



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:45 AM EDT

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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

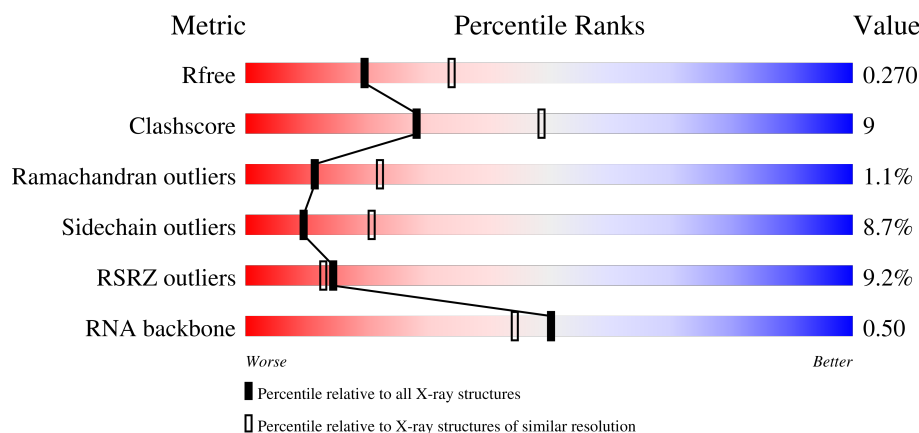
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

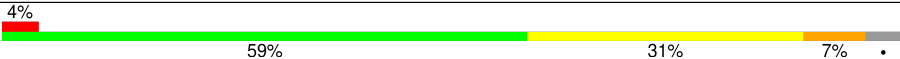
The reported resolution of this entry is 2.50 Å.

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)

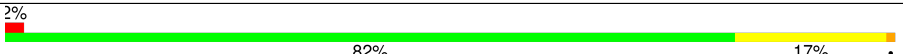
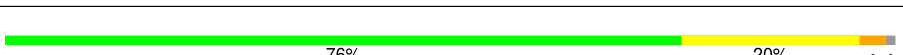
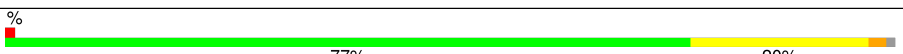
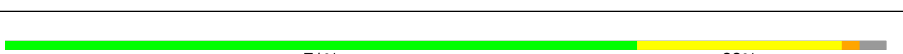
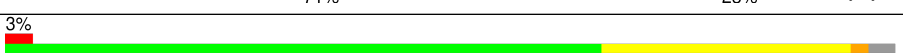
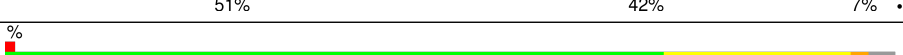
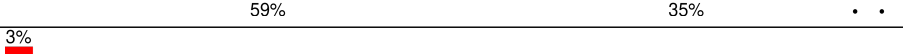
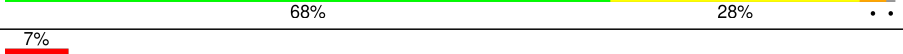
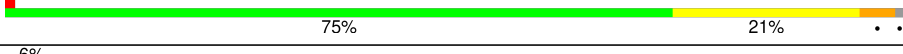
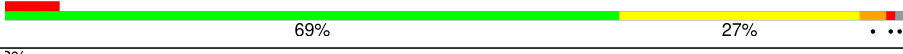
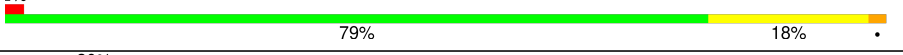
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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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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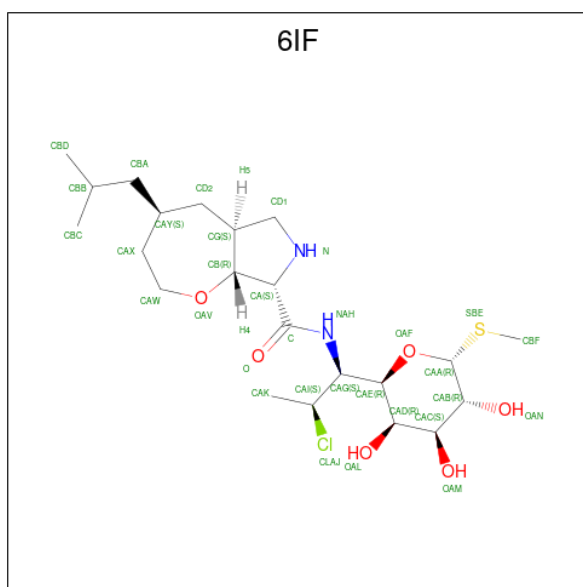
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2Q	1	Total 1	Mg 1	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 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: C₂₂H₃₉ClN₂O₆S).

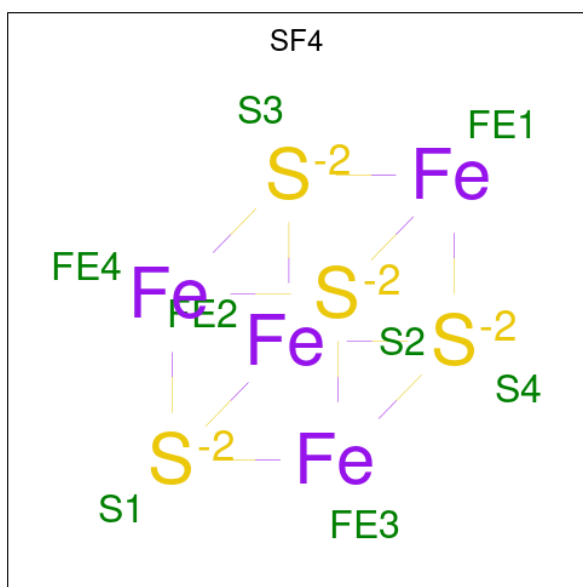


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
58	1A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		
58	2A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		

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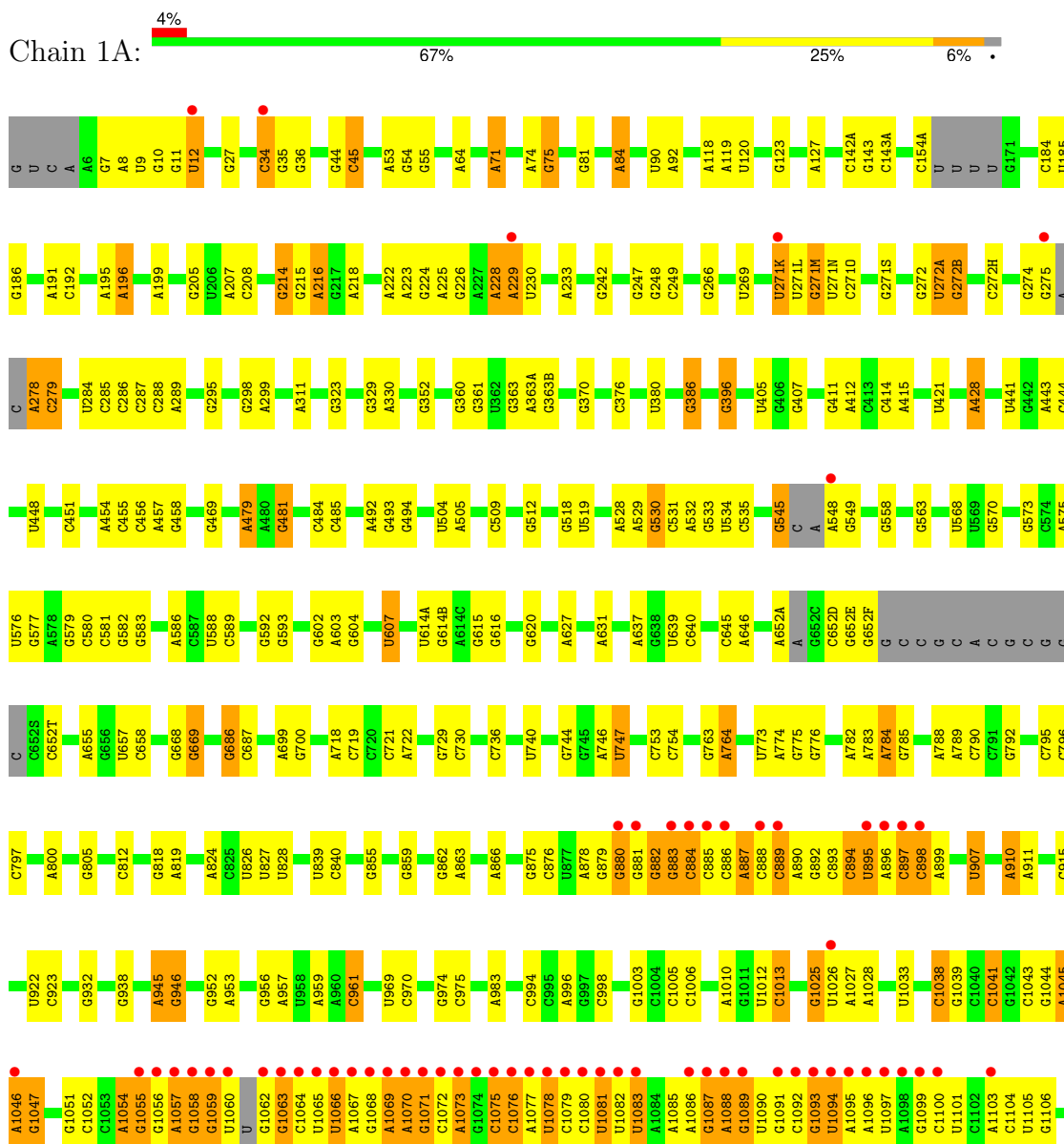
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2p	1	Total	O	0	0
			1	1		
62	2t	2	Total	O	0	0
			2	2		
62	2x	3	Total	O	0	0
			3	3		
62	2y	8	Total	O	0	0
			8	8		

