0
57	MG	2A	3354	1/1	0.82	0.13	71,71,71,71	0
57	MG	2A	3001	1/1	0.82	0.37	57,57,57,57	0
57	MG	1A	4088	1/1	0.82	0.11	64,64,64,64	0
57	MG	1A	3903	1/1	0.82	0.12	23,23,23,23	0
57	MG	2a	1633	1/1	0.82	0.41	67,67,67,67	0
57	MG	2a	1635	1/1	0.82	0.33	67,67,67,67	0
57	MG	2A	3052	1/1	0.82	0.29	66,66,66,66	0
57	MG	1A	3777	1/1	0.82	0.13	31,31,31,31	0
57	MG	2A	3635	1/1	0.82	0.18	55,55,55,55	0
57	MG	1a	1670	1/1	0.82	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3547	1/1	0.82	0.12	55,55,55,55	0
57	MG	2a	1649	1/1	0.82	0.20	66,66,66,66	0
57	MG	1A	4045	1/1	0.82	0.22	56,56,56,56	0
57	MG	2A	3445	1/1	0.82	0.14	48,48,48,48	0
57	MG	2a	1670	1/1	0.82	0.20	63,63,63,63	0
57	MG	2a	1696	1/1	0.82	0.18	66,66,66,66	0
57	MG	1A	3533	1/1	0.82	0.12	81,81,81,81	0
57	MG	1A	3164	1/1	0.82	0.23	55,55,55,55	0
57	MG	2A	3481	1/1	0.82	0.13	63,63,63,63	0
57	MG	2a	1784	1/1	0.82	0.16	71,71,71,71	0
57	MG	1A	3758	1/1	0.82	0.13	62,62,62,62	0
57	MG	2B	206	1/1	0.82	0.20	68,68,68,68	0
57	MG	1A	3490	1/1	0.83	0.21	63,63,63,63	0
57	MG	1A	3689	1/1	0.83	0.17	50,50,50,50	0
57	MG	2A	3303	1/1	0.83	0.34	59,59,59,59	0
57	MG	1x	108	1/1	0.83	0.24	68,68,68,68	0
57	MG	1A	3232	1/1	0.83	0.15	62,62,62,62	0
57	MG	1A	4048	1/1	0.83	0.18	53,53,53,53	0
57	MG	1A	3696	1/1	0.83	0.14	53,53,53,53	0
57	MG	1A	3026	1/1	0.83	0.17	63,63,63,63	0
57	MG	2a	1621	1/1	0.83	0.22	78,78,78,78	0
57	MG	1A	3016	1/1	0.83	0.25	56,56,56,56	0
57	MG	1A	3572	1/1	0.83	0.14	51,51,51,51	0
57	MG	1A	3900	1/1	0.83	0.12	37,37,37,37	0
57	MG	1A	4100	1/1	0.83	0.15	62,62,62,62	0
57	MG	2A	3057	1/1	0.83	0.14	61,61,61,61	0
57	MG	2A	3110	1/1	0.83	0.19	55,55,55,55	0
57	MG	2A	3605	1/1	0.83	0.16	70,70,70,70	0
57	MG	1a	1722	1/1	0.83	0.33	64,64,64,64	0
57	MG	2A	3607	1/1	0.83	0.14	60,60,60,60	0
57	MG	1A	3597	1/1	0.83	0.09	35,35,35,35	0
57	MG	1B	202	1/1	0.83	0.24	61,61,61,61	0
57	MG	2A	3170	1/1	0.83	0.09	57,57,57,57	0
57	MG	2a	1665	1/1	0.83	0.29	67,67,67,67	0
57	MG	1A	3931	1/1	0.83	0.13	72,72,72,72	0
57	MG	2a	1692	1/1	0.83	0.21	74,74,74,74	0
57	MG	2A	3224	1/1	0.83	0.15	58,58,58,58	0
57	MG	2a	1709	1/1	0.83	0.26	78,78,78,78	0
57	MG	2A	3226	1/1	0.83	0.21	74,74,74,74	0
57	MG	2A	3230	1/1	0.83	0.29	63,63,63,63	0
57	MG	1A	4019	1/1	0.83	0.12	35,35,35,35	0
57	MG	2a	1775	1/1	0.83	0.33	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	2a	1778	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3259	1/1	0.83	0.28	71,71,71,71	0
57	MG	1A	4037	1/1	0.83	0.18	72,72,72,72	0
57	MG	2A	3268	1/1	0.83	0.21	54,54,54,54	0
57	MG	1A	3268	1/1	0.84	0.10	57,57,57,57	0
57	MG	1A	3538	1/1	0.84	0.33	65,65,65,65	0
57	MG	2A	3300	1/1	0.84	0.33	64,64,64,64	0
57	MG	15	108	1/1	0.84	0.14	40,40,40,40	0
57	MG	1a	1628	1/1	0.84	0.23	61,61,61,61	0
57	MG	2A	3059	1/1	0.84	0.30	61,61,61,61	0
57	MG	2A	3343	1/1	0.84	0.28	58,58,58,58	0
57	MG	2A	3539	1/1	0.84	0.14	66,66,66,66	0
57	MG	2A	3632	1/1	0.84	0.16	64,64,64,64	0
57	MG	1A	4028	1/1	0.84	0.10	66,66,66,66	0
57	MG	1A	3205	1/1	0.84	0.16	59,59,59,59	0
57	MG	2a	1653	1/1	0.84	0.44	69,69,69,69	0
57	MG	1B	212	1/1	0.84	0.11	59,59,59,59	0
57	MG	1a	1669	1/1	0.84	0.17	57,57,57,57	0
57	MG	1A	3529	1/1	0.84	0.23	66,66,66,66	0
57	MG	1a	1676	1/1	0.84	0.17	64,64,64,64	0
57	MG	2A	3716	1/1	0.84	0.17	60,60,60,60	0
57	MG	2A	3216	1/1	0.84	0.28	60,60,60,60	0
57	MG	1A	3255	1/1	0.84	0.10	61,61,61,61	0
57	MG	2a	1711	1/1	0.84	0.41	71,71,71,71	0
57	MG	2a	1724	1/1	0.84	0.30	65,65,65,65	0
57	MG	2a	1728	1/1	0.84	0.36	64,64,64,64	0
57	MG	1A	4093	1/1	0.84	0.13	55,55,55,55	0
57	MG	1a	1696	1/1	0.84	0.31	72,72,72,72	0
57	MG	2A	3563	1/1	0.84	0.15	61,61,61,61	0
57	MG	2a	1756	1/1	0.84	0.41	73,73,73,73	0
57	MG	1a	1717	1/1	0.84	0.20	66,66,66,66	0
57	MG	1S	203	1/1	0.84	0.10	63,63,63,63	0
57	MG	2a	1779	1/1	0.84	0.31	62,62,62,62	0
57	MG	2A	3581	1/1	0.84	0.16	63,63,63,63	0
57	MG	2A	3003	1/1	0.84	0.28	61,61,61,61	0
57	MG	2A	3491	1/1	0.84	0.14	70,70,70,70	0
57	MG	1a	1791	1/1	0.85	0.15	56,56,56,56	0
57	MG	1A	3363	1/1	0.85	0.15	63,63,63,63	0
57	MG	1A	4086	1/1	0.85	0.18	49,49,49,49	0
57	MG	1a	1640	1/1	0.85	0.18	61,61,61,61	0
57	MG	1A	3942	1/1	0.85	0.10	49,49,49,49	0
57	MG	2A	3260	1/1	0.85	0.17	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	3988	1/1	0.85	0.12	60,60,60,60	0
57	MG	1A	3813	1/1	0.85	0.14	53,53,53,53	0
57	MG	1A	4027	1/1	0.85	0.23	65,65,65,65	0
57	MG	1A	3358	1/1	0.85	0.16	82,82,82,82	0
57	MG	1A	3822	1/1	0.85	0.12	42,42,42,42	0
57	MG	2a	1618	1/1	0.85	0.13	73,73,73,73	0
57	MG	1a	1682	1/1	0.85	0.30	63,63,63,63	0
57	MG	2a	1620	1/1	0.85	0.19	79,79,79,79	0
57	MG	2A	3021	1/1	0.85	0.26	70,70,70,70	0
57	MG	1A	3837	1/1	0.85	0.14	52,52,52,52	0
57	MG	1a	1692	1/1	0.85	0.40	74,74,74,74	0
57	MG	1B	228	1/1	0.85	0.23	73,73,73,73	0
57	MG	2A	3562	1/1	0.85	0.11	46,46,46,46	0
57	MG	1A	3589	1/1	0.85	0.22	58,58,58,58	0
57	MG	2A	3383	1/1	0.85	0.11	55,55,55,55	0
57	MG	2A	3386	1/1	0.85	0.26	72,72,72,72	0
57	MG	1A	3429	1/1	0.85	0.19	58,58,58,58	0
57	MG	2A	3398	1/1	0.85	0.10	44,44,44,44	0
57	MG	2a	1647	1/1	0.85	0.18	76,76,76,76	0
57	MG	2A	3583	1/1	0.85	0.17	55,55,55,55	0
57	MG	2A	3062	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3708	1/1	0.85	0.12	34,34,34,34	0
57	MG	2A	3594	1/1	0.85	0.12	66,66,66,66	0
57	MG	1O	201	1/1	0.85	0.12	72,72,72,72	0
57	MG	1A	4049	1/1	0.85	0.12	59,59,59,59	0
57	MG	2a	1678	1/1	0.85	0.28	76,76,76,76	0
57	MG	2A	3428	1/1	0.85	0.23	41,41,41,41	0
57	MG	2a	1694	1/1	0.85	0.12	60,60,60,60	0
57	MG	1A	3610	1/1	0.85	0.16	57,57,57,57	0
57	MG	2A	3168	1/1	0.85	0.27	67,67,67,67	0
57	MG	1A	3914	1/1	0.85	0.17	62,62,62,62	0
57	MG	2a	1716	1/1	0.85	0.10	56,56,56,56	0
57	MG	2A	3478	1/1	0.85	0.23	64,64,64,64	0
57	MG	2A	3628	1/1	0.85	0.17	66,66,66,66	0
57	MG	1A	4065	1/1	0.85	0.19	50,50,50,50	0
57	MG	2A	3187	1/1	0.85	0.16	56,56,56,56	0
57	MG	2A	3490	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3640	1/1	0.85	0.17	66,66,66,66	0
57	MG	2a	1766	1/1	0.85	0.33	62,62,62,62	0
57	MG	2a	1767	1/1	0.85	0.24	57,57,57,57	0
57	MG	2A	3648	1/1	0.85	0.14	76,76,76,76	0
57	MG	2A	3654	1/1	0.85	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	3193	1/1	0.85	0.32	66,66,66,66	0
57	MG	2a	1780	1/1	0.85	0.16	67,67,67,67	0
57	MG	2A	3212	1/1	0.85	0.22	66,66,66,66	0
57	MG	1a	1784	1/1	0.85	0.15	69,69,69,69	0
57	MG	2A	3703	1/1	0.85	0.17	67,67,67,67	0
57	MG	1A	3092	1/1	0.86	0.13	59,59,59,59	0
57	MG	1a	1708	1/1	0.86	0.19	58,58,58,58	0
57	MG	1a	1715	1/1	0.86	0.16	59,59,59,59	0
57	MG	1A	3724	1/1	0.86	0.22	64,64,64,64	0
57	MG	2A	3050	1/1	0.86	0.17	56,56,56,56	0
57	MG	2a	1609	1/1	0.86	0.23	68,68,68,68	0
57	MG	1A	3457	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3915	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3058	1/1	0.86	0.20	55,55,55,55	0
57	MG	2A	3359	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3373	1/1	0.86	0.29	62,62,62,62	0
57	MG	1A	3312	1/1	0.86	0.14	56,56,56,56	0
57	MG	1a	1734	1/1	0.86	0.25	54,54,54,54	0
57	MG	2A	3569	1/1	0.86	0.18	61,61,61,61	0
57	MG	2A	3091	1/1	0.86	0.14	56,56,56,56	0
57	MG	2A	3101	1/1	0.86	0.26	69,69,69,69	0
57	MG	1A	3932	1/1	0.86	0.13	70,70,70,70	0
57	MG	1A	3938	1/1	0.86	0.10	32,32,32,32	0
57	MG	1a	1623	1/1	0.86	0.24	68,68,68,68	0
57	MG	1a	1759	1/1	0.86	0.13	58,58,58,58	0
57	MG	1a	1760	1/1	0.86	0.13	80,80,80,80	0
57	MG	2A	3591	1/1	0.86	0.17	61,61,61,61	0
57	MG	2A	3419	1/1	0.86	0.11	51,51,51,51	0
57	MG	2A	3598	1/1	0.86	0.12	57,57,57,57	0
57	MG	2a	1659	1/1	0.86	0.22	62,62,62,62	0
57	MG	1A	3202	1/1	0.86	0.11	48,48,48,48	0
57	MG	2A	3442	1/1	0.86	0.21	69,69,69,69	0
57	MG	1A	3848	1/1	0.86	0.13	50,50,50,50	0
57	MG	2a	1677	1/1	0.86	0.43	71,71,71,71	0
57	MG	1A	4094	1/1	0.86	0.12	41,41,41,41	0
57	MG	2a	1686	1/1	0.86	0.21	69,69,69,69	0
57	MG	2A	3449	1/1	0.86	0.17	48,48,48,48	0
57	MG	2A	3188	1/1	0.86	0.15	52,52,52,52	0
57	MG	2A	3461	1/1	0.86	0.10	65,65,65,65	0
57	MG	2A	3466	1/1	0.86	0.11	54,54,54,54	0
57	MG	2A	3476	1/1	0.86	0.18	52,52,52,52	0
57	MG	1A	3855	1/1	0.86	0.13	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	2a	1722	1/1	0.86	0.25	56,56,56,56	0
57	MG	2A	3210	1/1	0.86	0.26	69,69,69,69	0
57	MG	2a	1727	1/1	0.86	0.28	71,71,71,71	0
57	MG	1a	1829	1/1	0.86	0.27	60,60,60,60	0
57	MG	1A	4097	1/1	0.86	0.17	64,64,64,64	0
57	MG	1r	101	1/1	0.86	0.21	68,68,68,68	0
57	MG	1A	3869	1/1	0.86	0.11	48,48,48,48	0
57	MG	1A	3874	1/1	0.86	0.16	58,58,58,58	0
57	MG	2A	3506	1/1	0.86	0.17	46,46,46,46	0
57	MG	2A	3692	1/1	0.86	0.10	71,71,71,71	0
57	MG	1A	3509	1/1	0.86	0.09	44,44,44,44	0
57	MG	2A	3706	1/1	0.86	0.27	56,56,56,56	0
57	MG	1A	3878	1/1	0.86	0.16	41,41,41,41	0
57	MG	1A	3886	1/1	0.86	0.13	50,50,50,50	0
57	MG	1B	230	1/1	0.86	0.16	75,75,75,75	0
57	MG	2l	201	1/1	0.86	0.26	70,70,70,70	0
57	MG	1A	3398	1/1	0.86	0.14	67,67,67,67	0
57	MG	2A	3275	1/1	0.86	0.25	65,65,65,65	0
57	MG	1A	3659	1/1	0.87	0.12	69,69,69,69	0
57	MG	2A	3094	1/1	0.87	0.23	66,66,66,66	0
57	MG	1A	4096	1/1	0.87	0.29	54,54,54,54	0
57	MG	1a	1702	1/1	0.87	0.33	67,67,67,67	0
57	MG	2A	3460	1/1	0.87	0.16	73,73,73,73	0
57	MG	1A	3489	1/1	0.87	0.12	61,61,61,61	0
57	MG	2A	3114	1/1	0.87	0.19	64,64,64,64	0
57	MG	1A	4098	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3477	1/1	0.87	0.23	65,65,65,65	0
57	MG	2A	3160	1/1	0.87	0.20	59,59,59,59	0
57	MG	2B	204	1/1	0.87	0.24	67,67,67,67	0
57	MG	1A	3348	1/1	0.87	0.19	58,58,58,58	0
57	MG	2B	211	1/1	0.87	0.26	62,62,62,62	0
57	MG	2A	3167	1/1	0.87	0.13	57,57,57,57	0
57	MG	1A	3827	1/1	0.87	0.21	61,61,61,61	0
57	MG	2B	218	1/1	0.87	0.21	64,64,64,64	0
57	MG	1A	3956	1/1	0.87	0.12	26,26,26,26	0
57	MG	2Z	301	1/1	0.87	0.24	76,76,76,76	0
57	MG	20	101	1/1	0.87	0.31	62,62,62,62	0
57	MG	1A	3508	1/1	0.87	0.11	53,53,53,53	0
57	MG	26	101	1/1	0.87	0.22	61,61,61,61	0
57	MG	28	102	1/1	0.87	0.24	59,59,59,59	0
57	MG	2a	1603	1/1	0.87	0.15	65,65,65,65	0
57	MG	1A	4008	1/1	0.87	0.12	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	2a	1611	1/1	0.87	0.22	66,66,66,66	0
57	MG	1A	3845	1/1	0.87	0.14	50,50,50,50	0
57	MG	1B	233	1/1	0.87	0.16	73,73,73,73	0
57	MG	2A	3199	1/1	0.87	0.35	64,64,64,64	0
57	MG	1A	3847	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3158	1/1	0.87	0.10	49,49,49,49	0
57	MG	1A	4031	1/1	0.87	0.11	58,58,58,58	0
57	MG	1a	1763	1/1	0.87	0.18	70,70,70,70	0
57	MG	1a	1778	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3335	1/1	0.87	0.21	54,54,54,54	0
57	MG	2A	3231	1/1	0.87	0.24	65,65,65,65	0
57	MG	2A	3243	1/1	0.87	0.14	52,52,52,52	0
57	MG	2A	3251	1/1	0.87	0.22	71,71,71,71	0
57	MG	1O	206	1/1	0.87	0.10	64,64,64,64	0
57	MG	1R	201	1/1	0.87	0.14	56,56,56,56	0
57	MG	1A	4038	1/1	0.87	0.23	57,57,57,57	0
57	MG	1a	1828	1/1	0.87	0.25	59,59,59,59	0
57	MG	1A	3469	1/1	0.87	0.16	56,56,56,56	0
57	MG	2a	1656	1/1	0.87	0.18	84,84,84,84	0
57	MG	2A	3274	1/1	0.87	0.26	48,48,48,48	0
57	MG	1A	3530	1/1	0.87	0.15	55,55,55,55	0
57	MG	2A	3288	1/1	0.87	0.26	60,60,60,60	0
57	MG	2A	3570	1/1	0.87	0.15	57,57,57,57	0
57	MG	2a	1668	1/1	0.87	0.32	71,71,71,71	0
57	MG	1f	201	1/1	0.87	0.17	55,55,55,55	0
57	MG	15	105	1/1	0.87	0.19	54,54,54,54	0
57	MG	1A	3310	1/1	0.87	0.33	66,66,66,66	0
57	MG	1A	3604	1/1	0.87	0.12	47,47,47,47	0
57	MG	2A	3304	1/1	0.87	0.40	70,70,70,70	0
57	MG	2A	3313	1/1	0.87	0.21	55,55,55,55	0
57	MG	1A	3609	1/1	0.87	0.13	56,56,56,56	0
57	MG	2a	1698	1/1	0.87	0.17	62,62,62,62	0
57	MG	2a	1705	1/1	0.87	0.18	66,66,66,66	0
57	MG	1a	1629	1/1	0.87	0.10	51,51,51,51	0
57	MG	1a	1630	1/1	0.87	0.27	59,59,59,59	0
57	MG	1a	1636	1/1	0.87	0.24	76,76,76,76	0
57	MG	1A	4050	1/1	0.87	0.11	57,57,57,57	0
57	MG	1A	3478	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3375	1/1	0.87	0.30	45,45,45,45	0
57	MG	1A	3895	1/1	0.87	0.14	35,35,35,35	0
57	MG	2A	3613	1/1	0.87	0.12	56,56,56,56	0
57	MG	2a	1740	1/1	0.87	0.35	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	3534	1/1	0.87	0.12	58,58,58,58	0
57	MG	1A	3901	1/1	0.87	0.08	29,29,29,29	0
57	MG	1A	4081	1/1	0.87	0.11	58,58,58,58	0
57	MG	1a	1675	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3055	1/1	0.87	0.20	65,65,65,65	0
57	MG	1A	3778	1/1	0.87	0.11	34,34,34,34	0
57	MG	1A	3906	1/1	0.87	0.27	46,46,46,46	0
57	MG	1A	3781	1/1	0.87	0.08	16,16,16,16	0
57	MG	1A	3652	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3651	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3082	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3087	1/1	0.87	0.23	70,70,70,70	0
57	MG	2A	3668	1/1	0.87	0.11	53,53,53,53	0
57	MG	2x	103	1/1	0.87	0.17	66,66,66,66	0
57	MG	2A	3051	1/1	0.88	0.18	68,68,68,68	0
57	MG	2E	302	1/1	0.88	0.25	66,66,66,66	0
57	MG	1A	3535	1/1	0.88	0.11	69,69,69,69	0
57	MG	1A	3208	1/1	0.88	0.11	64,64,64,64	0
57	MG	2A	3293	1/1	0.88	0.25	53,53,53,53	0
57	MG	1a	1709	1/1	0.88	0.46	67,67,67,67	0
57	MG	1a	1712	1/1	0.88	0.12	79,79,79,79	0
57	MG	1A	3541	1/1	0.88	0.21	45,45,45,45	0
57	MG	2A	3060	1/1	0.88	0.22	58,58,58,58	0
57	MG	2a	1606	1/1	0.88	0.16	71,71,71,71	0
57	MG	1O	204	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3071	1/1	0.88	0.23	58,58,58,58	0
57	MG	1A	3520	1/1	0.88	0.20	62,62,62,62	0
57	MG	1A	3844	1/1	0.88	0.09	33,33,33,33	0
57	MG	1S	201	1/1	0.88	0.39	46,46,46,46	0
57	MG	2A	3355	1/1	0.88	0.24	68,68,68,68	0
57	MG	1A	3917	1/1	0.88	0.17	56,56,56,56	0
57	MG	2a	1622	1/1	0.88	0.23	68,68,68,68	0
57	MG	2A	3100	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3611	1/1	0.88	0.17	48,48,48,48	0
57	MG	2a	1631	1/1	0.88	0.21	64,64,64,64	0
57	MG	1A	3622	1/1	0.88	0.16	53,53,53,53	0
57	MG	1A	3480	1/1	0.88	0.21	74,74,74,74	0
57	MG	2A	3382	1/1	0.88	0.10	52,52,52,52	0
57	MG	1A	3941	1/1	0.88	0.08	60,60,60,60	0
57	MG	2A	3122	1/1	0.88	0.24	48,48,48,48	0
57	MG	2A	3127	1/1	0.88	0.18	66,66,66,66	0
57	MG	17	103	1/1	0.88	0.10	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	1603	1/1	0.88	0.15	64,64,64,64	0
57	MG	1a	1607	1/1	0.88	0.31	62,62,62,62	0
57	MG	2a	1650	1/1	0.88	0.22	74,74,74,74	0
57	MG	1A	4082	1/1	0.88	0.12	44,44,44,44	0
57	MG	2a	1655	1/1	0.88	0.21	73,73,73,73	0
57	MG	1A	3650	1/1	0.88	0.08	26,26,26,26	0
57	MG	1A	3950	1/1	0.88	0.12	58,58,58,58	0
57	MG	1A	3867	1/1	0.88	0.13	49,49,49,49	0
57	MG	2A	3178	1/1	0.88	0.12	57,57,57,57	0
57	MG	2A	3180	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3619	1/1	0.88	0.09	44,44,44,44	0
57	MG	2A	3622	1/1	0.88	0.11	51,51,51,51	0
57	MG	1a	1827	1/1	0.88	0.36	70,70,70,70	0
57	MG	2A	3627	1/1	0.88	0.11	72,72,72,72	0
57	MG	1A	3977	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3438	1/1	0.88	0.12	43,43,43,43	0
57	MG	1A	3997	1/1	0.88	0.11	38,38,38,38	0
57	MG	2A	3207	1/1	0.88	0.12	56,56,56,56	0
57	MG	1A	4002	1/1	0.88	0.09	86,86,86,86	0
57	MG	2a	1703	1/1	0.88	0.20	65,65,65,65	0
57	MG	2A	3470	1/1	0.88	0.11	62,62,62,62	0
57	MG	2A	3475	1/1	0.88	0.20	58,58,58,58	0
57	MG	1a	1643	1/1	0.88	0.28	69,69,69,69	0
57	MG	1A	3767	1/1	0.88	0.21	50,50,50,50	0
57	MG	2a	1718	1/1	0.88	0.17	65,65,65,65	0
57	MG	1A	3163	1/1	0.88	0.15	50,50,50,50	0
57	MG	2A	3225	1/1	0.88	0.28	60,60,60,60	0
57	MG	1A	3676	1/1	0.88	0.14	31,31,31,31	0
57	MG	1A	4107	1/1	0.88	0.19	65,65,65,65	0
57	MG	2a	1729	1/1	0.88	0.28	63,63,63,63	0
57	MG	2a	1730	1/1	0.88	0.40	72,72,72,72	0
57	MG	1A	3679	1/1	0.88	0.12	31,31,31,31	0
57	MG	1A	3889	1/1	0.88	0.11	40,40,40,40	0
57	MG	2A	3244	1/1	0.88	0.13	65,65,65,65	0
57	MG	2A	3714	1/1	0.88	0.17	73,73,73,73	0
57	MG	2A	3499	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3717	1/1	0.88	0.15	57,57,57,57	0
57	MG	1a	1681	1/1	0.88	0.23	71,71,71,71	0
57	MG	1A	4035	1/1	0.88	0.10	80,80,80,80	0
57	MG	1A	3799	1/1	0.88	0.08	38,38,38,38	0
57	MG	2B	203	1/1	0.88	0.16	62,62,62,62	0
57	MG	2A	3517	1/1	0.88	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1781	1/1	0.88	0.16	67,67,67,67	0
57	MG	1a	1684	1/1	0.88	0.10	58,58,58,58	0
57	MG	2B	207	1/1	0.88	0.18	71,71,71,71	0
57	MG	2q	203	1/1	0.88	0.14	74,74,74,74	0
57	MG	1A	3342	1/1	0.88	0.23	62,62,62,62	0
57	MG	1A	3274	1/1	0.88	0.12	52,52,52,52	0
57	MG	2A	3537	1/1	0.88	0.11	60,60,60,60	0
57	MG	2B	209	1/1	0.89	0.21	65,65,65,65	0
57	MG	1A	3863	1/1	0.89	0.08	50,50,50,50	0
57	MG	1A	3959	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3214	1/1	0.89	0.26	69,69,69,69	0
57	MG	1A	3967	1/1	0.89	0.11	49,49,49,49	0
57	MG	2A	3218	1/1	0.89	0.10	53,53,53,53	0
57	MG	1A	3554	1/1	0.89	0.26	58,58,58,58	0
57	MG	1A	3555	1/1	0.89	0.23	59,59,59,59	0
57	MG	1A	3776	1/1	0.89	0.10	28,28,28,28	0
57	MG	1w	105	1/1	0.89	0.23	70,70,70,70	0
57	MG	1x	103	1/1	0.89	0.11	61,61,61,61	0
57	MG	2A	3235	1/1	0.89	0.14	60,60,60,60	0
57	MG	2A	3239	1/1	0.89	0.12	55,55,55,55	0
57	MG	1A	3532	1/1	0.89	0.15	71,71,71,71	0
57	MG	1x	110	1/1	0.89	0.15	69,69,69,69	0
57	MG	1a	1665	1/1	0.89	0.09	55,55,55,55	0
57	MG	1A	3245	1/1	0.89	0.16	59,59,59,59	0
57	MG	1A	3574	1/1	0.89	0.25	48,48,48,48	0
57	MG	1a	1673	1/1	0.89	0.19	65,65,65,65	0
57	MG	1A	3251	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3265	1/1	0.89	0.18	56,56,56,56	0
57	MG	1A	3891	1/1	0.89	0.13	46,46,46,46	0
57	MG	2a	1625	1/1	0.89	0.11	57,57,57,57	0
57	MG	2A	3016	1/1	0.89	0.21	73,73,73,73	0
57	MG	1B	224	1/1	0.89	0.14	70,70,70,70	0
57	MG	1a	1680	1/1	0.89	0.24	70,70,70,70	0
57	MG	2A	3290	1/1	0.89	0.20	45,45,45,45	0
57	MG	1A	4029	1/1	0.89	0.11	77,77,77,77	0
57	MG	1A	3808	1/1	0.89	0.09	20,20,20,20	0
57	MG	1A	3511	1/1	0.89	0.10	64,64,64,64	0
57	MG	1A	3405	1/1	0.89	0.18	46,46,46,46	0
57	MG	1a	1691	1/1	0.89	0.25	72,72,72,72	0
57	MG	1A	3027	1/1	0.89	0.18	69,69,69,69	0
57	MG	2A	3306	1/1	0.89	0.33	62,62,62,62	0
57	MG	2a	1648	1/1	0.89	0.15	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	4042	1/1	0.89	0.16	60,60,60,60	0
57	MG	2A	3340	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3428	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3459	1/1	0.89	0.17	70,70,70,70	0
57	MG	2A	3352	1/1	0.89	0.17	56,56,56,56	0
57	MG	1A	3828	1/1	0.89	0.31	34,34,34,34	0
57	MG	2A	3603	1/1	0.89	0.16	60,60,60,60	0
57	MG	1A	3619	1/1	0.89	0.09	27,27,27,27	0
57	MG	1A	3549	1/1	0.89	0.34	65,65,65,65	0
57	MG	2a	1666	1/1	0.89	0.11	59,59,59,59	0
57	MG	1A	3731	1/1	0.89	0.10	40,40,40,40	0
57	MG	2A	3368	1/1	0.89	0.27	63,63,63,63	0
57	MG	2a	1672	1/1	0.89	0.22	70,70,70,70	0
57	MG	1A	4053	1/1	0.89	0.09	28,28,28,28	0
57	MG	1A	3733	1/1	0.89	0.09	53,53,53,53	0
57	MG	2a	1679	1/1	0.89	0.20	66,66,66,66	0
57	MG	2a	1681	1/1	0.89	0.13	68,68,68,68	0
57	MG	13	103	1/1	0.89	0.15	57,57,57,57	0
57	MG	1a	1724	1/1	0.89	0.41	72,72,72,72	0
57	MG	2a	1693	1/1	0.89	0.19	78,78,78,78	0
57	MG	2A	3103	1/1	0.89	0.10	64,64,64,64	0
57	MG	2a	1695	1/1	0.89	0.23	64,64,64,64	0
57	MG	2A	3625	1/1	0.89	0.21	65,65,65,65	0
57	MG	1A	4059	1/1	0.89	0.14	70,70,70,70	0
57	MG	2a	1699	1/1	0.89	0.38	73,73,73,73	0
57	MG	1A	3937	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3626	1/1	0.89	0.10	10,10,10,10	0
57	MG	2a	1706	1/1	0.89	0.19	71,71,71,71	0
57	MG	1a	1742	1/1	0.89	0.22	56,56,56,56	0
57	MG	2a	1710	1/1	0.89	0.14	59,59,59,59	0
57	MG	2A	3637	1/1	0.89	0.15	67,67,67,67	0
57	MG	2a	1714	1/1	0.89	0.25	74,74,74,74	0
57	MG	2A	3126	1/1	0.89	0.27	67,67,67,67	0
57	MG	1a	1744	1/1	0.89	0.23	67,67,67,67	0
57	MG	2a	1719	1/1	0.89	0.23	67,67,67,67	0
57	MG	2a	1720	1/1	0.89	0.14	65,65,65,65	0
57	MG	18	3406	1/1	0.89	0.21	53,53,53,53	0
57	MG	2A	3152	1/1	0.89	0.22	55,55,55,55	0
57	MG	2A	3422	1/1	0.89	0.14	62,62,62,62	0
57	MG	1A	3854	1/1	0.89	0.13	51,51,51,51	0
57	MG	1A	3493	1/1	0.89	0.10	46,46,46,46	0
57	MG	1a	1616	1/1	0.89	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3685	1/1	0.89	0.15	46,46,46,46	0
57	MG	1a	1771	1/1	0.89	0.11	56,56,56,56	0
57	MG	2a	1741	1/1	0.89	0.21	45,45,45,45	0
57	MG	1a	1622	1/1	0.89	0.26	63,63,63,63	0
57	MG	1a	1779	1/1	0.89	0.09	55,55,55,55	0
57	MG	2a	1754	1/1	0.89	0.33	57,57,57,57	0
57	MG	1A	3945	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3179	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3710	1/1	0.89	0.29	60,60,60,60	0
57	MG	2a	1770	1/1	0.89	0.30	65,65,65,65	0
57	MG	2a	1773	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3712	1/1	0.89	0.17	58,58,58,58	0
57	MG	2a	1777	1/1	0.89	0.23	73,73,73,73	0
57	MG	2A	3462	1/1	0.89	0.10	67,67,67,67	0
57	MG	1a	1625	1/1	0.89	0.27	54,54,54,54	0
57	MG	1a	1788	1/1	0.89	0.09	85,85,85,85	0
57	MG	1a	1627	1/1	0.89	0.18	59,59,59,59	0
57	MG	2A	3190	1/1	0.89	0.24	40,40,40,40	0
57	MG	1a	1796	1/1	0.89	0.12	45,45,45,45	0
57	MG	1A	3857	1/1	0.89	0.17	51,51,51,51	0
57	MG	2A	3201	1/1	0.89	0.14	77,77,77,77	0
57	MG	2A	3203	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	3955	1/1	0.89	0.09	25,25,25,25	0
57	MG	2y	102	1/1	0.89	0.08	81,81,81,81	0
57	MG	2y	103	1/1	0.89	0.28	58,58,58,58	0
57	MG	2A	3128	1/1	0.90	0.16	61,61,61,61	0
57	MG	2A	3426	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3165	1/1	0.90	0.12	45,45,45,45	0
57	MG	2A	3438	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	3169	1/1	0.90	0.25	62,62,62,62	0
57	MG	1A	3182	1/1	0.90	0.10	51,51,51,51	0
57	MG	1a	1745	1/1	0.90	0.15	68,68,68,68	0
57	MG	1a	1748	1/1	0.90	0.16	60,60,60,60	0
57	MG	2B	213	1/1	0.90	0.21	64,64,64,64	0
57	MG	2A	3451	1/1	0.90	0.12	60,60,60,60	0
57	MG	2B	215	1/1	0.90	0.18	65,65,65,65	0
57	MG	2B	216	1/1	0.90	0.27	75,75,75,75	0
57	MG	1A	3359	1/1	0.90	0.17	62,62,62,62	0
57	MG	18	3405	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3171	1/1	0.90	0.10	47,47,47,47	0
57	MG	2E	306	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3174	1/1	0.90	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	1A	3361	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3468	1/1	0.90	0.14	67,67,67,67	0
57	MG	2A	3177	1/1	0.90	0.30	60,60,60,60	0
57	MG	1a	1601	1/1	0.90	0.29	66,66,66,66	0
57	MG	27	101	1/1	0.90	0.25	63,63,63,63	0
57	MG	1A	3460	1/1	0.90	0.18	55,55,55,55	0
57	MG	2a	1602	1/1	0.90	0.31	71,71,71,71	0
57	MG	1a	1605	1/1	0.90	0.11	59,59,59,59	0
57	MG	1A	3809	1/1	0.90	0.07	34,34,34,34	0
57	MG	2a	1607	1/1	0.90	0.23	69,69,69,69	0
57	MG	1A	3930	1/1	0.90	0.08	72,72,72,72	0
57	MG	2A	3485	1/1	0.90	0.09	32,32,32,32	0
57	MG	1A	3467	1/1	0.90	0.17	64,64,64,64	0
57	MG	1A	4064	1/1	0.90	0.12	68,68,68,68	0
57	MG	1A	3294	1/1	0.90	0.07	30,30,30,30	0
57	MG	1A	3933	1/1	0.90	0.15	33,33,33,33	0
57	MG	1a	1800	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	4080	1/1	0.90	0.15	52,52,52,52	0
57	MG	1A	3540	1/1	0.90	0.19	34,34,34,34	0
57	MG	1A	3820	1/1	0.90	0.13	46,46,46,46	0
57	MG	1a	1632	1/1	0.90	0.30	59,59,59,59	0
57	MG	2a	1630	1/1	0.90	0.40	74,74,74,74	0
57	MG	1b	301	1/1	0.90	0.09	80,80,80,80	0
57	MG	2A	3518	1/1	0.90	0.09	54,54,54,54	0
57	MG	2A	3519	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3523	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3666	1/1	0.90	0.09	44,44,44,44	0
57	MG	2A	3530	1/1	0.90	0.14	67,67,67,67	0
57	MG	2a	1642	1/1	0.90	0.23	59,59,59,59	0
57	MG	1A	3673	1/1	0.90	0.09	49,49,49,49	0
57	MG	1a	1638	1/1	0.90	0.15	50,50,50,50	0
57	MG	1v	101	1/1	0.90	0.20	71,71,71,71	0
57	MG	1w	101	1/1	0.90	0.18	76,76,76,76	0
57	MG	1w	103	1/1	0.90	0.15	63,63,63,63	0
57	MG	1A	4090	1/1	0.90	0.11	50,50,50,50	0
57	MG	2a	1651	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3308	1/1	0.90	0.17	49,49,49,49	0
57	MG	2A	3240	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3549	1/1	0.90	0.12	66,66,66,66	0
57	MG	1A	3376	1/1	0.90	0.23	58,58,58,58	0
57	MG	1a	1646	1/1	0.90	0.14	63,63,63,63	0
57	MG	2a	1661	1/1	0.90	0.21	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	3250	1/1	0.90	0.18	59,59,59,59	0
57	MG	1A	3547	1/1	0.90	0.20	52,52,52,52	0
57	MG	1x	113	1/1	0.90	0.19	72,72,72,72	0
57	MG	1a	1664	1/1	0.90	0.29	68,68,68,68	0
57	MG	1A	3378	1/1	0.90	0.14	53,53,53,53	0
57	MG	2a	1671	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3261	1/1	0.90	0.12	54,54,54,54	0
57	MG	2a	1676	1/1	0.90	0.19	64,64,64,64	0
57	MG	1A	3957	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3264	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3483	1/1	0.90	0.15	41,41,41,41	0
57	MG	1A	3700	1/1	0.90	0.11	26,26,26,26	0
57	MG	2a	1684	1/1	0.90	0.17	76,76,76,76	0
57	MG	2a	1685	1/1	0.90	0.17	67,67,67,67	0
57	MG	2A	3273	1/1	0.90	0.11	58,58,58,58	0
57	MG	1A	3972	1/1	0.90	0.10	40,40,40,40	0
57	MG	1A	3974	1/1	0.90	0.07	24,24,24,24	0
57	MG	2A	3280	1/1	0.90	0.08	58,58,58,58	0
57	MG	2A	3286	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3852	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3383	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3033	1/1	0.90	0.28	56,56,56,56	0
57	MG	1A	3996	1/1	0.90	0.12	26,26,26,26	0
57	MG	1A	3250	1/1	0.90	0.09	56,56,56,56	0
57	MG	2A	3301	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3100	1/1	0.90	0.09	61,61,61,61	0
57	MG	1A	3723	1/1	0.90	0.09	56,56,56,56	0
57	MG	1a	1687	1/1	0.90	0.22	48,48,48,48	0
57	MG	2a	1712	1/1	0.90	0.19	68,68,68,68	0
57	MG	1a	1690	1/1	0.90	0.16	74,74,74,74	0
57	MG	2A	3616	1/1	0.90	0.16	42,42,42,42	0
57	MG	2A	3307	1/1	0.90	0.25	69,69,69,69	0
57	MG	2A	3309	1/1	0.90	0.27	56,56,56,56	0
57	MG	2A	3311	1/1	0.90	0.22	56,56,56,56	0
57	MG	2A	3623	1/1	0.90	0.20	58,58,58,58	0
57	MG	1A	3495	1/1	0.90	0.07	41,41,41,41	0
57	MG	2a	1726	1/1	0.90	0.42	68,68,68,68	0
57	MG	2A	3335	1/1	0.90	0.19	62,62,62,62	0
57	MG	1E	301	1/1	0.90	0.13	32,32,32,32	0
57	MG	1a	1693	1/1	0.90	0.11	69,69,69,69	0
57	MG	1a	1694	1/1	0.90	0.11	59,59,59,59	0
57	MG	2a	1733	1/1	0.90	0.38	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1734	1/1	0.90	0.32	55,55,55,55	0
57	MG	2a	1737	1/1	0.90	0.40	64,64,64,64	0
57	MG	2A	3065	1/1	0.90	0.20	65,65,65,65	0
57	MG	1A	4023	1/1	0.90	0.08	41,41,41,41	0
57	MG	2A	3075	1/1	0.90	0.23	65,65,65,65	0
57	MG	1A	3318	1/1	0.90	0.08	50,50,50,50	0
57	MG	2a	1747	1/1	0.90	0.28	61,61,61,61	0
57	MG	2a	1748	1/1	0.90	0.35	62,62,62,62	0
57	MG	2A	3643	1/1	0.90	0.14	66,66,66,66	0
57	MG	1G	203	1/1	0.90	0.11	68,68,68,68	0
57	MG	1A	3006	1/1	0.90	0.14	54,54,54,54	0
57	MG	2a	1758	1/1	0.90	0.29	57,57,57,57	0
57	MG	2a	1761	1/1	0.90	0.29	59,59,59,59	0
57	MG	2a	1762	1/1	0.90	0.34	69,69,69,69	0
57	MG	2A	3369	1/1	0.90	0.31	61,61,61,61	0
57	MG	2A	3371	1/1	0.90	0.30	59,59,59,59	0
57	MG	2a	1768	1/1	0.90	0.26	61,61,61,61	0
57	MG	1a	1710	1/1	0.90	0.18	63,63,63,63	0
57	MG	1A	3421	1/1	0.90	0.10	57,57,57,57	0
57	MG	1A	3736	1/1	0.90	0.14	60,60,60,60	0
57	MG	1A	3747	1/1	0.90	0.20	49,49,49,49	0
57	MG	1A	3596	1/1	0.90	0.11	43,43,43,43	0
57	MG	2A	3694	1/1	0.90	0.12	41,41,41,41	0
57	MG	1S	202	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3705	1/1	0.90	0.22	59,59,59,59	0
57	MG	2A	3388	1/1	0.90	0.16	53,53,53,53	0
57	MG	2a	1786	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3264	1/1	0.90	0.10	44,44,44,44	0
57	MG	2A	3116	1/1	0.90	0.21	64,64,64,64	0
57	MG	2A	3121	1/1	0.90	0.32	67,67,67,67	0
57	MG	1A	3519	1/1	0.90	0.12	52,52,52,52	0
57	MG	2A	3125	1/1	0.90	0.14	50,50,50,50	0
57	MG	2y	101	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	3339	1/1	0.90	0.13	54,54,54,54	0
57	MG	1Z	3703	1/1	0.90	0.17	52,52,52,52	0
59	ZN	24	501	1/1	0.90	0.14	135,135,135,135	0
57	MG	1A	3510	1/1	0.91	0.14	69,69,69,69	0
57	MG	1x	105	1/1	0.91	0.08	59,59,59,59	0
57	MG	1A	3060	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3463	1/1	0.91	0.27	63,63,63,63	0
57	MG	1A	3408	1/1	0.91	0.13	48,48,48,48	0
57	MG	2A	3222	1/1	0.91	0.07	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	3469	1/1	0.91	0.14	65,65,65,65	0
57	MG	1x	111	1/1	0.91	0.13	62,62,62,62	0
57	MG	2F	306	1/1	0.91	0.07	62,62,62,62	0
57	MG	2A	3473	1/1	0.91	0.20	68,68,68,68	0
57	MG	1A	3647	1/1	0.91	0.08	35,35,35,35	0
57	MG	1A	3414	1/1	0.91	0.15	59,59,59,59	0
57	MG	1A	3061	1/1	0.91	0.15	50,50,50,50	0
57	MG	25	101	1/1	0.91	0.20	59,59,59,59	0
57	MG	1B	227	1/1	0.91	0.08	53,53,53,53	0
57	MG	2A	3232	1/1	0.91	0.17	62,62,62,62	0
57	MG	2A	3484	1/1	0.91	0.10	35,35,35,35	0
57	MG	1A	3655	1/1	0.91	0.09	33,33,33,33	0
57	MG	1B	229	1/1	0.91	0.11	61,61,61,61	0
57	MG	2a	1604	1/1	0.91	0.13	59,59,59,59	0
57	MG	1A	3657	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3242	1/1	0.91	0.29	67,67,67,67	0
57	MG	2A	3005	1/1	0.91	0.25	62,62,62,62	0
57	MG	2A	3007	1/1	0.91	0.13	53,53,53,53	0
57	MG	2a	1613	1/1	0.91	0.19	63,63,63,63	0
57	MG	2A	3245	1/1	0.91	0.09	49,49,49,49	0
57	MG	2A	3247	1/1	0.91	0.10	53,53,53,53	0
57	MG	1A	3419	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3513	1/1	0.91	0.14	45,45,45,45	0
57	MG	1A	3663	1/1	0.91	0.09	42,42,42,42	0
57	MG	2A	3255	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3336	1/1	0.91	0.12	43,43,43,43	0
57	MG	1A	3018	1/1	0.91	0.12	36,36,36,36	0
57	MG	2A	3522	1/1	0.91	0.28	66,66,66,66	0
57	MG	2A	3038	1/1	0.91	0.19	52,52,52,52	0
57	MG	2A	3524	1/1	0.91	0.10	72,72,72,72	0
57	MG	2A	3039	1/1	0.91	0.17	66,66,66,66	0
57	MG	2a	1634	1/1	0.91	0.18	72,72,72,72	0
57	MG	1E	315	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3850	1/1	0.91	0.24	56,56,56,56	0
57	MG	1A	3093	1/1	0.91	0.13	58,58,58,58	0
57	MG	2A	3534	1/1	0.91	0.20	60,60,60,60	0
57	MG	1A	4010	1/1	0.91	0.17	27,27,27,27	0
57	MG	2a	1643	1/1	0.91	0.11	73,73,73,73	0
57	MG	2A	3053	1/1	0.91	0.32	74,74,74,74	0
57	MG	1A	4014	1/1	0.91	0.08	69,69,69,69	0
57	MG	2A	3542	1/1	0.91	0.12	69,69,69,69	0
57	MG	1A	3435	1/1	0.91	0.25	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	3180	1/1	0.91	0.22	56,56,56,56	0
57	MG	1A	3856	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3256	1/1	0.91	0.11	66,66,66,66	0
57	MG	2A	3289	1/1	0.91	0.22	43,43,43,43	0
57	MG	2a	1654	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3355	1/1	0.91	0.12	58,58,58,58	0
57	MG	1V	205	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3297	1/1	0.91	0.15	56,56,56,56	0
57	MG	1A	3864	1/1	0.91	0.07	21,21,21,21	0
57	MG	1A	4033	1/1	0.91	0.08	80,80,80,80	0
57	MG	2A	3561	1/1	0.91	0.12	73,73,73,73	0
57	MG	1A	3444	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3868	1/1	0.91	0.22	35,35,35,35	0
57	MG	2A	3565	1/1	0.91	0.09	75,75,75,75	0
57	MG	1a	1726	1/1	0.91	0.12	53,53,53,53	0
57	MG	1A	3707	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3445	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3449	1/1	0.91	0.17	41,41,41,41	0