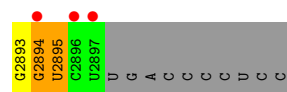
3 Residue-property plots [i](#)

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

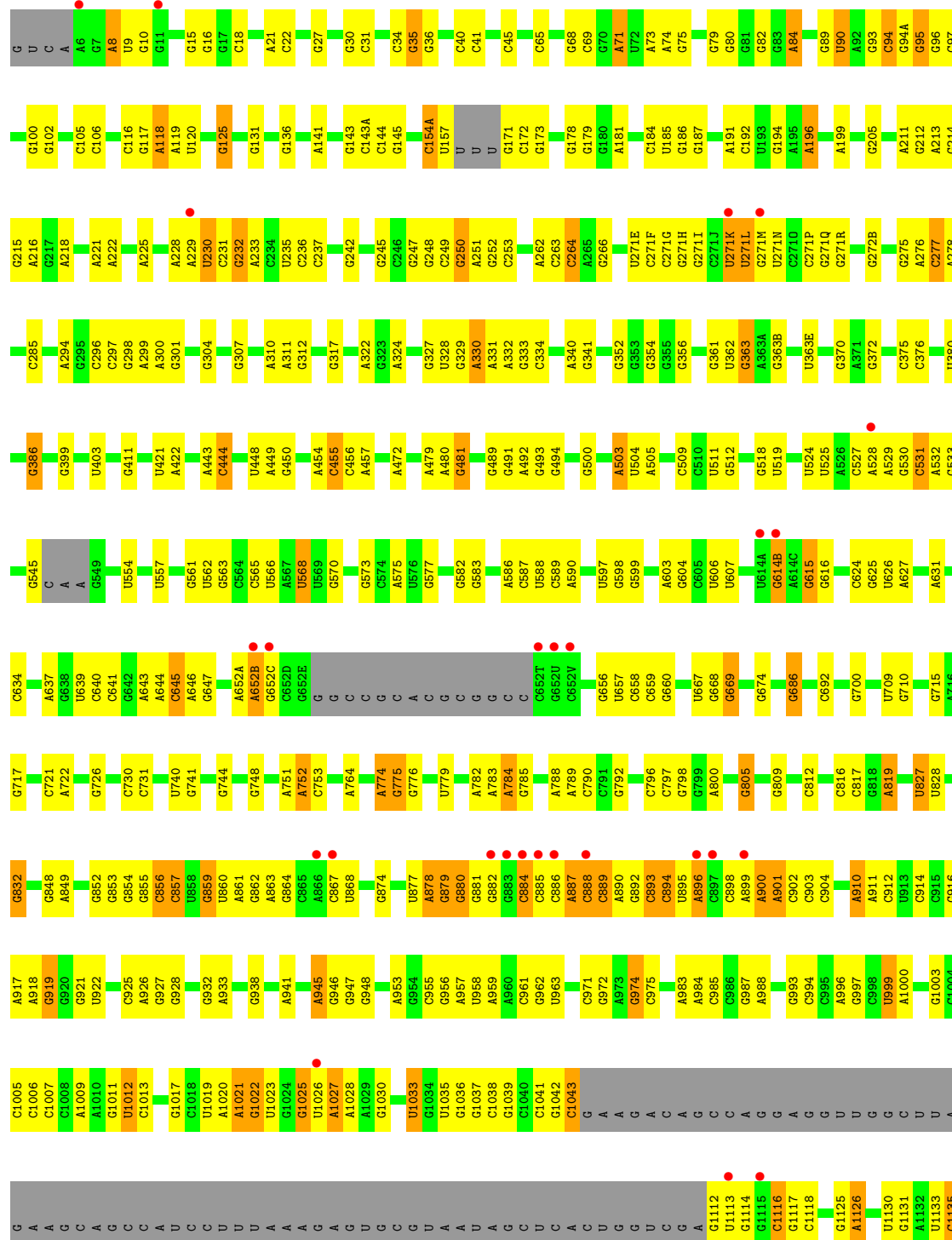
• Molecule 1: 23S Ribosomal RNA



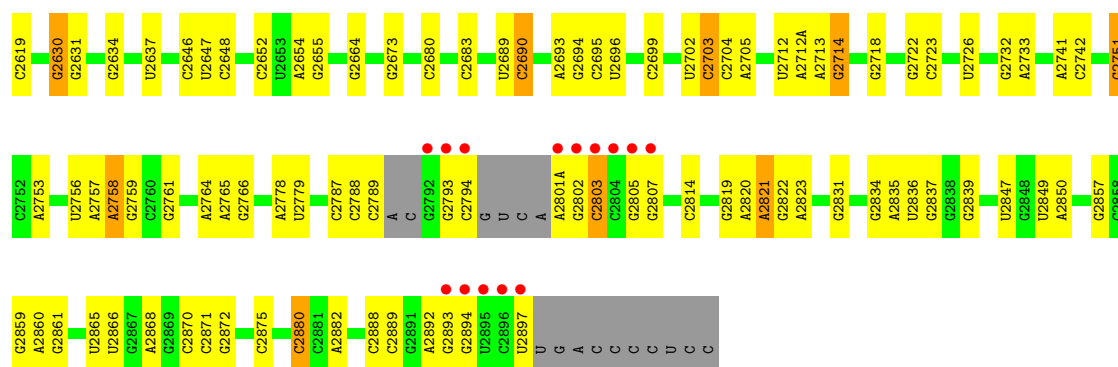




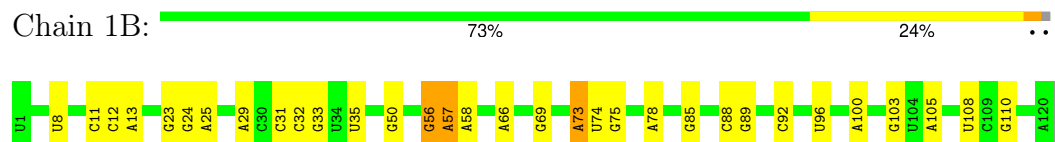
- Molecule 1: 23S Ribosomal RNA



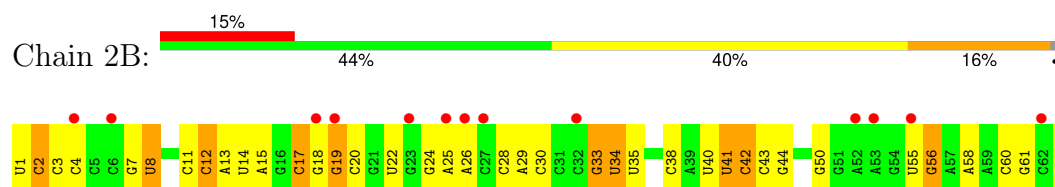




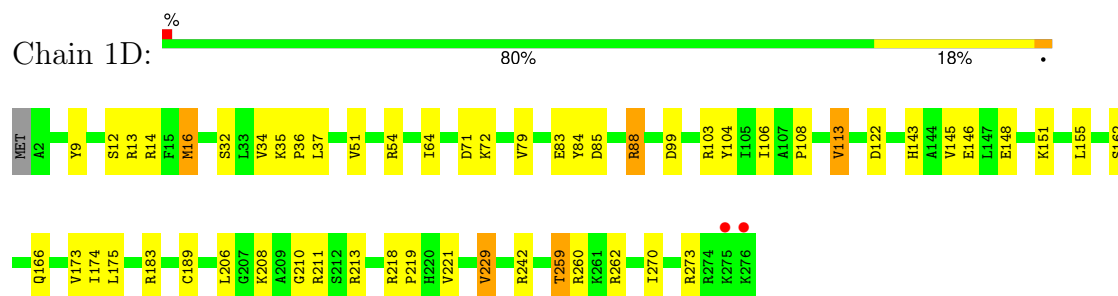
• Molecule 2: 5S Ribosomal RNA



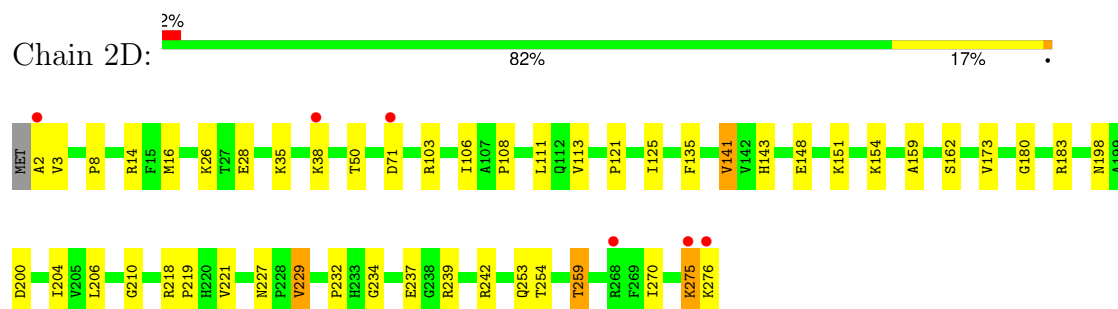
• Molecule 2: 5S Ribosomal RNA



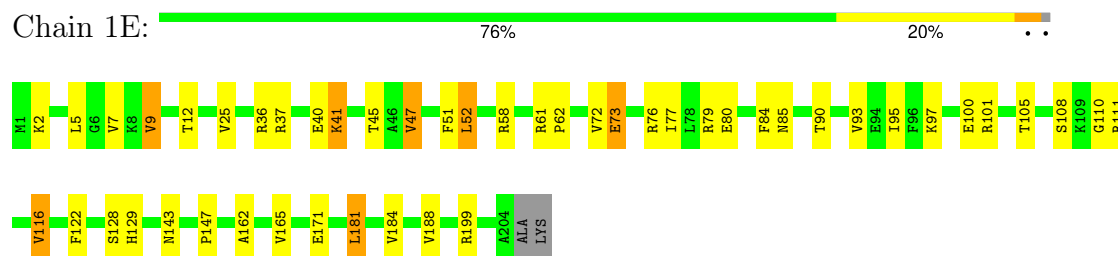