57	MG	1A	3545	1/1	0.91	0.27	59,59,59,59	0
57	MG	2A	3107	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3312	1/1	0.91	0.12	69,69,69,69	0
57	MG	2a	1680	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3722	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3316	1/1	0.91	0.25	53,53,53,53	0
57	MG	2A	3590	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3318	1/1	0.91	0.21	48,48,48,48	0
57	MG	1A	3262	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3339	1/1	0.91	0.18	56,56,56,56	0
57	MG	1a	1602	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3098	1/1	0.91	0.23	58,58,58,58	0
57	MG	2A	3342	1/1	0.91	0.49	60,60,60,60	0
57	MG	2A	3119	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3344	1/1	0.91	0.11	53,53,53,53	0
57	MG	2a	1702	1/1	0.91	0.27	57,57,57,57	0
57	MG	2A	3351	1/1	0.91	0.17	54,54,54,54	0
57	MG	2a	1704	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3265	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3191	1/1	0.91	0.16	51,51,51,51	0
57	MG	2a	1707	1/1	0.91	0.12	70,70,70,70	0
57	MG	1A	3194	1/1	0.91	0.35	36,36,36,36	0
57	MG	1A	3370	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	3559	1/1	0.91	0.12	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	3905	1/1	0.91	0.08	43,43,43,43	0
57	MG	1A	3754	1/1	0.91	0.09	59,59,59,59	0
57	MG	2a	1715	1/1	0.91	0.16	69,69,69,69	0
57	MG	2A	3370	1/1	0.91	0.16	60,60,60,60	0
57	MG	1A	3034	1/1	0.91	0.08	47,47,47,47	0
57	MG	2A	3372	1/1	0.91	0.12	54,54,54,54	0
57	MG	1a	1787	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3374	1/1	0.91	0.24	40,40,40,40	0
57	MG	2A	3162	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3164	1/1	0.91	0.24	61,61,61,61	0
57	MG	1A	3479	1/1	0.91	0.12	40,40,40,40	0
57	MG	1A	3148	1/1	0.91	0.22	38,38,38,38	0
57	MG	1A	3929	1/1	0.91	0.08	31,31,31,31	0
57	MG	1a	1797	1/1	0.91	0.09	56,56,56,56	0
57	MG	2a	1731	1/1	0.91	0.39	61,61,61,61	0
57	MG	2A	3653	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3390	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3394	1/1	0.91	0.13	50,50,50,50	0
57	MG	2A	3667	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3395	1/1	0.91	0.12	63,63,63,63	0
57	MG	1a	1633	1/1	0.91	0.21	56,56,56,56	0
57	MG	1a	1823	1/1	0.91	0.14	61,61,61,61	0
57	MG	2a	1745	1/1	0.91	0.18	49,49,49,49	0
57	MG	1A	3379	1/1	0.91	0.21	52,52,52,52	0
57	MG	2A	3690	1/1	0.91	0.08	51,51,51,51	0
57	MG	2a	1749	1/1	0.91	0.53	68,68,68,68	0
57	MG	2a	1750	1/1	0.91	0.34	55,55,55,55	0
57	MG	2a	1752	1/1	0.91	0.34	52,52,52,52	0
57	MG	1A	3770	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3484	1/1	0.91	0.13	43,43,43,43	0
57	MG	2A	3696	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	4092	1/1	0.91	0.13	63,63,63,63	0
57	MG	2a	1760	1/1	0.91	0.25	54,54,54,54	0
57	MG	1a	1641	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	3048	1/1	0.91	0.06	16,16,16,16	0
57	MG	2a	1763	1/1	0.91	0.24	64,64,64,64	0
57	MG	1A	3388	1/1	0.91	0.12	64,64,64,64	0
57	MG	2A	3708	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3395	1/1	0.91	0.09	48,48,48,48	0
57	MG	2a	1769	1/1	0.91	0.27	60,60,60,60	0
57	MG	2A	3711	1/1	0.91	0.15	61,61,61,61	0
57	MG	2a	1771	1/1	0.91	0.24	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	2A	3431	1/1	0.91	0.16	48,48,48,48	0
57	MG	2A	3434	1/1	0.91	0.08	36,36,36,36	0
57	MG	2a	1776	1/1	0.91	0.26	63,63,63,63	0
57	MG	2A	3715	1/1	0.91	0.17	68,68,68,68	0
57	MG	1t	201	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3198	1/1	0.91	0.34	68,68,68,68	0
57	MG	2A	3444	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3720	1/1	0.91	0.12	41,41,41,41	0
57	MG	1A	3397	1/1	0.91	0.26	42,42,42,42	0
57	MG	1a	1663	1/1	0.91	0.11	48,48,48,48	0
57	MG	2A	3724	1/1	0.91	0.20	44,44,44,44	0
57	MG	2A	3725	1/1	0.91	0.27	62,62,62,62	0
57	MG	2B	202	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3212	1/1	0.91	0.12	42,42,42,42	0
57	MG	1A	3223	1/1	0.91	0.10	47,47,47,47	0
57	MG	1a	1667	1/1	0.91	0.21	56,56,56,56	0
57	MG	2A	3455	1/1	0.91	0.24	62,62,62,62	0
57	MG	2A	3457	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3458	1/1	0.91	0.14	55,55,55,55	0
61	K	2A	3330	1/1	0.91	0.18	75,75,75,75	0
57	MG	2A	3358	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3591	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3361	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3366	1/1	0.92	0.28	68,68,68,68	0
57	MG	1A	3357	1/1	0.92	0.16	48,48,48,48	0
57	MG	2A	3069	1/1	0.92	0.25	67,67,67,67	0
57	MG	1A	3498	1/1	0.92	0.17	55,55,55,55	0
57	MG	2A	3073	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	3417	1/1	0.92	0.14	48,48,48,48	0
57	MG	2A	3076	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3077	1/1	0.92	0.12	66,66,66,66	0
57	MG	2A	3080	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3607	1/1	0.92	0.26	64,64,64,64	0
57	MG	2A	3083	1/1	0.92	0.15	55,55,55,55	0
57	MG	2A	3085	1/1	0.92	0.18	62,62,62,62	0
57	MG	2A	3384	1/1	0.92	0.13	40,40,40,40	0
57	MG	2A	3385	1/1	0.92	0.28	60,60,60,60	0
57	MG	2B	205	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3921	1/1	0.92	0.24	36,36,36,36	0
57	MG	2A	3387	1/1	0.92	0.08	36,36,36,36	0
57	MG	2A	3089	1/1	0.92	0.18	46,46,46,46	0
57	MG	2B	210	1/1	0.92	0.19	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	3924	1/1	0.92	0.11	30,30,30,30	0
57	MG	2B	212	1/1	0.92	0.12	65,65,65,65	0
57	MG	1A	3926	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3298	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3766	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3301	1/1	0.92	0.46	68,68,68,68	0
57	MG	2A	3104	1/1	0.92	0.20	50,50,50,50	0
57	MG	1A	4099	1/1	0.92	0.21	53,53,53,53	0
57	MG	1A	3769	1/1	0.92	0.06	16,16,16,16	0
57	MG	1A	3422	1/1	0.92	0.08	49,49,49,49	0
57	MG	2F	302	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3772	1/1	0.92	0.09	20,20,20,20	0
57	MG	1A	3049	1/1	0.92	0.17	32,32,32,32	0
57	MG	1B	203	1/1	0.92	0.06	31,31,31,31	0
57	MG	2A	3120	1/1	0.92	0.25	70,70,70,70	0
57	MG	1B	204	1/1	0.92	0.28	63,63,63,63	0
57	MG	1B	206	1/1	0.92	0.20	47,47,47,47	0
57	MG	1B	208	1/1	0.92	0.28	59,59,59,59	0
57	MG	2A	3440	1/1	0.92	0.09	40,40,40,40	0
57	MG	1a	1703	1/1	0.92	0.19	51,51,51,51	0
57	MG	1a	1704	1/1	0.92	0.25	52,52,52,52	0
57	MG	1B	210	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3141	1/1	0.92	0.28	54,54,54,54	0
57	MG	1B	211	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3151	1/1	0.92	0.07	45,45,45,45	0
57	MG	1A	3086	1/1	0.92	0.11	35,35,35,35	0
57	MG	2a	1610	1/1	0.92	0.28	73,73,73,73	0
57	MG	2A	3454	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3156	1/1	0.92	0.29	61,61,61,61	0
57	MG	2A	3158	1/1	0.92	0.26	67,67,67,67	0
57	MG	2a	1617	1/1	0.92	0.10	67,67,67,67	0
57	MG	1B	221	1/1	0.92	0.15	57,57,57,57	0
57	MG	1a	1714	1/1	0.92	0.15	46,46,46,46	0
57	MG	1B	222	1/1	0.92	0.07	51,51,51,51	0
57	MG	2A	3165	1/1	0.92	0.18	53,53,53,53	0
57	MG	1B	223	1/1	0.92	0.09	55,55,55,55	0
57	MG	2a	1623	1/1	0.92	0.24	68,68,68,68	0
57	MG	1a	1719	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3104	1/1	0.92	0.10	36,36,36,36	0
57	MG	1A	3632	1/1	0.92	0.07	24,24,24,24	0
57	MG	1A	3634	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3803	1/1	0.92	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3807	1/1	0.92	0.12	26,26,26,26	0
57	MG	1a	1728	1/1	0.92	0.26	58,58,58,58	0
57	MG	1a	1729	1/1	0.92	0.11	65,65,65,65	0
57	MG	1B	232	1/1	0.92	0.11	43,43,43,43	0
57	MG	1a	1735	1/1	0.92	0.20	48,48,48,48	0
57	MG	2A	3482	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3181	1/1	0.92	0.35	61,61,61,61	0
57	MG	2A	3185	1/1	0.92	0.13	72,72,72,72	0
57	MG	1A	3114	1/1	0.92	0.21	46,46,46,46	0
57	MG	1A	3374	1/1	0.92	0.24	43,43,43,43	0
57	MG	1A	3966	1/1	0.92	0.09	52,52,52,52	0
57	MG	2A	3192	1/1	0.92	0.12	54,54,54,54	0
57	MG	1E	303	1/1	0.92	0.21	44,44,44,44	0
57	MG	2A	3498	1/1	0.92	0.09	45,45,45,45	0
57	MG	2A	3195	1/1	0.92	0.13	38,38,38,38	0
57	MG	1E	307	1/1	0.92	0.20	49,49,49,49	0
57	MG	2A	3507	1/1	0.92	0.21	65,65,65,65	0
57	MG	1A	3649	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3968	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3202	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3516	1/1	0.92	0.09	50,50,50,50	0
57	MG	2a	1660	1/1	0.92	0.19	56,56,56,56	0
57	MG	1A	3375	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3442	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3209	1/1	0.92	0.36	59,59,59,59	0
57	MG	1G	204	1/1	0.92	0.09	68,68,68,68	0
57	MG	1a	1767	1/1	0.92	0.19	64,64,64,64	0
57	MG	1N	205	1/1	0.92	0.13	54,54,54,54	0
57	MG	1a	1777	1/1	0.92	0.14	71,71,71,71	0
57	MG	2A	3529	1/1	0.92	0.12	73,73,73,73	0
57	MG	2A	3217	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3531	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3975	1/1	0.92	0.27	50,50,50,50	0
57	MG	1A	3653	1/1	0.92	0.13	72,72,72,72	0
57	MG	2A	3223	1/1	0.92	0.26	72,72,72,72	0
57	MG	2A	3535	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3986	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3538	1/1	0.92	0.09	58,58,58,58	0
57	MG	1P	205	1/1	0.92	0.24	49,49,49,49	0
57	MG	2a	1687	1/1	0.92	0.13	67,67,67,67	0
57	MG	2a	1691	1/1	0.92	0.14	58,58,58,58	0
57	MG	1a	1785	1/1	0.92	0.12	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	3327	1/1	0.92	0.17	45,45,45,45	0
57	MG	1A	3994	1/1	0.92	0.12	73,73,73,73	0
57	MG	1A	3330	1/1	0.92	0.22	52,52,52,52	0
57	MG	1a	1792	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3236	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3237	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3331	1/1	0.92	0.21	54,54,54,54	0
57	MG	1T	202	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3554	1/1	0.92	0.17	60,60,60,60	0
57	MG	1U	209	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	4001	1/1	0.92	0.07	28,28,28,28	0
57	MG	1W	201	1/1	0.92	0.17	44,44,44,44	0
57	MG	1A	3829	1/1	0.92	0.08	41,41,41,41	0
57	MG	2A	3246	1/1	0.92	0.27	66,66,66,66	0
57	MG	1Z	3701	1/1	0.92	0.10	60,60,60,60	0
57	MG	1A	3453	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	4009	1/1	0.92	0.09	16,16,16,16	0
57	MG	2A	3252	1/1	0.92	0.11	71,71,71,71	0
57	MG	10	103	1/1	0.92	0.06	47,47,47,47	0
57	MG	2a	1717	1/1	0.92	0.10	75,75,75,75	0
57	MG	10	107	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3257	1/1	0.92	0.13	57,57,57,57	0
57	MG	1l	203	1/1	0.92	0.15	62,62,62,62	0
57	MG	2a	1721	1/1	0.92	0.29	47,47,47,47	0
57	MG	1A	3132	1/1	0.92	0.11	40,40,40,40	0
57	MG	2A	3586	1/1	0.92	0.11	39,39,39,39	0
57	MG	1A	4012	1/1	0.92	0.06	36,36,36,36	0
57	MG	2A	3262	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	3670	1/1	0.92	0.07	24,24,24,24	0
57	MG	1A	3385	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3248	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	4025	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3391	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3680	1/1	0.92	0.07	34,34,34,34	0
57	MG	2a	1735	1/1	0.92	0.33	61,61,61,61	0
57	MG	2a	1736	1/1	0.92	0.44	72,72,72,72	0
57	MG	1A	3269	1/1	0.92	0.32	53,53,53,53	0
57	MG	2a	1738	1/1	0.92	0.20	57,57,57,57	0
57	MG	1A	3691	1/1	0.92	0.09	32,32,32,32	0
57	MG	1A	3474	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1610	1/1	0.92	0.08	57,57,57,57	0
57	MG	1a	1612	1/1	0.92	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3137	1/1	0.92	0.16	40,40,40,40	0
57	MG	1y	101	1/1	0.92	0.06	68,68,68,68	0
57	MG	2A	3296	1/1	0.92	0.18	54,54,54,54	0
57	MG	2A	3621	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3552	1/1	0.92	0.28	51,51,51,51	0
57	MG	2a	1751	1/1	0.92	0.41	59,59,59,59	0
57	MG	1A	3701	1/1	0.92	0.11	23,23,23,23	0
57	MG	1A	3703	1/1	0.92	0.15	68,68,68,68	0
57	MG	1A	3706	1/1	0.92	0.09	36,36,36,36	0
57	MG	1A	3277	1/1	0.92	0.18	35,35,35,35	0
57	MG	1A	3400	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3630	1/1	0.92	0.24	61,61,61,61	0
57	MG	1A	3710	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3008	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3344	1/1	0.92	0.24	37,37,37,37	0
57	MG	2a	1764	1/1	0.92	0.42	67,67,67,67	0
57	MG	1A	3884	1/1	0.92	0.16	32,32,32,32	0
57	MG	2A	3026	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3402	1/1	0.92	0.22	40,40,40,40	0
57	MG	2A	3645	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	4054	1/1	0.92	0.07	32,32,32,32	0
57	MG	2A	3314	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3036	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3560	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3655	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3323	1/1	0.92	0.30	52,52,52,52	0
57	MG	2A	3662	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3561	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3040	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3671	1/1	0.92	0.09	53,53,53,53	0
57	MG	2a	1782	1/1	0.92	0.24	62,62,62,62	0
57	MG	2a	1783	1/1	0.92	0.14	73,73,73,73	0
57	MG	1A	4061	1/1	0.92	0.11	55,55,55,55	0
57	MG	2a	1785	1/1	0.92	0.27	69,69,69,69	0
57	MG	1A	3347	1/1	0.92	0.20	60,60,60,60	0
57	MG	2f	201	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3893	1/1	0.92	0.09	32,32,32,32	0
57	MG	1a	1645	1/1	0.92	0.15	65,65,65,65	0
57	MG	1A	3207	1/1	0.92	0.15	61,61,61,61	0
57	MG	2w	101	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3350	1/1	0.92	0.12	50,50,50,50	0
57	MG	1a	1651	1/1	0.92	0.22	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3701	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	4068	1/1	0.92	0.06	25,25,25,25	0
57	MG	1A	3411	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	3253	1/1	0.92	0.20	49,49,49,49	0
57	MG	1A	3735	1/1	0.92	0.14	55,55,55,55	0
57	MG	1Q	203	1/1	0.93	0.11	55,55,55,55	0
57	MG	1Q	205	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3400	1/1	0.93	0.08	42,42,42,42	0
57	MG	1a	1743	1/1	0.93	0.31	59,59,59,59	0
57	MG	2A	3153	1/1	0.93	0.18	57,57,57,57	0
57	MG	2A	3728	1/1	0.93	0.22	51,51,51,51	0
57	MG	2A	3730	1/1	0.93	0.14	66,66,66,66	0
57	MG	2B	201	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3408	1/1	0.93	0.16	48,48,48,48	0
57	MG	1A	3671	1/1	0.93	0.09	24,24,24,24	0
57	MG	2A	3410	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	4011	1/1	0.93	0.10	19,19,19,19	0
57	MG	2A	3417	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3846	1/1	0.93	0.18	60,60,60,60	0
57	MG	1a	1749	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1752	1/1	0.93	0.08	56,56,56,56	0
57	MG	1a	1754	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3433	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3296	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3435	1/1	0.93	0.16	56,56,56,56	0
57	MG	1U	202	1/1	0.93	0.19	40,40,40,40	0
57	MG	1A	4020	1/1	0.93	0.07	21,21,21,21	0
57	MG	2A	3441	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3677	1/1	0.93	0.07	25,25,25,25	0
57	MG	2E	301	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3297	1/1	0.93	0.12	59,59,59,59	0
57	MG	2E	305	1/1	0.93	0.12	39,39,39,39	0
57	MG	1a	1776	1/1	0.93	0.35	70,70,70,70	0
57	MG	1Y	202	1/1	0.93	0.23	56,56,56,56	0
57	MG	1A	3053	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3368	1/1	0.93	0.11	57,57,57,57	0
57	MG	2Q	201	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3439	1/1	0.93	0.13	54,54,54,54	0
57	MG	1A	3246	1/1	0.93	0.13	57,57,57,57	0
57	MG	2A	3182	1/1	0.93	0.12	55,55,55,55	0
57	MG	10	102	1/1	0.93	0.18	47,47,47,47	0
57	MG	1a	1786	1/1	0.93	0.09	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	3543	1/1	0.93	0.26	50,50,50,50	0
57	MG	1A	4034	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3373	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3307	1/1	0.93	0.41	63,63,63,63	0
57	MG	1A	3247	1/1	0.93	0.32	62,62,62,62	0
57	MG	2A	3197	1/1	0.93	0.27	64,64,64,64	0
57	MG	1A	3183	1/1	0.93	0.13	70,70,70,70	0
57	MG	2a	1608	1/1	0.93	0.32	68,68,68,68	0
57	MG	1A	3870	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3200	1/1	0.93	0.09	52,52,52,52	0
57	MG	1a	1813	1/1	0.93	0.07	68,68,68,68	0
57	MG	1a	1817	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3873	1/1	0.93	0.07	40,40,40,40	0
57	MG	2A	3205	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3550	1/1	0.93	0.26	47,47,47,47	0
57	MG	1a	1826	1/1	0.93	0.18	56,56,56,56	0
57	MG	1A	3454	1/1	0.93	0.12	62,62,62,62	0
57	MG	1A	3877	1/1	0.93	0.07	30,30,30,30	0
57	MG	1A	3311	1/1	0.93	0.25	50,50,50,50	0
57	MG	2A	3488	1/1	0.93	0.09	34,34,34,34	0
57	MG	1a	1606	1/1	0.93	0.14	53,53,53,53	0
57	MG	1A	3712	1/1	0.93	0.08	27,27,27,27	0
57	MG	1A	3187	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3888	1/1	0.93	0.09	50,50,50,50	0
57	MG	1a	1613	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3316	1/1	0.93	0.20	59,59,59,59	0
57	MG	2A	3501	1/1	0.93	0.17	54,54,54,54	0
57	MG	1A	3720	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3188	1/1	0.93	0.24	32,32,32,32	0
57	MG	1A	3468	1/1	0.93	0.09	50,50,50,50	0
57	MG	2a	1638	1/1	0.93	0.22	57,57,57,57	0
57	MG	2a	1639	1/1	0.93	0.21	53,53,53,53	0
57	MG	1A	3320	1/1	0.93	0.17	57,57,57,57	0
57	MG	1A	3899	1/1	0.93	0.11	25,25,25,25	0
57	MG	2A	3233	1/1	0.93	0.16	57,57,57,57	0
57	MG	1x	102	1/1	0.93	0.09	33,33,33,33	0
57	MG	2a	1645	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	4071	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3726	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3238	1/1	0.93	0.13	63,63,63,63	0
57	MG	1x	106	1/1	0.93	0.25	69,69,69,69	0
57	MG	1A	3471	1/1	0.93	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3325	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3393	1/1	0.93	0.22	44,44,44,44	0
57	MG	1x	112	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3587	1/1	0.93	0.07	37,37,37,37	0
57	MG	1A	3909	1/1	0.93	0.08	54,54,54,54	0
57	MG	2a	1657	1/1	0.93	0.14	65,65,65,65	0
57	MG	1A	3135	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3746	1/1	0.93	0.08	51,51,51,51	0
57	MG	1A	3045	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3919	1/1	0.93	0.12	64,64,64,64	0
57	MG	2A	3253	1/1	0.93	0.09	63,63,63,63	0
57	MG	2A	3254	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3748	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3752	1/1	0.93	0.08	21,21,21,21	0
57	MG	2A	3004	1/1	0.93	0.36	68,68,68,68	0
57	MG	1A	3594	1/1	0.93	0.14	43,43,43,43	0
57	MG	2A	3545	1/1	0.93	0.11	46,46,46,46	0
57	MG	2a	1674	1/1	0.93	0.15	65,65,65,65	0
57	MG	2a	1675	1/1	0.93	0.10	63,63,63,63	0
57	MG	1a	1657	1/1	0.93	0.20	52,52,52,52	0
57	MG	1a	1658	1/1	0.93	0.23	60,60,60,60	0
57	MG	2A	3009	1/1	0.93	0.11	45,45,45,45	0
57	MG	1A	3196	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3481	1/1	0.93	0.17	50,50,50,50	0
57	MG	2A	3553	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3261	1/1	0.93	0.16	62,62,62,62	0
57	MG	2A	3266	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3039	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3558	1/1	0.93	0.15	62,62,62,62	0
57	MG	2a	1689	1/1	0.93	0.17	48,48,48,48	0
57	MG	2A	3559	1/1	0.93	0.15	61,61,61,61	0
57	MG	2A	3269	1/1	0.93	0.16	65,65,65,65	0
57	MG	2A	3271	1/1	0.93	0.31	62,62,62,62	0
57	MG	2A	3029	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3030	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3564	1/1	0.93	0.15	56,56,56,56	0
57	MG	2a	1697	1/1	0.93	0.20	51,51,51,51	0
57	MG	1A	4105	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3278	1/1	0.93	0.11	60,60,60,60	0
57	MG	2A	3035	1/1	0.93	0.12	31,31,31,31	0
57	MG	2A	3571	1/1	0.93	0.15	66,66,66,66	0
57	MG	2A	3572	1/1	0.93	0.08	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	3574	1/1	0.93	0.08	77,77,77,77	0
57	MG	2A	3285	1/1	0.93	0.26	44,44,44,44	0
57	MG	1A	3263	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3040	1/1	0.93	0.11	39,39,39,39	0
57	MG	1a	1672	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3111	1/1	0.93	0.11	33,33,33,33	0
57	MG	2A	3291	1/1	0.93	0.23	48,48,48,48	0
57	MG	2A	3041	1/1	0.93	0.21	63,63,63,63	0
57	MG	2A	3043	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3494	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3048	1/1	0.93	0.14	63,63,63,63	0
57	MG	2A	3049	1/1	0.93	0.18	63,63,63,63	0
57	MG	1A	3410	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3496	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3602	1/1	0.93	0.09	58,58,58,58	0
57	MG	1a	1679	1/1	0.93	0.21	60,60,60,60	0
57	MG	1A	3629	1/1	0.93	0.11	50,50,50,50	0
57	MG	1A	3630	1/1	0.93	0.07	23,23,23,23	0
57	MG	1A	3794	1/1	0.93	0.06	64,64,64,64	0
57	MG	2A	3609	1/1	0.93	0.15	53,53,53,53	0
57	MG	1B	216	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	3052	1/1	0.93	0.11	46,46,46,46	0
57	MG	1a	1686	1/1	0.93	0.15	51,51,51,51	0
57	MG	2a	1732	1/1	0.93	0.31	56,56,56,56	0
57	MG	1A	3800	1/1	0.93	0.09	20,20,20,20	0
57	MG	2A	3618	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3063	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3315	1/1	0.93	0.30	59,59,59,59	0
57	MG	2A	3064	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3801	1/1	0.93	0.25	74,74,74,74	0
57	MG	1A	3501	1/1	0.93	0.07	46,46,46,46	0
57	MG	2A	3324	1/1	0.93	0.29	61,61,61,61	0
57	MG	2A	3626	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3332	1/1	0.93	0.07	49,49,49,49	0
57	MG	1A	3412	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3337	1/1	0.93	0.12	61,61,61,61	0
57	MG	1A	3970	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3644	1/1	0.93	0.12	38,38,38,38	0
57	MG	1a	1695	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3973	1/1	0.93	0.08	56,56,56,56	0
57	MG	1a	1697	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1698	1/1	0.93	0.06	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	2A	3346	1/1	0.93	0.20	43,43,43,43	0
57	MG	1A	3115	1/1	0.93	0.16	42,42,42,42	0
57	MG	1A	3217	1/1	0.93	0.08	46,46,46,46	0
57	MG	2a	1759	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3349	1/1	0.93	0.23	49,49,49,49	0
57	MG	1D	312	1/1	0.93	0.14	37,37,37,37	0
57	MG	1A	3981	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3352	1/1	0.93	0.15	49,49,49,49	0
57	MG	2A	3095	1/1	0.93	0.39	61,61,61,61	0
57	MG	2a	1765	1/1	0.93	0.46	68,68,68,68	0
57	MG	1A	3515	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3360	1/1	0.93	0.41	63,63,63,63	0
57	MG	1E	312	1/1	0.93	0.10	25,25,25,25	0
57	MG	2A	3672	1/1	0.93	0.08	40,40,40,40	0
57	MG	2A	3365	1/1	0.93	0.33	61,61,61,61	0
57	MG	2A	3684	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3420	1/1	0.93	0.12	41,41,41,41	0
57	MG	1a	1716	1/1	0.93	0.11	57,57,57,57	0
57	MG	1A	3823	1/1	0.93	0.08	61,61,61,61	0
57	MG	1A	3122	1/1	0.93	0.14	45,45,45,45	0
57	MG	1F	312	1/1	0.93	0.15	56,56,56,56	0
57	MG	2A	3695	1/1	0.93	0.10	62,62,62,62	0
57	MG	1G	202	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3697	1/1	0.93	0.06	47,47,47,47	0
57	MG	1A	3999	1/1	0.93	0.07	24,24,24,24	0
57	MG	1A	3224	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3704	1/1	0.93	0.08	53,53,53,53	0
57	MG	1a	1725	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3426	1/1	0.93	0.09	60,60,60,60	0
57	MG	2e	201	1/1	0.93	0.08	72,72,72,72	0
57	MG	1A	4003	1/1	0.93	0.11	74,74,74,74	0
57	MG	2f	202	1/1	0.93	0.18	73,73,73,73	0
57	MG	2A	3124	1/1	0.93	0.18	62,62,62,62	0
57	MG	2l	203	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3709	1/1	0.93	0.20	64,64,64,64	0
57	MG	1O	202	1/1	0.93	0.19	53,53,53,53	0
57	MG	1A	4004	1/1	0.93	0.07	54,54,54,54	0
57	MG	1A	3131	1/1	0.93	0.09	43,43,43,43	0
57	MG	1a	1736	1/1	0.93	0.30	54,54,54,54	0
57	MG	2A	3129	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3138	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3295	1/1	0.93	0.15	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	3718	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3144	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3393	1/1	0.94	0.12	48,48,48,48	0
57	MG	1A	3369	1/1	0.94	0.21	48,48,48,48	0
57	MG	2A	3140	1/1	0.94	0.37	63,63,63,63	0
57	MG	1R	204	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3142	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3097	1/1	0.94	0.06	37,37,37,37	0
57	MG	1a	1746	1/1	0.94	0.19	57,57,57,57	0
57	MG	2A	3406	1/1	0.94	0.10	66,66,66,66	0
57	MG	1A	3674	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3539	1/1	0.94	0.09	38,38,38,38	0
57	MG	1a	1751	1/1	0.94	0.08	54,54,54,54	0
57	MG	1T	201	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3413	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3727	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3443	1/1	0.94	0.23	52,52,52,52	0
57	MG	2A	3159	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3418	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	4017	1/1	0.94	0.05	23,23,23,23	0
57	MG	2A	3161	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	4018	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3371	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3429	1/1	0.94	0.06	48,48,48,48	0
57	MG	1A	3144	1/1	0.94	0.16	46,46,46,46	0
57	MG	2A	3433	1/1	0.94	0.11	56,56,56,56	0
57	MG	1W	202	1/1	0.94	0.10	48,48,48,48	0
57	MG	1a	1769	1/1	0.94	0.08	57,57,57,57	0
57	MG	1Y	201	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3439	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3447	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3448	1/1	0.94	0.17	62,62,62,62	0
57	MG	2A	3173	1/1	0.94	0.26	68,68,68,68	0
57	MG	2A	3443	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3057	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3693	1/1	0.94	0.09	22,22,22,22	0
57	MG	2A	3176	1/1	0.94	0.18	42,42,42,42	0
57	MG	1A	3859	1/1	0.94	0.15	43,43,43,43	0
57	MG	1A	4030	1/1	0.94	0.07	61,61,61,61	0
57	MG	2F	301	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3861	1/1	0.94	0.14	35,35,35,35	0
57	MG	10	105	1/1	0.94	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3195	1/1	0.94	0.25	52,52,52,52	0
57	MG	2O	201	1/1	0.94	0.13	70,70,70,70	0
57	MG	11	105	1/1	0.94	0.10	68,68,68,68	0
57	MG	2T	202	1/1	0.94	0.17	60,60,60,60	0
57	MG	2W	201	1/1	0.94	0.15	40,40,40,40	0
57	MG	2X	101	1/1	0.94	0.10	51,51,51,51	0
57	MG	12	101	1/1	0.94	0.07	39,39,39,39	0
57	MG	1A	3699	1/1	0.94	0.08	31,31,31,31	0
57	MG	14	101	1/1	0.94	0.13	64,64,64,64	0
57	MG	20	103	1/1	0.94	0.14	64,64,64,64	0
57	MG	1A	3062	1/1	0.94	0.21	48,48,48,48	0
57	MG	1A	3377	1/1	0.94	0.36	58,58,58,58	0
57	MG	1a	1812	1/1	0.94	0.11	62,62,62,62	0
57	MG	15	109	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3196	1/1	0.94	0.18	52,52,52,52	0
57	MG	1a	1816	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3472	1/1	0.94	0.10	34,34,34,34	0
57	MG	2a	1605	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3702	1/1	0.94	0.07	26,26,26,26	0
57	MG	1a	1820	1/1	0.94	0.22	51,51,51,51	0
57	MG	1A	3314	1/1	0.94	0.26	59,59,59,59	0
57	MG	1A	3315	1/1	0.94	0.26	54,54,54,54	0
57	MG	1A	3462	1/1	0.94	0.09	61,61,61,61	0
57	MG	1A	3064	1/1	0.94	0.08	47,47,47,47	0
57	MG	2a	1612	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3557	1/1	0.94	0.21	55,55,55,55	0
57	MG	2a	1615	1/1	0.94	0.20	58,58,58,58	0
57	MG	2A	3483	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3711	1/1	0.94	0.10	30,30,30,30	0
57	MG	1A	3880	1/1	0.94	0.18	35,35,35,35	0
57	MG	1A	4052	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3487	1/1	0.94	0.07	44,44,44,44	0
57	MG	1d	301	1/1	0.94	0.25	58,58,58,58	0
57	MG	2A	3489	1/1	0.94	0.10	43,43,43,43	0
57	MG	1e	201	1/1	0.94	0.12	67,67,67,67	0
57	MG	1A	3384	1/1	0.94	0.15	37,37,37,37	0
57	MG	1l	201	1/1	0.94	0.08	65,65,65,65	0
57	MG	2A	3495	1/1	0.94	0.09	38,38,38,38	0
57	MG	1l	202	1/1	0.94	0.09	64,64,64,64	0
57	MG	2A	3497	1/1	0.94	0.18	58,58,58,58	0
57	MG	2a	1632	1/1	0.94	0.28	60,60,60,60	0
57	MG	2A	3219	1/1	0.94	0.16	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	3317	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	3257	1/1	0.94	0.10	27,27,27,27	0
57	MG	1a	1615	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3258	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3509	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	4060	1/1	0.94	0.06	17,17,17,17	0
57	MG	2A	3227	1/1	0.94	0.20	59,59,59,59	0
57	MG	2A	3228	1/1	0.94	0.29	59,59,59,59	0
57	MG	1w	102	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3568	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	4062	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3321	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3521	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3259	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3584	1/1	0.94	0.16	44,44,44,44	0
57	MG	1x	104	1/1	0.94	0.24	68,68,68,68	0
57	MG	1A	4066	1/1	0.94	0.14	46,46,46,46	0
57	MG	2A	3528	1/1	0.94	0.16	63,63,63,63	0
57	MG	1a	1631	1/1	0.94	0.24	62,62,62,62	0
57	MG	1x	107	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	4067	1/1	0.94	0.05	34,34,34,34	0
57	MG	1A	3326	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3588	1/1	0.94	0.30	40,40,40,40	0
57	MG	1A	3067	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3734	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3328	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3248	1/1	0.94	0.19	57,57,57,57	0
57	MG	1A	3206	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3744	1/1	0.94	0.10	49,49,49,49	0
57	MG	2a	1667	1/1	0.94	0.17	52,52,52,52	0
57	MG	1A	3745	1/1	0.94	0.07	48,48,48,48	0
57	MG	1a	1644	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3078	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3002	1/1	0.94	0.26	58,58,58,58	0
57	MG	1A	3333	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1648	1/1	0.94	0.13	49,49,49,49	0
57	MG	1a	1649	1/1	0.94	0.13	45,45,45,45	0
57	MG	2A	3006	1/1	0.94	0.22	46,46,46,46	0
57	MG	1A	3601	1/1	0.94	0.15	36,36,36,36	0
57	MG	1a	1652	1/1	0.94	0.09	45,45,45,45	0