• Molecule 3: 50S ribosomal protein L2



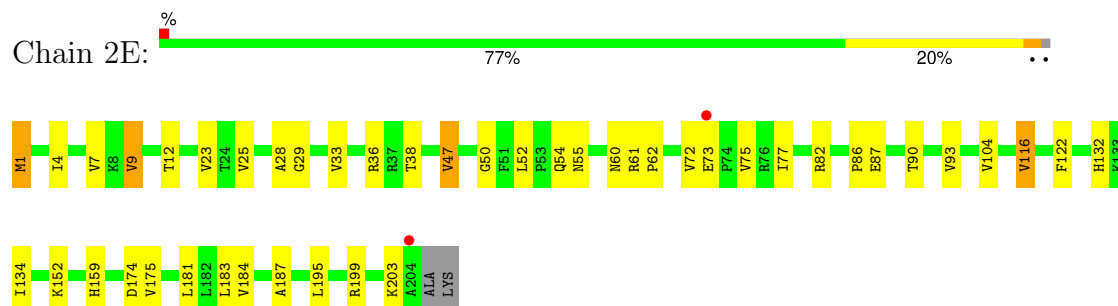
• Molecule 3: 50S ribosomal protein L2



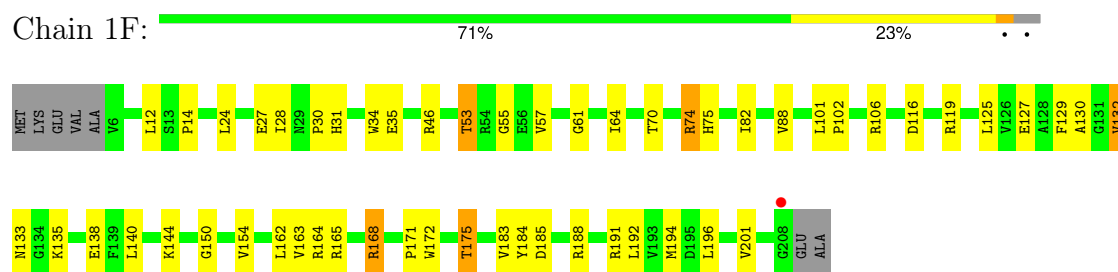
- Molecule 4: 50S ribosomal protein L3



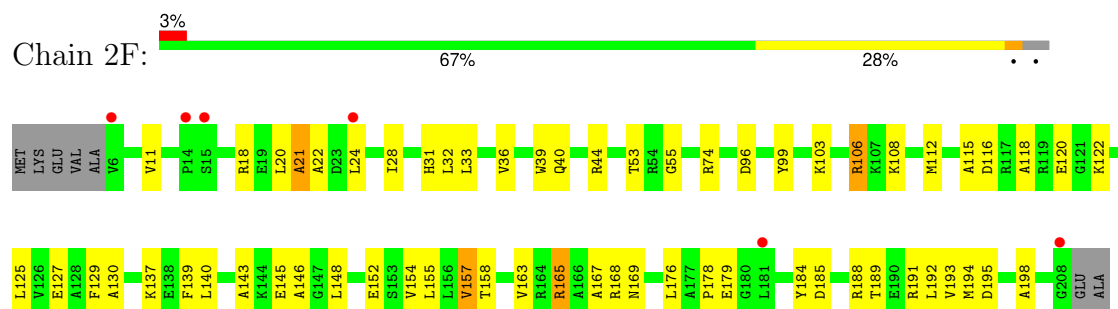
- Molecule 4: 50S ribosomal protein L3



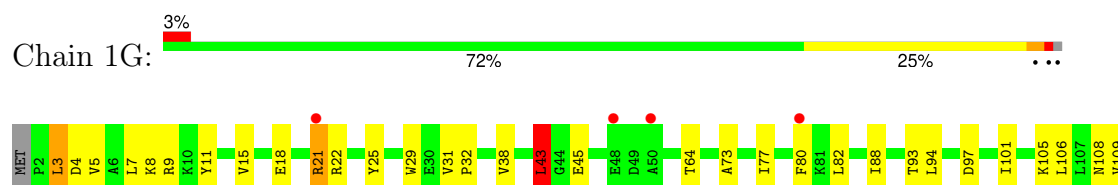
- Molecule 5: 50S ribosomal protein L4

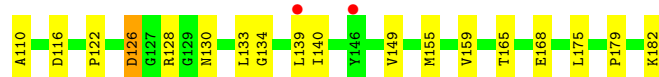


- Molecule 5: 50S ribosomal protein L4

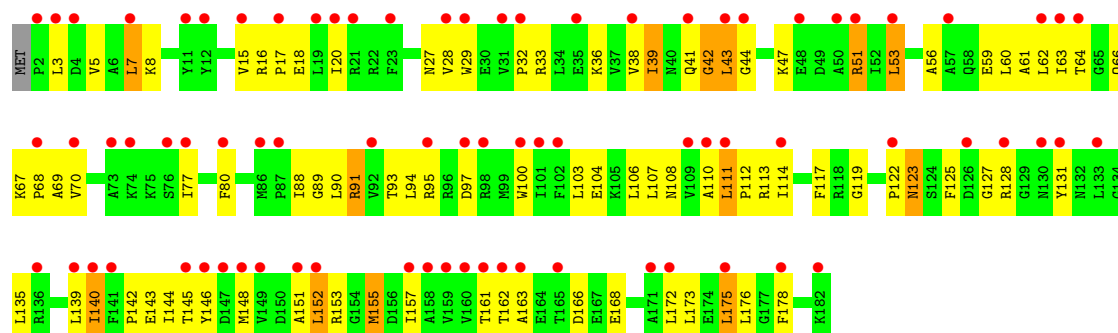
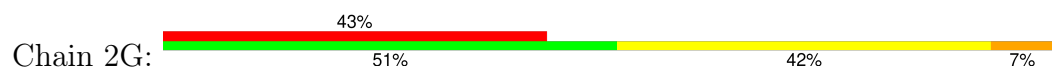