57	MG	1a	1655	1/1	0.94	0.16	54,54,54,54	0
57	MG	2A	3010	1/1	0.94	0.18	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	1682	1/1	0.94	0.17	66,66,66,66	0
57	MG	1A	3749	1/1	0.94	0.07	50,50,50,50	0
57	MG	1A	3166	1/1	0.94	0.20	32,32,32,32	0
57	MG	2A	3023	1/1	0.94	0.27	41,41,41,41	0
57	MG	1A	3058	1/1	0.94	0.19	54,54,54,54	0
57	MG	2A	3027	1/1	0.94	0.08	46,46,46,46	0
57	MG	2a	1690	1/1	0.94	0.24	61,61,61,61	0
57	MG	1a	1660	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3928	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3170	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3276	1/1	0.94	0.13	59,59,59,59	0
57	MG	2A	3567	1/1	0.94	0.07	68,68,68,68	0
57	MG	1A	3218	1/1	0.94	0.20	39,39,39,39	0
57	MG	1A	3413	1/1	0.94	0.13	33,33,33,33	0
57	MG	2A	3281	1/1	0.94	0.11	58,58,58,58	0
57	MG	1A	3765	1/1	0.94	0.07	42,42,42,42	0
57	MG	2a	1700	1/1	0.94	0.21	68,68,68,68	0
57	MG	2a	1701	1/1	0.94	0.06	75,75,75,75	0
57	MG	2A	3037	1/1	0.94	0.21	57,57,57,57	0
57	MG	2A	3287	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3578	1/1	0.94	0.07	28,28,28,28	0
57	MG	1A	3613	1/1	0.94	0.08	36,36,36,36	0
57	MG	1a	1671	1/1	0.94	0.26	58,58,58,58	0
57	MG	1A	3934	1/1	0.94	0.08	32,32,32,32	0
57	MG	1B	201	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3614	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3044	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3768	1/1	0.94	0.08	49,49,49,49	0
57	MG	1a	1677	1/1	0.94	0.13	64,64,64,64	0
57	MG	1A	3618	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3593	1/1	0.94	0.05	47,47,47,47	0
57	MG	1A	3340	1/1	0.94	0.08	51,51,51,51	0
57	MG	2A	3595	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3596	1/1	0.94	0.17	68,68,68,68	0
57	MG	1A	3620	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3273	1/1	0.94	0.19	36,36,36,36	0
57	MG	1A	3087	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3054	1/1	0.94	0.16	51,51,51,51	0
57	MG	2a	1725	1/1	0.94	0.28	66,66,66,66	0
57	MG	2A	3604	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3181	1/1	0.94	0.15	47,47,47,47	0
57	MG	1A	3289	1/1	0.94	0.10	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	1B	219	1/1	0.94	0.13	45,45,45,45	0
57	MG	1A	3958	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3612	1/1	0.94	0.08	41,41,41,41	0
57	MG	1a	1689	1/1	0.94	0.20	60,60,60,60	0
57	MG	1A	3785	1/1	0.94	0.06	36,36,36,36	0
57	MG	1A	3964	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3965	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3225	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3321	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3291	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3423	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3643	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3517	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3336	1/1	0.94	0.28	49,49,49,49	0
57	MG	2a	1743	1/1	0.94	0.20	68,68,68,68	0
57	MG	2a	1744	1/1	0.94	0.29	55,55,55,55	0
57	MG	1A	3518	1/1	0.94	0.14	45,45,45,45	0
57	MG	2a	1746	1/1	0.94	0.21	58,58,58,58	0
57	MG	1a	1701	1/1	0.94	0.28	47,47,47,47	0
57	MG	2A	3078	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3648	1/1	0.94	0.07	40,40,40,40	0
57	MG	1D	301	1/1	0.94	0.18	28,28,28,28	0
57	MG	2A	3634	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3292	1/1	0.94	0.11	60,60,60,60	0
57	MG	2A	3636	1/1	0.94	0.08	51,51,51,51	0
57	MG	1a	1706	1/1	0.94	0.23	58,58,58,58	0
57	MG	2a	1755	1/1	0.94	0.32	60,60,60,60	0
57	MG	1a	1707	1/1	0.94	0.20	57,57,57,57	0
57	MG	2A	3348	1/1	0.94	0.18	58,58,58,58	0
57	MG	2A	3088	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3089	1/1	0.94	0.18	50,50,50,50	0
57	MG	1A	3980	1/1	0.94	0.12	37,37,37,37	0
57	MG	2A	3650	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3092	1/1	0.94	0.15	47,47,47,47	0
57	MG	2A	3652	1/1	0.94	0.10	80,80,80,80	0
57	MG	1A	3522	1/1	0.94	0.15	34,34,34,34	0
57	MG	1A	3527	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3357	1/1	0.94	0.25	64,64,64,64	0
57	MG	2A	3096	1/1	0.94	0.24	51,51,51,51	0
57	MG	2A	3657	1/1	0.94	0.07	65,65,65,65	0
57	MG	2A	3660	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3099	1/1	0.94	0.10	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	2A	3666	1/1	0.94	0.10	54,54,54,54	0
57	MG	2a	1774	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3987	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3235	1/1	0.94	0.08	63,63,63,63	0
57	MG	2A	3362	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3992	1/1	0.94	0.06	68,68,68,68	0
57	MG	2A	3674	1/1	0.94	0.06	50,50,50,50	0
57	MG	2A	3680	1/1	0.94	0.07	69,69,69,69	0
57	MG	1A	3993	1/1	0.94	0.12	64,64,64,64	0
57	MG	1G	201	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3238	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3059	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3661	1/1	0.94	0.08	41,41,41,41	0
57	MG	1I	201	1/1	0.94	0.12	64,64,64,64	0
57	MG	2d	301	1/1	0.94	0.29	56,56,56,56	0
57	MG	1N	201	1/1	0.94	0.20	51,51,51,51	0
57	MG	1A	3998	1/1	0.94	0.12	36,36,36,36	0
57	MG	1A	3185	1/1	0.94	0.13	39,39,39,39	0
57	MG	2A	3377	1/1	0.94	0.27	56,56,56,56	0
57	MG	2A	3698	1/1	0.94	0.08	41,41,41,41	0
57	MG	2q	201	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3004	1/1	0.94	0.08	26,26,26,26	0
57	MG	2r	101	1/1	0.94	0.11	61,61,61,61	0
57	MG	2t	201	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3702	1/1	0.94	0.07	44,44,44,44	0
57	MG	1A	3305	1/1	0.94	0.06	29,29,29,29	0
57	MG	1O	205	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3838	1/1	0.94	0.13	43,43,43,43	0
57	MG	2x	105	1/1	0.94	0.15	54,54,54,54	0
57	MG	1A	3841	1/1	0.94	0.12	40,40,40,40	0
57	MG	1A	4007	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3842	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3133	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3135	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3403	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3143	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3017	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3145	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3146	1/1	0.95	0.18	56,56,56,56	0
57	MG	2A	3147	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3332	1/1	0.95	0.14	42,42,42,42	0
57	MG	2A	3150	1/1	0.95	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3879	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3198	1/1	0.95	0.12	40,40,40,40	0
57	MG	1a	1770	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3155	1/1	0.95	0.08	47,47,47,47	0
57	MG	2A	3420	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3881	1/1	0.95	0.06	29,29,29,29	0
57	MG	2A	3425	1/1	0.95	0.11	43,43,43,43	0
57	MG	1a	1772	1/1	0.95	0.18	68,68,68,68	0
57	MG	1A	3882	1/1	0.95	0.14	34,34,34,34	0
57	MG	1A	3381	1/1	0.95	0.09	49,49,49,49	0
57	MG	2B	208	1/1	0.95	0.18	62,62,62,62	0
57	MG	1A	3334	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	4047	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3163	1/1	0.95	0.18	56,56,56,56	0
57	MG	1a	1780	1/1	0.95	0.08	60,60,60,60	0
57	MG	1l	102	1/1	0.95	0.08	49,49,49,49	0
57	MG	1a	1783	1/1	0.95	0.07	71,71,71,71	0
57	MG	1A	3101	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3103	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3740	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	4051	1/1	0.95	0.12	28,28,28,28	0
57	MG	2D	302	1/1	0.95	0.15	44,44,44,44	0
57	MG	2D	304	1/1	0.95	0.22	62,62,62,62	0
57	MG	1A	3743	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3337	1/1	0.95	0.18	43,43,43,43	0
57	MG	2E	303	1/1	0.95	0.10	43,43,43,43	0
57	MG	2E	304	1/1	0.95	0.23	57,57,57,57	0
57	MG	1A	3621	1/1	0.95	0.11	38,38,38,38	0
57	MG	1a	1795	1/1	0.95	0.09	74,74,74,74	0
57	MG	1A	3525	1/1	0.95	0.12	49,49,49,49	0
57	MG	17	105	1/1	0.95	0.12	54,54,54,54	0
57	MG	1a	1799	1/1	0.95	0.08	55,55,55,55	0
57	MG	18	3401	1/1	0.95	0.16	54,54,54,54	0
57	MG	1a	1804	1/1	0.95	0.07	67,67,67,67	0
57	MG	18	3402	1/1	0.95	0.12	37,37,37,37	0
57	MG	2R	201	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3623	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3186	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3171	1/1	0.95	0.27	41,41,41,41	0
57	MG	19	101	1/1	0.95	0.13	44,44,44,44	0
57	MG	2A	3189	1/1	0.95	0.16	43,43,43,43	0
57	MG	2A	3467	1/1	0.95	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3252	1/1	0.95	0.07	53,53,53,53	0
57	MG	2I	101	1/1	0.95	0.19	52,52,52,52	0
57	MG	1a	1821	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3904	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3194	1/1	0.95	0.09	52,52,52,52	0
57	MG	27	102	1/1	0.95	0.07	46,46,46,46	0
57	MG	27	103	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3750	1/1	0.95	0.06	52,52,52,52	0
57	MG	2a	1601	1/1	0.95	0.15	53,53,53,53	0
57	MG	2A	3474	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3176	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3451	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3633	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3396	1/1	0.95	0.38	46,46,46,46	0
57	MG	1A	3760	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	4070	1/1	0.95	0.07	48,48,48,48	0
57	MG	1a	1614	1/1	0.95	0.29	54,54,54,54	0
57	MG	1A	3055	1/1	0.95	0.20	50,50,50,50	0
57	MG	1e	202	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3206	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	4072	1/1	0.95	0.10	15,15,15,15	0
57	MG	1a	1618	1/1	0.95	0.07	48,48,48,48	0
57	MG	1a	1620	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3920	1/1	0.95	0.12	32,32,32,32	0
57	MG	2A	3213	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3492	1/1	0.95	0.12	56,56,56,56	0
57	MG	1n	101	1/1	0.95	0.30	53,53,53,53	0
57	MG	2A	3494	1/1	0.95	0.07	39,39,39,39	0
57	MG	1n	102	1/1	0.95	0.15	55,55,55,55	0
57	MG	1A	4075	1/1	0.95	0.10	23,23,23,23	0
57	MG	2a	1624	1/1	0.95	0.13	59,59,59,59	0
57	MG	1a	1624	1/1	0.95	0.16	64,64,64,64	0
57	MG	1A	3456	1/1	0.95	0.18	54,54,54,54	0
57	MG	2a	1627	1/1	0.95	0.11	59,59,59,59	0
57	MG	2a	1628	1/1	0.95	0.08	83,83,83,83	0
57	MG	2A	3221	1/1	0.95	0.18	47,47,47,47	0
57	MG	1a	1626	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3502	1/1	0.95	0.10	37,37,37,37	0
57	MG	2A	3503	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3504	1/1	0.95	0.21	59,59,59,59	0
57	MG	1A	3343	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3925	1/1	0.95	0.07	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	1A	4083	1/1	0.95	0.12	43,43,43,43	0
57	MG	2A	3510	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3537	1/1	0.95	0.09	48,48,48,48	0
57	MG	1x	101	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3143	1/1	0.95	0.10	55,55,55,55	0
57	MG	2a	1641	1/1	0.95	0.19	63,63,63,63	0
57	MG	2A	3229	1/1	0.95	0.10	60,60,60,60	0
57	MG	1A	4089	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3345	1/1	0.95	0.18	51,51,51,51	0
57	MG	1A	3306	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3520	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3463	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3774	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	1639	1/1	0.95	0.18	43,43,43,43	0
57	MG	1A	3216	1/1	0.95	0.21	40,40,40,40	0
57	MG	1A	3406	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3656	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3779	1/1	0.95	0.11	26,26,26,26	0
57	MG	2A	3241	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3939	1/1	0.95	0.08	36,36,36,36	0
57	MG	1x	115	1/1	0.95	0.09	68,68,68,68	0
57	MG	1A	3407	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3470	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	4103	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3786	1/1	0.95	0.08	61,61,61,61	0
57	MG	1a	1650	1/1	0.95	0.07	64,64,64,64	0
57	MG	2a	1664	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3790	1/1	0.95	0.06	29,29,29,29	0
57	MG	1A	3792	1/1	0.95	0.14	53,53,53,53	0
57	MG	1A	3024	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3028	1/1	0.95	0.11	39,39,39,39	0
57	MG	2a	1669	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3665	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3220	1/1	0.95	0.07	40,40,40,40	0
57	MG	1B	207	1/1	0.95	0.17	62,62,62,62	0
57	MG	2a	1673	1/1	0.95	0.23	57,57,57,57	0
57	MG	1a	1661	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3258	1/1	0.95	0.15	53,53,53,53	0
57	MG	1a	1662	1/1	0.95	0.12	63,63,63,63	0
57	MG	1A	3962	1/1	0.95	0.08	80,80,80,80	0
57	MG	1A	3802	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	3667	1/1	0.95	0.11	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	1666	1/1	0.95	0.23	65,65,65,65	0
57	MG	1A	3669	1/1	0.95	0.06	31,31,31,31	0
57	MG	1a	1668	1/1	0.95	0.07	57,57,57,57	0
57	MG	2a	1683	1/1	0.95	0.30	64,64,64,64	0
57	MG	1A	3221	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3152	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3032	1/1	0.95	0.04	33,33,33,33	0
57	MG	1A	3969	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3272	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3051	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3162	1/1	0.95	0.27	33,33,33,33	0
57	MG	1A	3482	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3416	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3226	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3488	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3978	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3573	1/1	0.95	0.10	57,57,57,57	0
57	MG	2A	3282	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3283	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3042	1/1	0.95	0.08	54,54,54,54	0
57	MG	1B	231	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3824	1/1	0.95	0.15	55,55,55,55	0
57	MG	1A	3825	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3982	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3585	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3984	1/1	0.95	0.08	56,56,56,56	0
57	MG	2A	3587	1/1	0.95	0.07	46,46,46,46	0
57	MG	1D	302	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3292	1/1	0.95	0.25	49,49,49,49	0
57	MG	1D	311	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3295	1/1	0.95	0.13	36,36,36,36	0
57	MG	1a	1688	1/1	0.95	0.12	64,64,64,64	0
57	MG	1A	3985	1/1	0.95	0.06	62,62,62,62	0
57	MG	2A	3298	1/1	0.95	0.38	58,58,58,58	0
57	MG	1A	3687	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3230	1/1	0.95	0.08	40,40,40,40	0
57	MG	1E	306	1/1	0.95	0.12	29,29,29,29	0
57	MG	1A	3366	1/1	0.95	0.13	49,49,49,49	0
57	MG	1E	309	1/1	0.95	0.16	53,53,53,53	0
57	MG	1E	310	1/1	0.95	0.24	69,69,69,69	0
57	MG	2A	3305	1/1	0.95	0.35	67,67,67,67	0
57	MG	1E	311	1/1	0.95	0.09	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	3835	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3492	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3319	1/1	0.95	0.11	51,51,51,51	0