- Molecule 6: 50S ribosomal protein L5

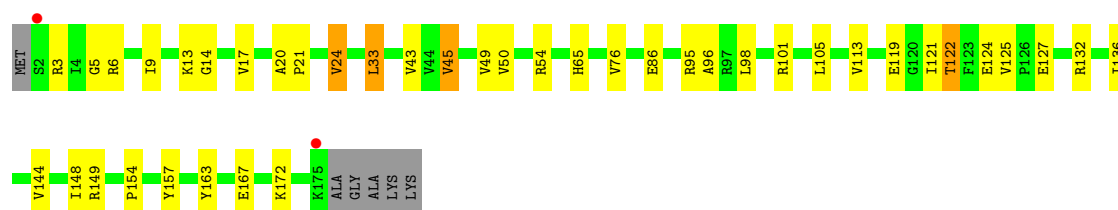
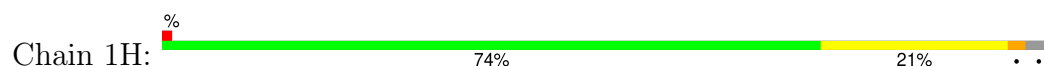




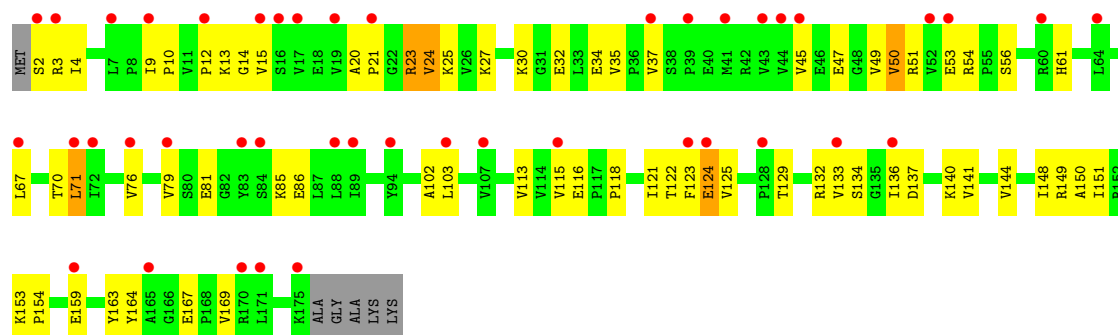
• Molecule 6: 50S ribosomal protein L5



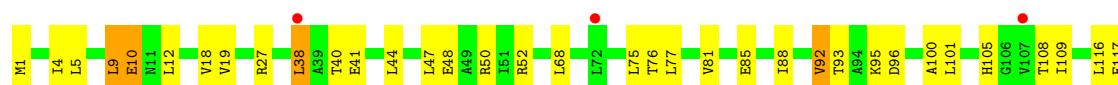
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

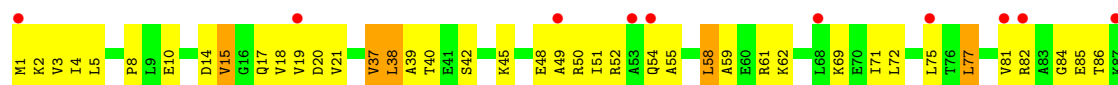


• Molecule 8: 50S ribosomal protein L9

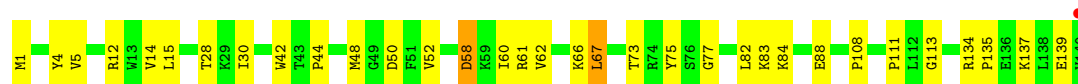
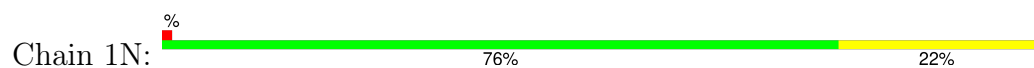




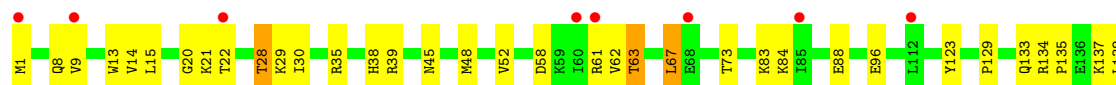
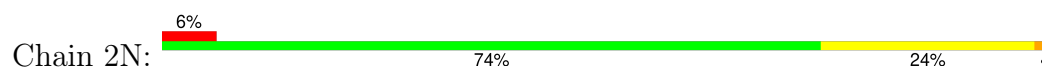
- Molecule 8: 50S ribosomal protein L9



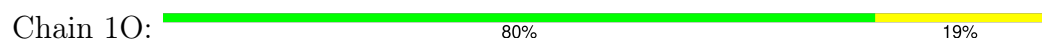
- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



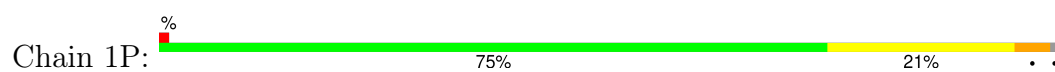
- Molecule 10: 50S ribosomal protein L14



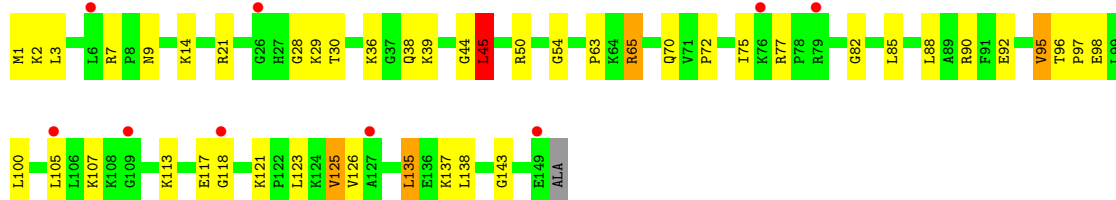
- Molecule 10: 50S ribosomal protein L14



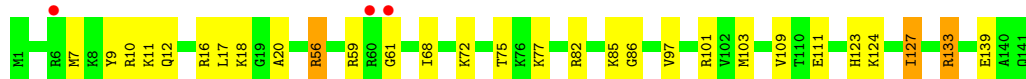
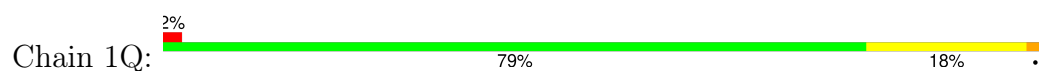
- Molecule 11: 50S ribosomal protein L15



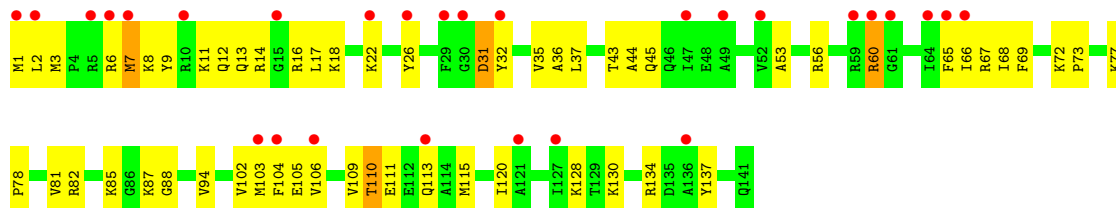
- Molecule 11: 50S ribosomal protein L15



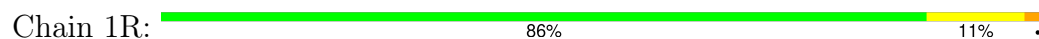
- Molecule 12: 50S ribosomal protein L16



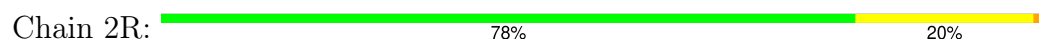
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



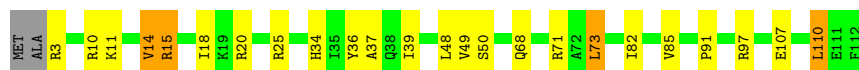
- Molecule 13: 50S ribosomal protein L17





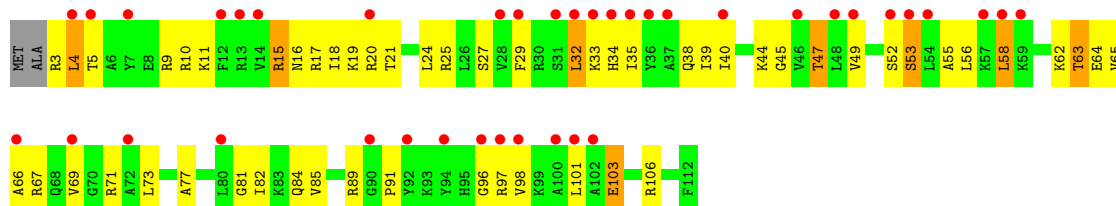
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 77% 18% . .



- Molecule 14: 50S ribosomal protein L18

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



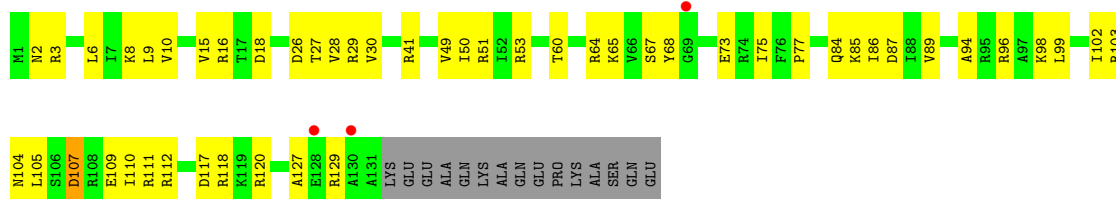
- Molecule 15: 50S ribosomal protein L19

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% . .

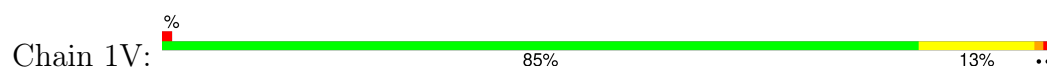


- Molecule 16: 50S ribosomal protein L20

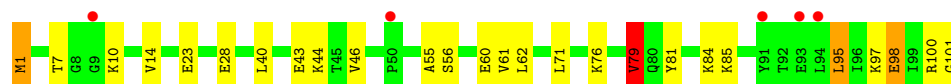
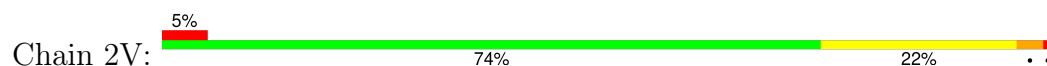
Chain 2U: 2% 75% 23% .



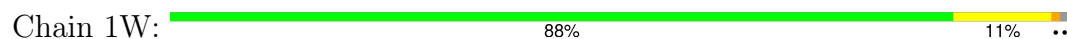
- Molecule 17: 50S ribosomal protein L21



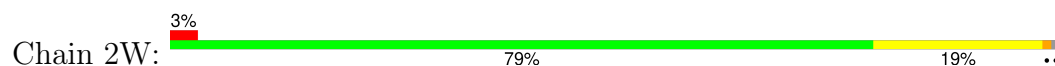
- Molecule 17: 50S ribosomal protein L21



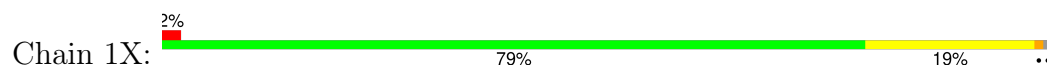
- Molecule 18: 50S ribosomal protein L22



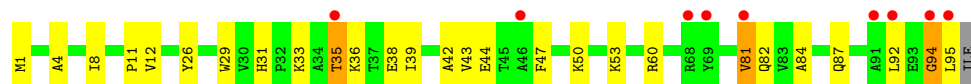
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



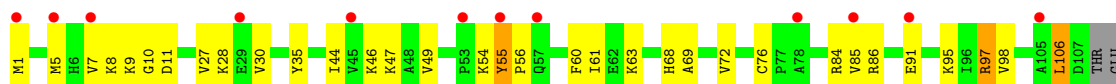
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

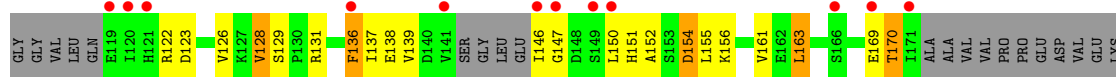
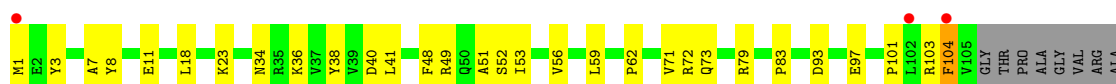


• Molecule 20: 50S ribosomal protein L24



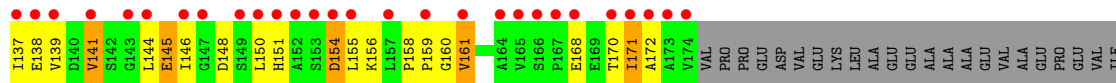
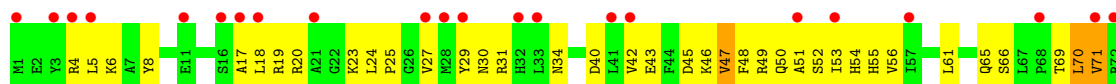
GLU

• Molecule 21: 50S ribosomal protein L25



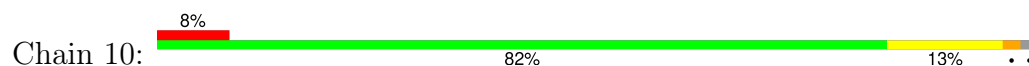
LEU
ALA
GLU
GLU
ALA
GLU
VAL
ALA
GLU
VAL
PRO
GLU
GLU
VAL
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

• Molecule 21: 50S ribosomal protein L25



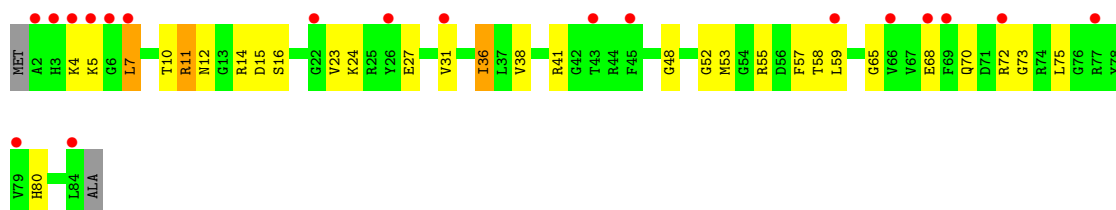
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU
GLU

• Molecule 22: 50S ribosomal protein L27

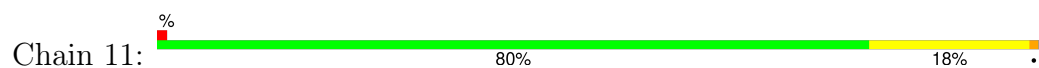




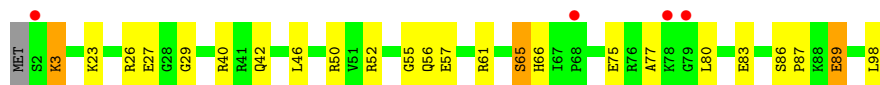
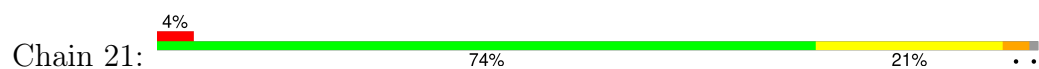
- Molecule 22: 50S ribosomal protein L27



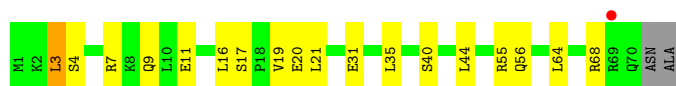
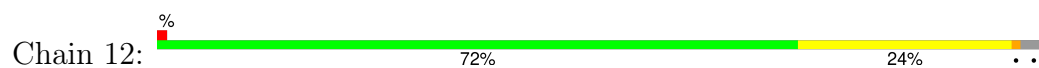
- Molecule 23: 50S ribosomal protein L28



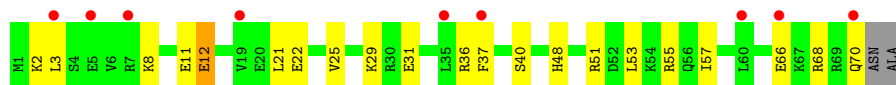
- Molecule 23: 50S ribosomal protein L28



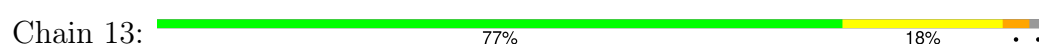
- Molecule 24: 50S ribosomal protein L29



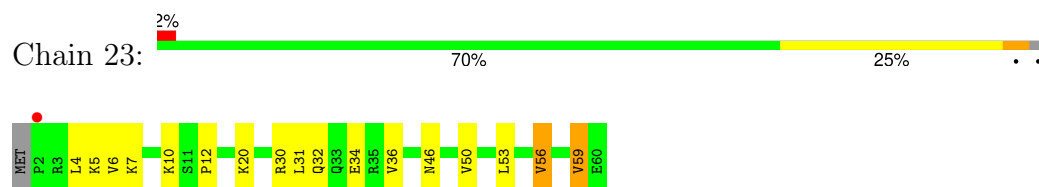
- Molecule 24: 50S ribosomal protein L29