57	MG	2A	3066	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3068	1/1	0.95	0.10	29,29,29,29	0
57	MG	1F	304	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3694	1/1	0.95	0.06	36,36,36,36	0
57	MG	1F	309	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3575	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3620	1/1	0.95	0.08	43,43,43,43	0
57	MG	2A	3319	1/1	0.95	0.23	56,56,56,56	0
57	MG	1A	3579	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3580	1/1	0.95	0.29	40,40,40,40	0
57	MG	1A	4000	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3582	1/1	0.95	0.29	39,39,39,39	0
57	MG	2A	3334	1/1	0.95	0.23	55,55,55,55	0
57	MG	2A	3081	1/1	0.95	0.05	34,34,34,34	0
57	MG	1a	1711	1/1	0.95	0.21	57,57,57,57	0
57	MG	1G	205	1/1	0.95	0.07	53,53,53,53	0
57	MG	2A	3338	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3633	1/1	0.95	0.05	34,34,34,34	0
57	MG	1a	1713	1/1	0.95	0.30	57,57,57,57	0
57	MG	1A	3189	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3119	1/1	0.95	0.10	40,40,40,40	0
57	MG	1N	202	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3849	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3639	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3704	1/1	0.95	0.09	21,21,21,21	0
57	MG	2A	3642	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3345	1/1	0.95	0.25	54,54,54,54	0
57	MG	1A	3276	1/1	0.95	0.06	40,40,40,40	0
57	MG	2a	1757	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3647	1/1	0.95	0.09	53,53,53,53	0
57	MG	1O	203	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3649	1/1	0.95	0.06	53,53,53,53	0
57	MG	2A	3349	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3236	1/1	0.95	0.15	27,27,27,27	0
57	MG	2A	3098	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3288	1/1	0.95	0.20	46,46,46,46	0
57	MG	2A	3353	1/1	0.95	0.33	61,61,61,61	0
57	MG	1A	3502	1/1	0.95	0.08	60,60,60,60	0
57	MG	1A	3595	1/1	0.95	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3102	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	4013	1/1	0.95	0.11	53,53,53,53	0
57	MG	1Q	204	1/1	0.95	0.11	54,54,54,54	0
57	MG	2A	3665	1/1	0.95	0.10	45,45,45,45	0
57	MG	2a	1772	1/1	0.95	0.15	57,57,57,57	0
57	MG	2A	3105	1/1	0.95	0.07	48,48,48,48	0
57	MG	2A	3106	1/1	0.95	0.10	50,50,50,50	0
57	MG	1a	1731	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3108	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3504	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3713	1/1	0.95	0.05	14,14,14,14	0
57	MG	1A	3715	1/1	0.95	0.05	25,25,25,25	0
57	MG	1A	3506	1/1	0.95	0.09	41,41,41,41	0
57	MG	2A	3683	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3118	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3865	1/1	0.95	0.08	17,17,17,17	0
57	MG	1A	3718	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3042	1/1	0.95	0.21	30,30,30,30	0
57	MG	1A	4026	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3602	1/1	0.95	0.14	37,37,37,37	0
57	MG	1U	203	1/1	0.95	0.14	28,28,28,28	0
57	MG	1a	1747	1/1	0.95	0.17	57,57,57,57	0
57	MG	2A	3379	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3721	1/1	0.95	0.06	45,45,45,45	0
57	MG	1V	202	1/1	0.95	0.29	38,38,38,38	0
57	MG	1A	3871	1/1	0.95	0.05	35,35,35,35	0
57	MG	2A	3130	1/1	0.95	0.15	58,58,58,58	0
57	MG	2A	3132	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3434	1/1	0.95	0.28	52,52,52,52	0
57	MG	2A	3134	1/1	0.95	0.10	59,59,59,59	0
57	MG	2A	3389	1/1	0.95	0.06	24,24,24,24	0
57	MG	2x	101	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3606	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3137	1/1	0.95	0.15	58,58,58,58	0
57	MG	1a	1756	1/1	0.95	0.11	56,56,56,56	0
57	MG	2A	3139	1/1	0.95	0.09	37,37,37,37	0
57	MG	1a	1757	1/1	0.95	0.09	73,73,73,73	0
57	MG	1X	101	1/1	0.95	0.31	38,38,38,38	0
57	MG	1A	3130	1/1	0.95	0.13	74,74,74,74	0
57	MG	2A	3401	1/1	0.95	0.08	44,44,44,44	0
57	MG	1B	218	1/1	0.96	0.11	60,60,60,60	0
57	MG	1A	3102	1/1	0.96	0.25	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	1B	220	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3081	1/1	0.96	0.15	41,41,41,41	0
57	MG	1A	3658	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3082	1/1	0.96	0.20	42,42,42,42	0
57	MG	1A	3322	1/1	0.96	0.13	29,29,29,29	0
57	MG	2A	3471	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3805	1/1	0.96	0.05	19,19,19,19	0
57	MG	1A	3083	1/1	0.96	0.19	38,38,38,38	0
57	MG	2D	301	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3112	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3047	1/1	0.96	0.11	28,28,28,28	0
57	MG	2D	306	1/1	0.96	0.31	42,42,42,42	0
57	MG	1A	3544	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3668	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3002	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3546	1/1	0.96	0.20	41,41,41,41	0
57	MG	2A	3011	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3234	1/1	0.96	0.08	61,61,61,61	0
57	MG	2A	3015	1/1	0.96	0.11	46,46,46,46	0
57	MG	1B	236	1/1	0.96	0.07	40,40,40,40	0
57	MG	2F	304	1/1	0.96	0.24	47,47,47,47	0
57	MG	2F	305	1/1	0.96	0.28	47,47,47,47	0
57	MG	2A	3017	1/1	0.96	0.15	56,56,56,56	0
57	MG	2A	3018	1/1	0.96	0.07	41,41,41,41	0
57	MG	2N	201	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3329	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3022	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3461	1/1	0.96	0.06	38,38,38,38	0
57	MG	2T	201	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3024	1/1	0.96	0.07	40,40,40,40	0
57	MG	2T	203	1/1	0.96	0.10	48,48,48,48	0
57	MG	1D	305	1/1	0.96	0.08	35,35,35,35	0
57	MG	1D	308	1/1	0.96	0.07	48,48,48,48	0
57	MG	2Y	201	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3167	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3270	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3826	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3551	1/1	0.96	0.07	17,17,17,17	0
57	MG	1A	3464	1/1	0.96	0.21	48,48,48,48	0
57	MG	23	102	1/1	0.96	0.07	59,59,59,59	0
57	MG	1A	3466	1/1	0.96	0.21	49,49,49,49	0
57	MG	25	102	1/1	0.96	0.20	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	3500	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3990	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3831	1/1	0.96	0.04	24,24,24,24	0
57	MG	1A	3832	1/1	0.96	0.07	27,27,27,27	0
57	MG	28	101	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3833	1/1	0.96	0.08	31,31,31,31	0
57	MG	28	103	1/1	0.96	0.09	75,75,75,75	0
57	MG	2A	3505	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3995	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3834	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3508	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3684	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3685	1/1	0.96	0.08	21,21,21,21	0
57	MG	2A	3511	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3394	1/1	0.96	0.19	24,24,24,24	0
57	MG	1F	310	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3840	1/1	0.96	0.09	55,55,55,55	0
57	MG	2A	3515	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3271	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3690	1/1	0.96	0.08	56,56,56,56	0
57	MG	2a	1614	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3556	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3117	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3088	1/1	0.96	0.11	34,34,34,34	0
57	MG	1a	1700	1/1	0.96	0.18	45,45,45,45	0
57	MG	2A	3270	1/1	0.96	0.19	49,49,49,49	0
57	MG	1A	3120	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3056	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3399	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3526	1/1	0.96	0.12	49,49,49,49	0
57	MG	2A	3527	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3698	1/1	0.96	0.06	22,22,22,22	0
57	MG	1N	204	1/1	0.96	0.12	51,51,51,51	0
57	MG	1a	1705	1/1	0.96	0.24	49,49,49,49	0
57	MG	2A	3277	1/1	0.96	0.16	61,61,61,61	0
57	MG	1A	3475	1/1	0.96	0.06	47,47,47,47	0
57	MG	2A	3279	1/1	0.96	0.21	68,68,68,68	0
57	MG	1N	206	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3563	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3536	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3853	1/1	0.96	0.05	55,55,55,55	0
57	MG	1A	3172	1/1	0.96	0.09	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	2A	3284	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	4015	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3571	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3477	1/1	0.96	0.12	51,51,51,51	0
57	MG	1P	203	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3281	1/1	0.96	0.15	28,28,28,28	0
57	MG	1A	3858	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	4022	1/1	0.96	0.04	30,30,30,30	0
57	MG	1A	3010	1/1	0.96	0.06	39,39,39,39	0
57	MG	1Q	206	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3294	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3179	1/1	0.96	0.12	34,34,34,34	0
57	MG	1R	203	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3862	1/1	0.96	0.16	56,56,56,56	0
57	MG	1A	3227	1/1	0.96	0.21	36,36,36,36	0
57	MG	2A	3557	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3709	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3341	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3866	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3090	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3228	1/1	0.96	0.23	24,24,24,24	0
57	MG	1A	3129	1/1	0.96	0.10	31,31,31,31	0
57	MG	2A	3093	1/1	0.96	0.23	57,57,57,57	0
57	MG	1A	3487	1/1	0.96	0.12	39,39,39,39	0
57	MG	1U	205	1/1	0.96	0.11	30,30,30,30	0
57	MG	1a	1737	1/1	0.96	0.20	44,44,44,44	0
57	MG	2A	3310	1/1	0.96	0.25	53,53,53,53	0
57	MG	2A	3097	1/1	0.96	0.17	62,62,62,62	0
57	MG	1a	1738	1/1	0.96	0.26	62,62,62,62	0
57	MG	1A	3714	1/1	0.96	0.10	42,42,42,42	0
57	MG	1a	1740	1/1	0.96	0.21	57,57,57,57	0
57	MG	1A	3231	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3576	1/1	0.96	0.07	70,70,70,70	0
57	MG	2A	3577	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3091	1/1	0.96	0.15	25,25,25,25	0
57	MG	2A	3317	1/1	0.96	0.07	53,53,53,53	0
57	MG	1V	206	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3346	1/1	0.96	0.15	41,41,41,41	0
57	MG	2A	3320	1/1	0.96	0.26	55,55,55,55	0
57	MG	1A	4043	1/1	0.96	0.06	42,42,42,42	0
57	MG	1W	204	1/1	0.96	0.08	35,35,35,35	0
57	MG	1W	206	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	2A	3325	1/1	0.96	0.10	54,54,54,54	0
57	MG	2A	3326	1/1	0.96	0.09	65,65,65,65	0
57	MG	2A	3329	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3875	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3333	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3491	1/1	0.96	0.22	57,57,57,57	0
57	MG	1A	3234	1/1	0.96	0.21	42,42,42,42	0
57	MG	2A	3113	1/1	0.96	0.07	42,42,42,42	0
57	MG	2a	1688	1/1	0.96	0.20	62,62,62,62	0
57	MG	1A	3013	1/1	0.96	0.17	30,30,30,30	0
57	MG	2A	3600	1/1	0.96	0.10	57,57,57,57	0
57	MG	1A	3019	1/1	0.96	0.19	43,43,43,43	0
57	MG	2A	3117	1/1	0.96	0.26	52,52,52,52	0
57	MG	1A	3351	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3418	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3725	1/1	0.96	0.04	16,16,16,16	0
57	MG	1A	3184	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3500	1/1	0.96	0.15	49,49,49,49	0
57	MG	2A	3608	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3302	1/1	0.96	0.31	54,54,54,54	0
57	MG	2A	3610	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3611	1/1	0.96	0.14	55,55,55,55	0
57	MG	1a	1764	1/1	0.96	0.11	54,54,54,54	0
57	MG	2A	3347	1/1	0.96	0.17	39,39,39,39	0
57	MG	1a	1766	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	4056	1/1	0.96	0.07	44,44,44,44	0
57	MG	11	103	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3356	1/1	0.96	0.07	46,46,46,46	0
57	MG	2a	1708	1/1	0.96	0.24	60,60,60,60	0
57	MG	1A	3303	1/1	0.96	0.16	38,38,38,38	0
57	MG	12	102	1/1	0.96	0.19	43,43,43,43	0
57	MG	13	102	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3612	1/1	0.96	0.08	24,24,24,24	0
57	MG	13	104	1/1	0.96	0.07	51,51,51,51	0
57	MG	2A	3136	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3095	1/1	0.96	0.04	32,32,32,32	0
57	MG	15	102	1/1	0.96	0.10	35,35,35,35	0
57	MG	15	104	1/1	0.96	0.24	28,28,28,28	0
57	MG	1A	3425	1/1	0.96	0.07	40,40,40,40	0
57	MG	15	107	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3363	1/1	0.96	0.19	57,57,57,57	0
57	MG	1A	3896	1/1	0.96	0.09	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	1723	1/1	0.96	0.25	61,61,61,61	0
57	MG	1A	3615	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3617	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3136	1/1	0.96	0.11	28,28,28,28	0
57	MG	1a	1789	1/1	0.96	0.05	55,55,55,55	0
57	MG	1A	3360	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3043	1/1	0.96	0.12	34,34,34,34	0
57	MG	1a	1794	1/1	0.96	0.06	56,56,56,56	0
57	MG	18	3404	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	4069	1/1	0.96	0.05	39,39,39,39	0
57	MG	2A	3644	1/1	0.96	0.04	54,54,54,54	0
57	MG	1A	3513	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3432	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3362	1/1	0.96	0.09	51,51,51,51	0
57	MG	2A	3380	1/1	0.96	0.07	54,54,54,54	0
57	MG	2A	3381	1/1	0.96	0.08	60,60,60,60	0
57	MG	1a	1801	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3911	1/1	0.96	0.09	46,46,46,46	0
57	MG	1a	1809	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	3913	1/1	0.96	0.12	36,36,36,36	0
57	MG	1a	1604	1/1	0.96	0.16	54,54,54,54	0
57	MG	1A	4076	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	4078	1/1	0.96	0.05	28,28,28,28	0
57	MG	1a	1819	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	4079	1/1	0.96	0.15	55,55,55,55	0
57	MG	2A	3663	1/1	0.96	0.07	58,58,58,58	0
57	MG	2A	3392	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3625	1/1	0.96	0.05	37,37,37,37	0
57	MG	1a	1611	1/1	0.96	0.11	28,28,28,28	0
57	MG	2A	3169	1/1	0.96	0.13	62,62,62,62	0
57	MG	2A	3670	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3516	1/1	0.96	0.15	35,35,35,35	0
57	MG	1a	1825	1/1	0.96	0.09	49,49,49,49	0
57	MG	2A	3673	1/1	0.96	0.05	55,55,55,55	0
57	MG	2A	3172	1/1	0.96	0.07	51,51,51,51	0
57	MG	2A	3675	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3755	1/1	0.96	0.06	17,17,17,17	0
57	MG	1A	3628	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3682	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3757	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	4087	1/1	0.96	0.19	55,55,55,55	0
57	MG	1a	1617	1/1	0.96	0.07	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	3139	1/1	0.96	0.09	39,39,39,39	0
57	MG	1a	1619	1/1	0.96	0.07	54,54,54,54	0
57	MG	1A	3759	1/1	0.96	0.04	33,33,33,33	0
57	MG	1A	3141	1/1	0.96	0.07	20,20,20,20	0
57	MG	1A	3033	1/1	0.96	0.11	27,27,27,27	0