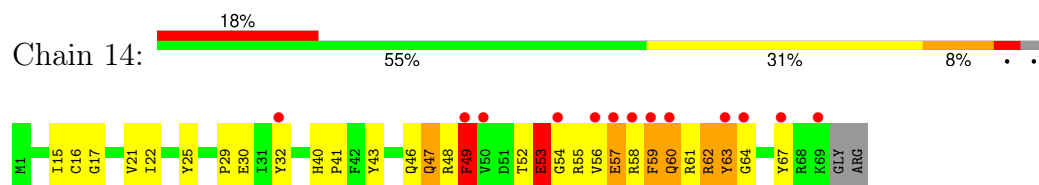
- Molecule 25: 50S ribosomal protein L30



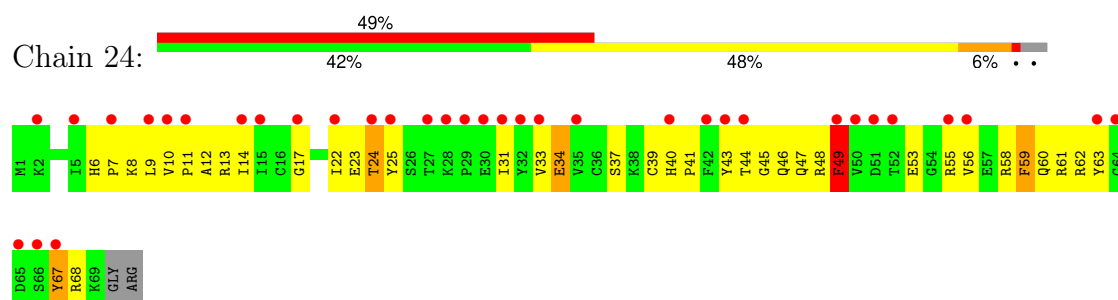
- Molecule 25: 50S ribosomal protein L30



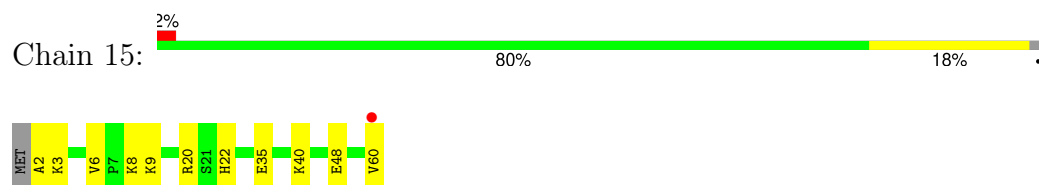
- Molecule 26: 50S ribosomal protein L31



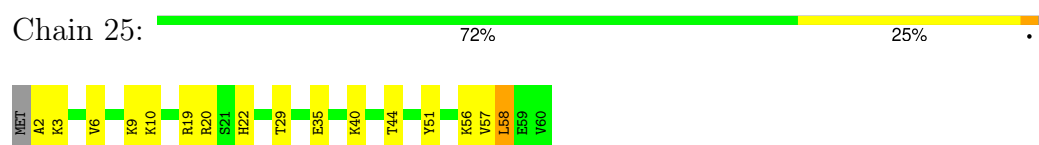
- Molecule 26: 50S ribosomal protein L31



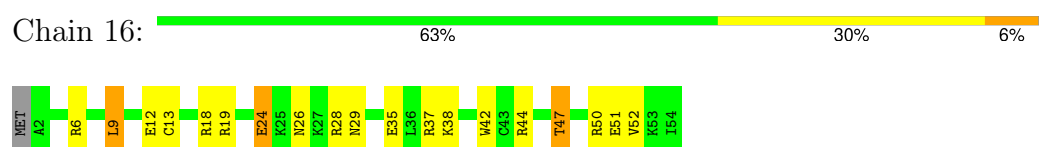
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

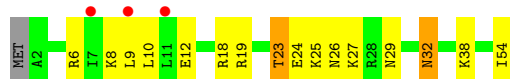


- Molecule 28: 50S ribosomal protein L33

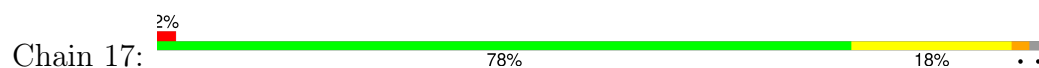


- Molecule 28: 50S ribosomal protein L33

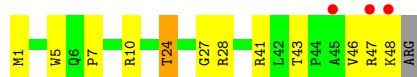
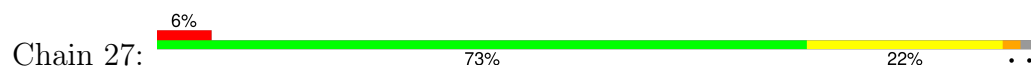




- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



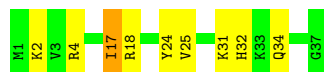
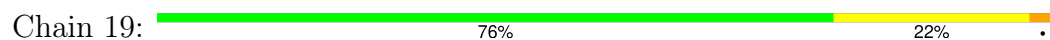
- Molecule 30: 50S ribosomal protein L35



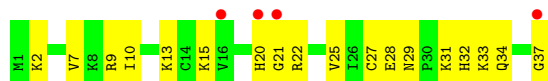
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



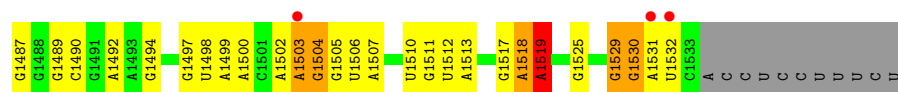
- Molecule 31: 50S ribosomal protein L36



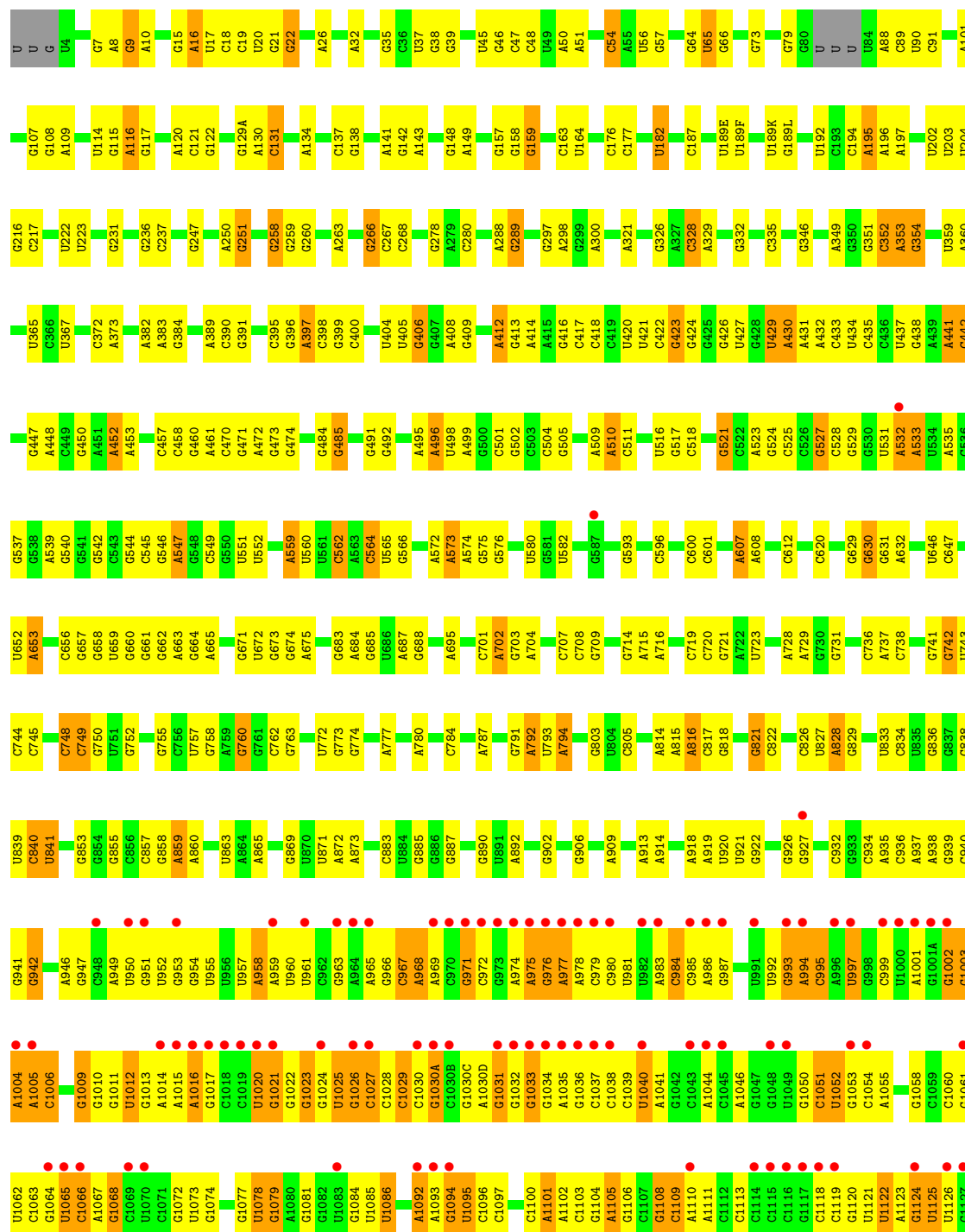
- Molecule 32: 16S Ribosomal RNA

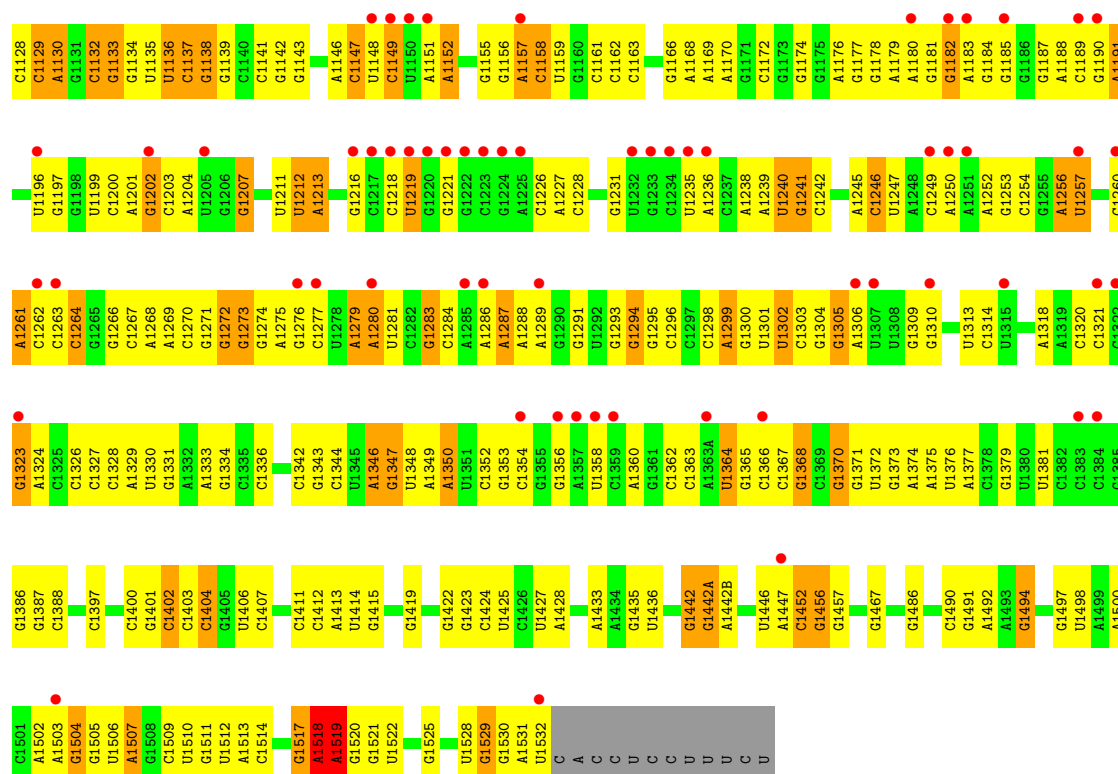


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U1358	G1266	C1147	U1040	A974	G629	A509	U404	U294	C187	G	G
A1359	C1270	U1148	A1044	A975	G630	A510	U405	U295	C188	U4	U4
A1360	C1271	A1152	C1045	A977	G631	C511	G406	U296	G189	G7	G7
C1363	G1273	C1158	G1053	U981	G632	U516	G410	A298	C189D	A8	A8
A1363A	G1274	U1159	G1054	U982	G633	G517	A411	G299	U189E	G9	G9
G1370	A1275	G1160	C1060	A983	A642	C518	A412	A300	G189J	A10	A10
C1277	G1276	C1161	U1061	C910	U646	C524	G413	A301	U189K	G11	G11
G1371	C1277	A1168	U1062	U911	G647	G524	A414	C311	G189L	U17	U17
U1278	U1278	A1169	C1063	C912	A648	G527	C418	G316	U190	C18	C18
G1373	A1279	C1176	G1068	A913	G649	C531	C419	G317	G191	C19	C19
A1374	A1280	C1177	C1069	A914	A653	A532	C422	G318	U192	U20	U20
C1378	C1284	A1179	U1073	A915	G662	A536	G423	G324	G193	G22	G22
U1381	A1285	A1180	C1074	C995	A663	A539	G424	A325	C110	C110	C110
A1287	A1286	C1183	C1075	A996	G664	G542	G424	A326	G111	A26	A26
A1288	A1288	G1184	U1076	U997	A665	G547	U429	A327	G115	A32	A32
C1289	G1290	C1189	U1077	G998	G667	A559	A430	A328	G116	C36	C36
G1291	U1291	C1190	U1078	C999	G674	G540	A431	A329	G117	U37	U37
U1292	U1292	C1191	U1079	U1000	G675	G541	A432	A330	U118	G38	G38
A1299	A1299	U1194	A1080	U1001	G676	A547	C433	G332	U202	C39	C39
G1300	G1300	C1195	G1081	G1001A	G677	A559	U434	C339	G121	G42	G42
U1301	C1301	U1196	U1086	G1002	A676	A560	G438	U340	G122	C43	C43
C1402	U1302	G1197	C1094	G1003	U677	U561	A439	C341	G123	C44	C44
C1403	C1303	C1200	U1095	C1005	A684	C564	A441	U343	G124	U45	U45
G1304	G1304	A1201	C1096	C1006	G685	C564	C442	A344	A130	G46	G46
G1305	G1305	U1202	G1097	C1007	U686	A572	A442	C344	C131	C47	C47
C1407	C1312	G1203	C1100	A1015	U687	A573	G445	G347	A134	C48	C48
G1410	U1312	G1204	A1101	A1016	A688	G567	G446	G348	G145	A51	A51
C1412	C1314	G1207	A1102	G1017	C689	G568	G447	C352	G146	G52	G52
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G1419	C1321	G1224	G1108	U1020	A695	G576	A453	G354	A149	C58	C58
G1422	C1322	A1227	C1112	G1021	G711	G577	C456	U367	G159	G61	G61
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A1428	U1329	A1236	U1121	G1023	G713	A583	A461	A373	A161	C67	C67
G1435	U1330	A1237	U1122	G1024	G714	G584	C470	A374	A162	G68	G68
U1436	G1331	A1238	A1123	U1025	A715	G585	G471	U375	C163	G69	G69
G1436	C1338	A1239	G1124	C1026	U850	C596	A472	G376	C165	G70	G70
G1442	A1339	U1240	U1125	C1027	G851	G597	G473	G377	G166	G73	G73
G1442A	A1340	A1250	C1126	C1028	A865	U598	G474	A382	G167	C76	C76
U1446	G1343	G1255	C1129	G1030A	G869	C599	G475	A383	G168	G79	G79
A1447	C1344	A1256	U1134	C1030B	U870	G610	G485	G384	A172	G	G
C1452	U1345	U1257	U1135	A1030C	A728	C613	A496	C390	U173	U	U
G1456	A1346	G1258	U1136	A965	G730	A614	U498	G391	C174	U	U
G1457	G1347	C1259	C1137	C967	G731	G615	G502	C396	C175	U	U
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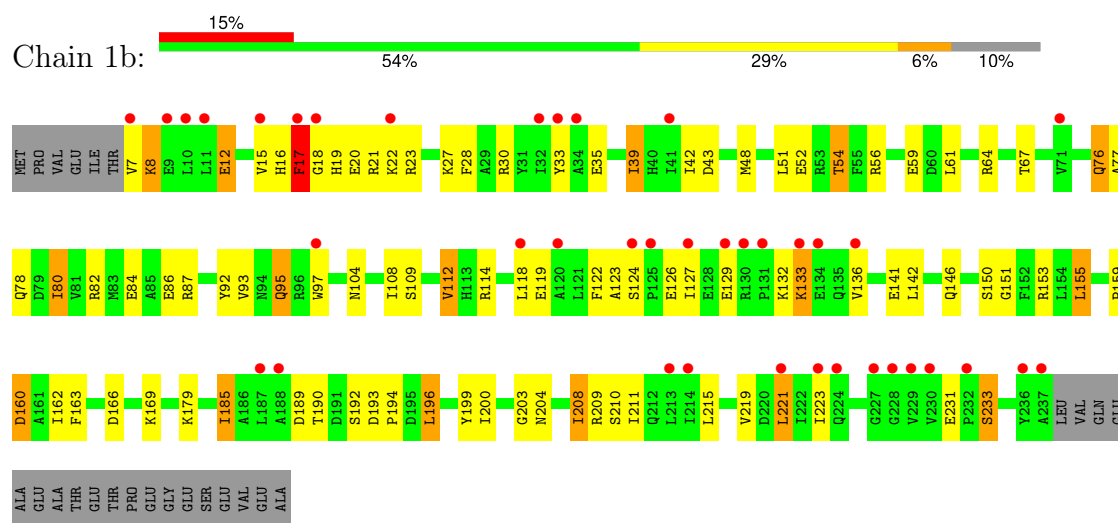