57	MG	2A	3183	1/1	0.96	0.21	58,58,58,58	0
57	MG	2A	3184	1/1	0.96	0.21	37,37,37,37	0
57	MG	1A	3367	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3072	1/1	0.96	0.24	52,52,52,52	0
57	MG	2A	3421	1/1	0.96	0.10	40,40,40,40	0
57	MG	1A	3313	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3424	1/1	0.96	0.07	33,33,33,33	0
57	MG	1m	3001	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3636	1/1	0.96	0.09	24,24,24,24	0
57	MG	2A	3427	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3638	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3639	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3640	1/1	0.96	0.04	19,19,19,19	0
57	MG	1A	3936	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3440	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3528	1/1	0.96	0.15	47,47,47,47	0
57	MG	2A	3437	1/1	0.96	0.10	45,45,45,45	0
57	MG	1a	1635	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3646	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	4106	1/1	0.96	0.12	43,43,43,43	0
57	MG	1A	3441	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3146	1/1	0.96	0.17	29,29,29,29	0
57	MG	1A	3046	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3201	1/1	0.96	0.07	32,32,32,32	0
57	MG	2q	202	1/1	0.96	0.05	75,75,75,75	0
57	MG	2A	3204	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3952	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3447	1/1	0.96	0.04	39,39,39,39	0
57	MG	1B	205	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3729	1/1	0.96	0.10	59,59,59,59	0
57	MG	2A	3450	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3953	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3150	1/1	0.96	0.15	32,32,32,32	0
57	MG	2x	104	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	3446	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3791	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3654	1/1	0.96	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3203	1/1	0.96	0.09	22,22,22,22	0
58	6IF	2A	3731	32/32	0.96	0.08	28,36,41,45	0
59	ZN	14	102	1/1	0.96	0.08	97,97,97,97	0
57	MG	2A	3215	1/1	0.96	0.06	54,54,54,54	0
59	ZN	2n	501	1/1	0.96	0.07	95,95,95,95	0
57	MG	1A	3797	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3324	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3219	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3991	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3105	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3107	1/1	0.97	0.29	34,34,34,34	0
57	MG	1A	3380	1/1	0.97	0.24	40,40,40,40	0
57	MG	1A	3108	1/1	0.97	0.14	26,26,26,26	0
57	MG	2A	3154	1/1	0.97	0.07	41,41,41,41	0
57	MG	1B	235	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3109	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3568	1/1	0.97	0.05	58,58,58,58	0
57	MG	1A	3523	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	3140	1/1	0.97	0.09	27,27,27,27	0
57	MG	1D	304	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3624	1/1	0.97	0.07	21,21,21,21	0
57	MG	1D	307	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3054	1/1	0.97	0.12	35,35,35,35	0
57	MG	1D	309	1/1	0.97	0.06	42,42,42,42	0
57	MG	1D	310	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3386	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3387	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3729	1/1	0.97	0.13	44,44,44,44	0
57	MG	2A	3580	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3730	1/1	0.97	0.06	53,53,53,53	0
57	MG	2A	3364	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	4005	1/1	0.97	0.06	38,38,38,38	0
57	MG	1a	1656	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4006	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3066	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3452	1/1	0.97	0.20	36,36,36,36	0
57	MG	1A	3631	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3389	1/1	0.97	0.08	43,43,43,43	0
57	MG	1E	313	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3390	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3738	1/1	0.97	0.09	52,52,52,52	0
57	MG	1E	316	1/1	0.97	0.06	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	1F	301	1/1	0.97	0.20	39,39,39,39	0
57	MG	1x	109	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3739	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3455	1/1	0.97	0.11	30,30,30,30	0
57	MG	1A	3279	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3392	1/1	0.97	0.17	37,37,37,37	0
57	MG	1F	311	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3458	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3094	1/1	0.97	0.14	34,34,34,34	0
57	MG	1a	1674	1/1	0.97	0.23	66,66,66,66	0
57	MG	1A	3284	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3642	1/1	0.97	0.05	23,23,23,23	0
57	MG	1A	3285	1/1	0.97	0.14	44,44,44,44	0
57	MG	1A	3286	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3645	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3287	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3044	1/1	0.97	0.06	38,38,38,38	0
57	MG	2a	1652	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3396	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3465	1/1	0.97	0.16	54,54,54,54	0
57	MG	1A	3116	1/1	0.97	0.19	30,30,30,30	0
57	MG	2A	3399	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3883	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	3084	1/1	0.97	0.15	27,27,27,27	0
57	MG	2A	3402	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3885	1/1	0.97	0.22	39,39,39,39	0
57	MG	1A	3651	1/1	0.97	0.04	15,15,15,15	0
57	MG	2a	1662	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3012	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3013	1/1	0.97	0.05	53,53,53,53	0
57	MG	2A	3014	1/1	0.97	0.10	45,45,45,45	0
57	MG	2A	3208	1/1	0.97	0.11	58,58,58,58	0
57	MG	2A	3629	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3887	1/1	0.97	0.14	30,30,30,30	0
57	MG	2A	3631	1/1	0.97	0.11	56,56,56,56	0
57	MG	2A	3411	1/1	0.97	0.10	44,44,44,44	0
57	MG	2A	3412	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3233	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3211	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3416	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3190	1/1	0.97	0.12	33,33,33,33	0
57	MG	1P	201	1/1	0.97	0.13	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	3019	1/1	0.97	0.10	30,30,30,30	0
57	MG	2A	3020	1/1	0.97	0.17	51,51,51,51	0
57	MG	1A	3403	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3404	1/1	0.97	0.21	29,29,29,29	0
57	MG	1A	3008	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3193	1/1	0.97	0.22	37,37,37,37	0
57	MG	2A	3025	1/1	0.97	0.20	56,56,56,56	0
57	MG	1A	3237	1/1	0.97	0.18	30,30,30,30	0
57	MG	1A	3898	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3153	1/1	0.97	0.07	37,37,37,37	0
57	MG	1R	202	1/1	0.97	0.21	46,46,46,46	0
57	MG	2A	3432	1/1	0.97	0.08	68,68,68,68	0
57	MG	1A	3409	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3773	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3902	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3034	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3240	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3659	1/1	0.97	0.06	77,77,77,77	0
57	MG	1A	3775	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	4055	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3664	1/1	0.97	0.06	50,50,50,50	0
57	MG	2A	3664	1/1	0.97	0.05	48,48,48,48	0
57	MG	1A	4057	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3558	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3300	1/1	0.97	0.21	45,45,45,45	0
57	MG	1U	206	1/1	0.97	0.25	33,33,33,33	0
57	MG	1A	3910	1/1	0.97	0.10	52,52,52,52	0
57	MG	1A	3350	1/1	0.97	0.26	37,37,37,37	0
57	MG	2A	3046	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3780	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3243	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3783	1/1	0.97	0.07	17,17,17,17	0
57	MG	2A	3678	1/1	0.97	0.05	50,50,50,50	0
57	MG	1a	1718	1/1	0.97	0.20	70,70,70,70	0
57	MG	1A	3784	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3456	1/1	0.97	0.09	55,55,55,55	0
57	MG	2a	1713	1/1	0.97	0.17	62,62,62,62	0
57	MG	1W	203	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3154	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3459	1/1	0.97	0.07	41,41,41,41	0
57	MG	1W	205	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3688	1/1	0.97	0.06	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	3157	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3787	1/1	0.97	0.06	45,45,45,45	0
57	MG	1X	105	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3788	1/1	0.97	0.04	21,21,21,21	0
57	MG	1A	3197	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3672	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3927	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3569	1/1	0.97	0.17	44,44,44,44	0
57	MG	1A	3793	1/1	0.97	0.08	25,25,25,25	0
57	MG	10	101	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3099	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3067	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3795	1/1	0.97	0.08	43,43,43,43	0
57	MG	10	104	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3796	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3072	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3480	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3675	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3074	1/1	0.97	0.14	55,55,55,55	0
57	MG	2A	3713	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3159	1/1	0.97	0.17	29,29,29,29	0
57	MG	1A	3935	1/1	0.97	0.06	68,68,68,68	0
57	MG	1A	3573	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	4085	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3678	1/1	0.97	0.04	22,22,22,22	0
57	MG	13	101	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3121	1/1	0.97	0.16	38,38,38,38	0
57	MG	2A	3721	1/1	0.97	0.17	45,45,45,45	0
57	MG	1A	3075	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3084	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3804	1/1	0.97	0.05	36,36,36,36	0
57	MG	2A	3086	1/1	0.97	0.12	34,34,34,34	0
57	MG	1a	1753	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3204	1/1	0.97	0.07	34,34,34,34	0
57	MG	15	101	1/1	0.97	0.18	26,26,26,26	0
57	MG	1A	3126	1/1	0.97	0.22	36,36,36,36	0
57	MG	15	103	1/1	0.97	0.17	29,29,29,29	0
57	MG	1A	3946	1/1	0.97	0.04	53,53,53,53	0
57	MG	1A	3127	1/1	0.97	0.26	40,40,40,40	0
57	MG	1a	1761	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3951	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3424	1/1	0.97	0.25	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	1A	3810	1/1	0.97	0.04	36,36,36,36	0
57	MG	17	101	1/1	0.97	0.04	29,29,29,29	0
57	MG	1a	1768	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3364	1/1	0.97	0.10	43,43,43,43	0
57	MG	1A	3128	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	3815	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3818	1/1	0.97	0.27	26,26,26,26	0
57	MG	18	3403	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	4102	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3499	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	4104	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3427	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3109	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3963	1/1	0.97	0.06	54,54,54,54	0
57	MG	2D	303	1/1	0.97	0.10	51,51,51,51	0
57	MG	1a	1782	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3821	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3077	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3209	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3308	1/1	0.97	0.17	52,52,52,52	0
57	MG	1A	3697	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3503	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3431	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	1608	1/1	0.97	0.07	50,50,50,50	0
57	MG	1a	1790	1/1	0.97	0.07	73,73,73,73	0
57	MG	1a	1609	1/1	0.97	0.20	48,48,48,48	0
57	MG	1A	3599	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3505	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3210	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3830	1/1	0.97	0.07	32,32,32,32	0
57	MG	1A	3603	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3507	1/1	0.97	0.13	38,38,38,38	0
57	MG	1B	213	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3322	1/1	0.97	0.22	48,48,48,48	0
57	MG	2A	3131	1/1	0.97	0.14	38,38,38,38	0
57	MG	1B	214	1/1	0.97	0.10	44,44,44,44	0
57	MG	1a	1803	1/1	0.97	0.12	68,68,68,68	0
57	MG	1B	215	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3327	1/1	0.97	0.07	41,41,41,41	0
57	MG	2A	3328	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3015	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3979	1/1	0.97	0.09	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3546	1/1	0.97	0.22	41,41,41,41	0
57	MG	1A	3090	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3608	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3080	1/1	0.97	0.12	38,38,38,38	0
57	MG	1a	1818	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3133	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3512	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3267	1/1	0.97	0.10	31,31,31,31	0
57	MG	1B	226	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3323	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	3200	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	3598	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3037	1/1	0.98	0.18	31,31,31,31	0
57	MG	1A	3600	1/1	0.98	0.13	35,35,35,35	0
57	MG	2A	3367	1/1	0.98	0.18	39,39,39,39	0
57	MG	1A	3254	1/1	0.98	0.05	32,32,32,32	0
57	MG	1P	206	1/1	0.98	0.14	50,50,50,50	0
57	MG	1Q	201	1/1	0.98	0.09	29,29,29,29	0
57	MG	1Q	202	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3123	1/1	0.98	0.14	31,31,31,31	0
57	MG	1A	3382	1/1	0.98	0.11	34,34,34,34	0
57	MG	1A	3124	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3605	1/1	0.98	0.07	29,29,29,29	0
57	MG	2A	3376	1/1	0.98	0.24	47,47,47,47	0
57	MG	1A	3160	1/1	0.98	0.17	27,27,27,27	0
57	MG	1A	3161	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3814	1/1	0.98	0.03	22,22,22,22	0
57	MG	1A	3125	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3705	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3450	1/1	0.98	0.12	32,32,32,32	0
57	MG	2A	3191	1/1	0.98	0.19	36,36,36,36	0
57	MG	1A	3260	1/1	0.98	0.08	53,53,53,53	0
57	MG	1A	3940	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3521	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	4077	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3076	1/1	0.98	0.08	33,33,33,33	0
57	MG	1U	204	1/1	0.98	0.19	32,32,32,32	0
57	MG	1A	3020	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3022	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3599	1/1	0.98	0.04	36,36,36,36	0
57	MG	1U	207	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3948	1/1	0.98	0.04	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1699	1/1	0.98	0.15	44,44,44,44	0
57	MG	1A	3949	1/1	0.98	0.04	30,30,30,30	0
57	MG	1V	203	1/1	0.98	0.14	30,30,30,30	0
57	MG	1V	204	1/1	0.98	0.11	30,30,30,30	0
57	MG	1A	3041	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	4084	1/1	0.98	0.03	32,32,32,32	0
57	MG	1A	3616	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3211	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3266	1/1	0.98	0.14	41,41,41,41	0
57	MG	1A	3954	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3405	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3056	1/1	0.98	0.05	28,28,28,28	0
57	MG	2A	3614	1/1	0.98	0.16	45,45,45,45	0
57	MG	1A	3213	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	4091	1/1	0.98	0.06	57,57,57,57	0
57	MG	1X	102	1/1	0.98	0.05	27,27,27,27	0
57	MG	1X	104	1/1	0.98	0.12	33,33,33,33	0
57	MG	1A	3214	1/1	0.98	0.08	47,47,47,47	0
57	MG	1A	3168	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3003	1/1	0.98	0.04	28,28,28,28	0
57	MG	2A	3414	1/1	0.98	0.04	55,55,55,55	0
57	MG	2A	3220	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3961	1/1	0.98	0.04	52,52,52,52	0
57	MG	1Y	204	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3025	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3001	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3836	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3275	1/1	0.98	0.15	39,39,39,39	0
57	MG	1A	3134	1/1	0.98	0.06	25,25,25,25	0
57	MG	2A	3423	1/1	0.98	0.10	26,26,26,26	0
57	MG	1A	3839	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3174	1/1	0.98	0.16	25,25,25,25	0
57	MG	1a	1727	1/1	0.98	0.23	40,40,40,40	0
57	MG	1A	3727	1/1	0.98	0.07	27,27,27,27	0
57	MG	10	106	1/1	0.98	0.05	46,46,46,46	0
57	MG	2A	3045	1/1	0.98	0.12	26,26,26,26	0
57	MG	2A	3430	1/1	0.98	0.08	34,34,34,34	0
57	MG	1a	1730	1/1	0.98	0.14	43,43,43,43	0
57	MG	1A	3222	1/1	0.98	0.14	28,28,28,28	0
57	MG	2A	3641	1/1	0.98	0.05	52,52,52,52	0
57	MG	1a	1732	1/1	0.98	0.13	42,42,42,42	0
57	MG	1a	1733	1/1	0.98	0.25	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	11	101	1/1	0.98	0.28	39,39,39,39	0
57	MG	2A	3436	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3843	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3280	1/1	0.98	0.21	38,38,38,38	0
57	MG	11	104	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3009	1/1	0.98	0.03	22,22,22,22	0
57	MG	1A	4108	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3283	1/1	0.98	0.44	35,35,35,35	0
57	MG	1A	3976	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3732	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3472	1/1	0.98	0.21	31,31,31,31	0
57	MG	1A	3473	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3249	1/1	0.98	0.05	49,49,49,49	0
57	MG	2A	3448	1/1	0.98	0.09	42,42,42,42	0
57	MG	2A	3061	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3661	1/1	0.98	0.04	62,62,62,62	0
57	MG	1A	3177	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3851	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3637	1/1	0.98	0.04	42,42,42,42	0
57	MG	2A	3453	1/1	0.98	0.04	24,24,24,24	0
57	MG	1B	209	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3737	1/1	0.98	0.04	52,52,52,52	0
57	MG	1a	1750	1/1	0.98	0.10	44,44,44,44	0
57	MG	2A	3669	1/1	0.98	0.08	41,41,41,41	0
57	MG	1A	3178	1/1	0.98	0.04	31,31,31,31	0
57	MG	15	106	1/1	0.98	0.06	29,29,29,29	0
57	MG	2A	3070	1/1	0.98	0.04	46,46,46,46	0
57	MG	1A	3005	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3110	1/1	0.98	0.19	34,34,34,34	0
57	MG	1a	1755	1/1	0.98	0.10	43,43,43,43	0
57	MG	2A	3677	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3741	1/1	0.98	0.06	26,26,26,26	0
57	MG	16	101	1/1	0.98	0.04	47,47,47,47	0
57	MG	1A	3989	1/1	0.98	0.10	57,57,57,57	0
57	MG	17	102	1/1	0.98	0.14	24,24,24,24	0
57	MG	2A	3267	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3641	1/1	0.98	0.05	29,29,29,29	0
57	MG	2A	3079	1/1	0.98	0.12	54,54,54,54	0
57	MG	17	104	1/1	0.98	0.07	31,31,31,31	0
57	MG	1B	217	1/1	0.98	0.05	34,34,34,34	0
57	MG	2A	3689	1/1	0.98	0.06	64,64,64,64	0
57	MG	1A	3138	1/1	0.98	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3691	1/1	0.98	0.05	30,30,30,30	0
57	MG	1a	1765	1/1	0.98	0.04	61,61,61,61	0
57	MG	2A	3693	1/1	0.98	0.03	63,63,63,63	0
57	MG	1A	3860	1/1	0.98	0.07	15,15,15,15	0
57	MG	1A	3229	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3031	1/1	0.98	0.12	30,30,30,30	0
57	MG	1A	3032	1/1	0.98	0.26	26,26,26,26	0
57	MG	1A	3354	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3699	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3113	1/1	0.98	0.06	33,33,33,33	0
57	MG	1B	225	1/1	0.98	0.07	36,36,36,36	0
57	MG	1a	1774	1/1	0.98	0.03	50,50,50,50	0
57	MG	1a	1775	1/1	0.98	0.07	51,51,51,51	0
57	MG	1A	3142	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3486	1/1	0.98	0.09	41,41,41,41	0
57	MG	1A	3753	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3186	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	3065	1/1	0.98	0.12	36,36,36,36	0
57	MG	1A	3011	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3872	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3145	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3299	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3564	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	3565	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3566	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3762	1/1	0.98	0.03	40,40,40,40	0
57	MG	1D	303	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3050	1/1	0.98	0.12	35,35,35,35	0
57	MG	1A	3239	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3660	1/1	0.98	0.09	46,46,46,46	0
57	MG	1A	3570	1/1	0.98	0.14	41,41,41,41	0
57	MG	1A	3662	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3112	1/1	0.98	0.16	42,42,42,42	0
57	MG	1a	1621	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3726	1/1	0.98	0.11	53,53,53,53	0
57	MG	1A	4016	1/1	0.98	0.03	21,21,21,21	0
57	MG	1A	3147	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3771	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3241	1/1	0.98	0.16	29,29,29,29	0
57	MG	1a	1802	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3242	1/1	0.98	0.20	33,33,33,33	0
57	MG	1E	304	1/1	0.98	0.08	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	1806	1/1	0.98	0.10	68,68,68,68	0
57	MG	1a	1807	1/1	0.98	0.05	60,60,60,60	0
57	MG	1a	1808	1/1	0.98	0.04	49,49,49,49	0
57	MG	1E	305	1/1	0.98	0.09	28,28,28,28	0
57	MG	1a	1810	1/1	0.98	0.04	50,50,50,50	0
57	MG	1a	1811	1/1	0.98	0.09	67,67,67,67	0
57	MG	1A	3497	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3192	1/1	0.98	0.17	30,30,30,30	0
57	MG	1a	1814	1/1	0.98	0.05	64,64,64,64	0
57	MG	1a	1815	1/1	0.98	0.04	64,64,64,64	0
57	MG	1A	3890	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3577	1/1	0.98	0.07	21,21,21,21	0
57	MG	1A	3430	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3244	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3581	1/1	0.98	0.21	30,30,30,30	0
57	MG	1A	3071	1/1	0.98	0.05	16,16,16,16	0
57	MG	1a	1822	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3583	1/1	0.98	0.12	44,44,44,44	0
57	MG	1A	4032	1/1	0.98	0.04	50,50,50,50	0
57	MG	2D	305	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3782	1/1	0.98	0.04	47,47,47,47	0
57	MG	1F	302	1/1	0.98	0.08	31,31,31,31	0
57	MG	1F	303	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3309	1/1	0.98	0.04	37,37,37,37	0
57	MG	1F	305	1/1	0.98	0.10	34,34,34,34	0
57	MG	1F	307	1/1	0.98	0.14	34,34,34,34	0
57	MG	2A	3148	1/1	0.98	0.11	37,37,37,37	0
57	MG	2E	307	1/1	0.98	0.09	35,35,35,35	0
57	MG	1A	3585	1/1	0.98	0.23	33,33,33,33	0
57	MG	2A	3541	1/1	0.98	0.05	43,43,43,43	0
57	MG	2F	303	1/1	0.98	0.11	53,53,53,53	0
57	MG	1a	1647	1/1	0.98	0.09	52,52,52,52	0
57	MG	1A	4036	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3586	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3149	1/1	0.98	0.29	30,30,30,30	0
57	MG	1A	3372	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3118	1/1	0.98	0.05	49,49,49,49	0
57	MG	2I	202	1/1	0.98	0.06	65,65,65,65	0
57	MG	2A	3548	1/1	0.98	0.05	57,57,57,57	0
57	MG	1a	1653	1/1	0.98	0.14	43,43,43,43	0
57	MG	2A	3157	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3789	1/1	0.98	0.07	25,25,25,25	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	0.98	0.07	43,43,43,43	0
57	MG	1A	3590	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3682	1/1	0.98	0.05	19,19,19,19	0
57	MG	1A	3683	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3012	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3592	1/1	0.98	0.06	37,37,37,37	0
57	MG	1N	203	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3593	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3688	1/1	0.98	0.05	27,27,27,27	0
57	MG	23	101	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3918	1/1	0.98	0.11	36,36,36,36	0
57	MG	1A	3249	1/1	0.98	0.15	34,34,34,34	0
58	6IF	1A	4109	32/32	0.98	0.07	18,25,31,31	0
57	MG	1A	3073	1/1	0.98	0.08	21,21,21,21	0
57	MG	25	103	1/1	0.98	0.08	56,56,56,56	0
59	ZN	2Y	202	1/1	0.98	0.04	95,95,95,95	0
57	MG	1A	3074	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3923	1/1	0.98	0.04	33,33,33,33	0
60	SF4	1d	302	8/8	0.98	0.05	57,60,69,76	0
60	SF4	2d	302	8/8	0.98	0.04	62,75,82,85	0
57	MG	2A	3566	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3272	1/1	0.99	0.12	38,38,38,38	0
57	MG	1A	3155	1/1	0.99	0.09	40,40,40,40	0
57	MG	17	106	1/1	0.99	0.03	43,43,43,43	0
57	MG	1A	3156	1/1	0.99	0.16	31,31,31,31	0
57	MG	2A	3331	1/1	0.99	0.11	25,25,25,25	0
57	MG	1A	3742	1/1	0.99	0.06	23,23,23,23	0
57	MG	1A	3007	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	3304	1/1	0.99	0.07	23,23,23,23	0
57	MG	1A	3023	1/1	0.99	0.07	18,18,18,18	0
57	MG	1A	3894	1/1	0.99	0.03	27,27,27,27	0
57	MG	1a	1762	1/1	0.99	0.04	41,41,41,41	0
57	MG	1A	3485	1/1	0.99	0.05	41,41,41,41	0
57	MG	1D	306	1/1	0.99	0.14	26,26,26,26	0
57	MG	1A	3014	1/1	0.99	0.10	23,23,23,23	0
57	MG	1U	201	1/1	0.99	0.11	30,30,30,30	0
57	MG	1A	3897	1/1	0.99	0.05	41,41,41,41	0
57	MG	1a	1685	1/1	0.99	0.04	43,43,43,43	0
57	MG	1A	3278	1/1	0.99	0.09	25,25,25,25	0
57	MG	1A	3627	1/1	0.99	0.09	37,37,37,37	0
57	MG	1A	4021	1/1	0.99	0.02	36,36,36,36	0
57	MG	1A	3960	1/1	0.99	0.04	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	3106	1/1	0.99	0.11	31,31,31,31	0
57	MG	1U	208	1/1	0.99	0.15	30,30,30,30	0
57	MG	1E	302	1/1	0.99	0.21	32,32,32,32	0
57	MG	1V	201	1/1	0.99	0.16	24,24,24,24	0
57	MG	1A	4024	1/1	0.99	0.08	33,33,33,33	0
57	MG	1A	3751	1/1	0.99	0.06	45,45,45,45	0
57	MG	1A	3798	1/1	0.99	0.02	36,36,36,36	0
57	MG	1A	3035	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3063	1/1	0.99	0.05	26,26,26,26	0
57	MG	1E	308	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3282	1/1	0.99	0.28	35,35,35,35	0
57	MG	1A	3036	1/1	0.99	0.10	23,23,23,23	0
57	MG	1A	3524	1/1	0.99	0.15	33,33,33,33	0
57	MG	1A	3908	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3029	1/1	0.99	0.06	31,31,31,31	0
57	MG	1A	3971	1/1	0.99	0.03	43,43,43,43	0
57	MG	1A	3526	1/1	0.99	0.12	25,25,25,25	0
57	MG	1X	103	1/1	0.99	0.08	51,51,51,51	0
57	MG	1A	3806	1/1	0.99	0.07	21,21,21,21	0
57	MG	1a	1793	1/1	0.99	0.03	56,56,56,56	0
57	MG	1A	3912	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3079	1/1	0.99	0.08	36,36,36,36	0
57	MG	1A	4039	1/1	0.99	0.04	45,45,45,45	0
57	MG	1A	4041	1/1	0.99	0.02	45,45,45,45	0
57	MG	1a	1798	1/1	0.99	0.05	64,64,64,64	0
57	MG	2A	3465	1/1	0.99	0.04	43,43,43,43	0
57	MG	1A	3038	1/1	0.99	0.20	30,30,30,30	0
57	MG	1F	306	1/1	0.99	0.13	28,28,28,28	0
57	MG	2A	3658	1/1	0.99	0.03	75,75,75,75	0
57	MG	1a	1634	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3717	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3096	1/1	0.99	0.12	22,22,22,22	0
57	MG	1A	3763	1/1	0.99	0.06	41,41,41,41	0
57	MG	1a	1805	1/1	0.99	0.03	40,40,40,40	0
57	MG	1A	3812	1/1	0.99	0.03	40,40,40,40	0
57	MG	1A	3764	1/1	0.99	0.02	25,25,25,25	0
57	MG	1A	3030	1/1	0.99	0.09	28,28,28,28	0
57	MG	1A	3983	1/1	0.99	0.05	50,50,50,50	0
57	MG	2A	3115	1/1	0.99	0.12	35,35,35,35	0
57	MG	1a	1723	1/1	0.99	0.14	38,38,38,38	0
57	MG	2A	3479	1/1	0.99	0.03	56,56,56,56	0
57	MG	1A	3922	1/1	0.99	0.02	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3068	1/1	0.99	0.09	26,26,26,26	0
57	MG	2A	3031	1/1	0.99	0.06	53,53,53,53	0
57	MG	10	108	1/1	0.99	0.03	46,46,46,46	0
57	MG	1A	3816	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3676	1/1	0.99	0.06	36,36,36,36	0
57	MG	2A	3391	1/1	0.99	0.07	43,43,43,43	0
57	MG	1A	3817	1/1	0.99	0.05	25,25,25,25	0
57	MG	2A	3679	1/1	0.99	0.04	45,45,45,45	0
57	MG	2A	3123	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3215	1/1	0.99	0.16	38,38,38,38	0
57	MG	1A	3567	1/1	0.99	0.13	31,31,31,31	0
57	MG	1A	3681	1/1	0.99	0.05	41,41,41,41	0
57	MG	2A	3584	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3069	1/1	0.99	0.11	21,21,21,21	0
57	MG	2A	3686	1/1	0.99	0.09	30,30,30,30	0
57	MG	1A	3151	1/1	0.99	0.12	31,31,31,31	0
57	MG	1A	3293	1/1	0.99	0.17	31,31,31,31	0
57	MG	1A	3536	1/1	0.99	0.05	48,48,48,48	0
57	MG	1a	1654	1/1	0.99	0.09	42,42,42,42	0
57	MG	1A	3686	1/1	0.99	0.04	26,26,26,26	0
57	MG	1A	3070	1/1	0.99	0.21	34,34,34,34	0
57	MG	2A	3592	1/1	0.99	0.03	52,52,52,52	0
57	MG	1A	3353	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3173	1/1	0.99	0.12	29,29,29,29	0
57	MG	1A	3085	1/1	0.99	0.13	32,32,32,32	0
57	MG	1A	3576	1/1	0.99	0.15	24,24,24,24	0
57	MG	2A	3597	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3175	1/1	0.99	0.07	26,26,26,26	0
57	MG	2A	3700	1/1	0.99	0.03	58,58,58,58	0
57	MG	1P	202	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3578	1/1	0.99	0.10	24,24,24,24	0
57	MG	1P	204	1/1	0.99	0.16	31,31,31,31	0
59	ZN	15	110	1/1	0.99	0.07	47,47,47,47	0
59	ZN	19	102	1/1	0.99	0.15	67,67,67,67	0
57	MG	1A	3021	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3695	1/1	0.99	0.03	23,23,23,23	0
59	ZN	25	104	1/1	0.99	0.05	57,57,57,57	0
59	ZN	26	102	1/1	0.99	0.06	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	66,66,66,66	0
57	MG	1A	3943	1/1	0.99	0.05	51,51,51,51	0
57	MG	1A	3944	1/1	0.99	0.05	12,12,12,12	0
57	MG	1A	4073	1/1	0.99	0.07	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	3199	1/1	0.99	0.12	24,24,24,24	0
57	MG	1A	4040	1/1	1.00	0.05	24,24,24,24	0
57	MG	2A	3464	1/1	1.00	0.05	38,38,38,38	0
57	MG	1A	3916	1/1	1.00	0.03	35,35,35,35	0
59	ZN	1Y	205	1/1	1.00	0.02	57,57,57,57	0
57	MG	2A	3646	1/1	1.00	0.03	48,48,48,48	0
57	MG	1A	3947	1/1	1.00	0.09	29,29,29,29	0
59	ZN	16	102	1/1	1.00	0.03	41,41,41,41	0
57	MG	1a	1773	1/1	1.00	0.07	57,57,57,57	0
59	ZN	1n	103	1/1	1.00	0.04	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.