• Molecule 32: 16S Ribosomal RNA

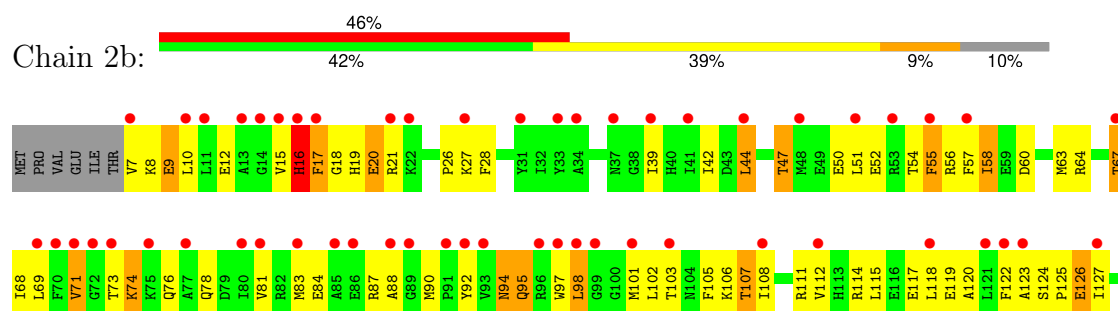


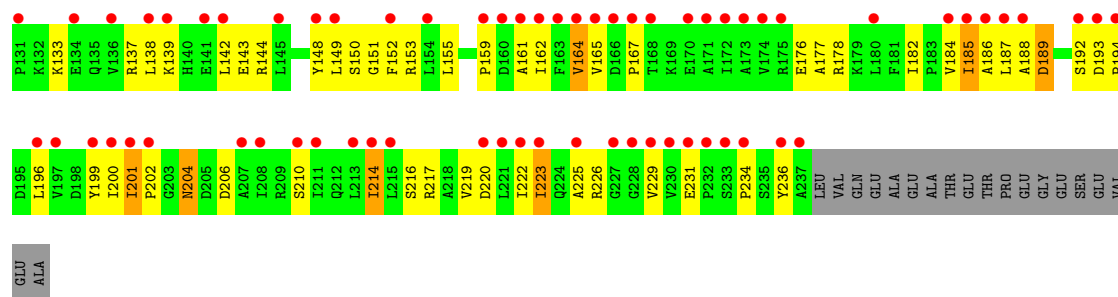


• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2





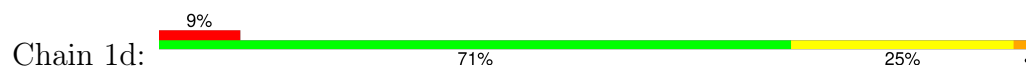
• Molecule 34: 30S ribosomal protein S3

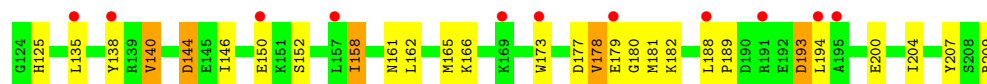


• Molecule 34: 30S ribosomal protein S3

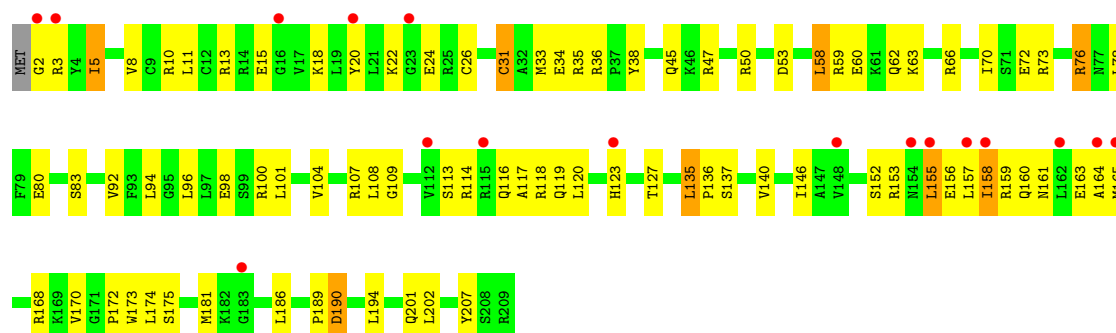


• Molecule 35: 30S ribosomal protein S4

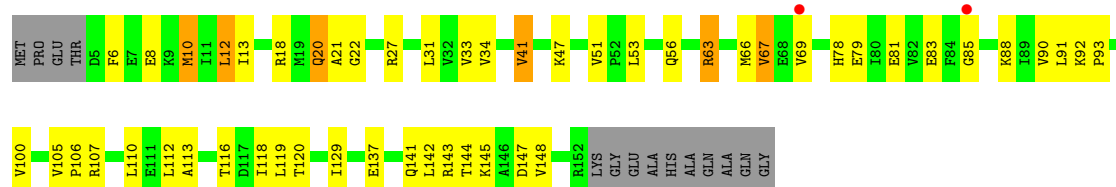




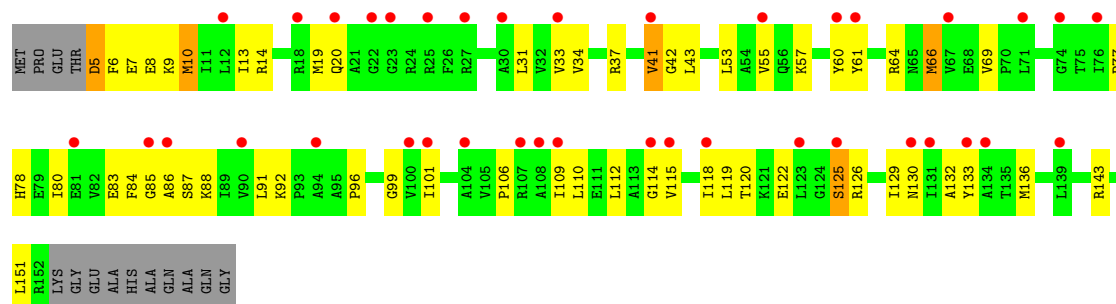
- Molecule 35: 30S ribosomal protein S4



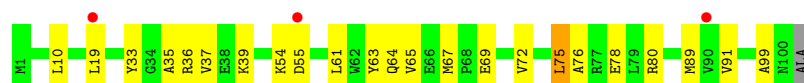
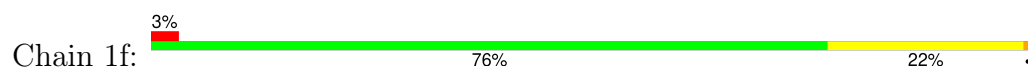
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



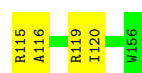
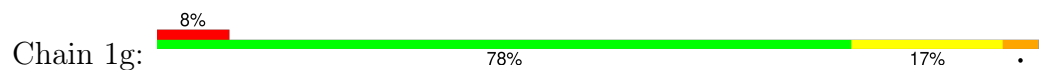
- Molecule 37: 30S ribosomal protein S6



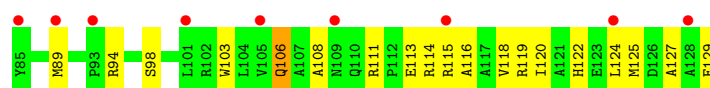
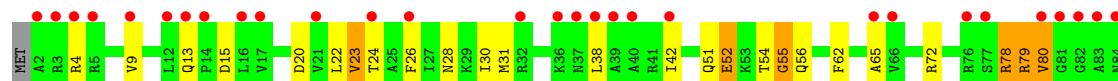
- Molecule 37: 30S ribosomal protein S6



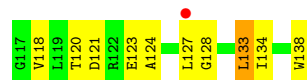
- Molecule 38: 30S ribosomal protein S7



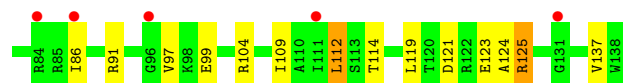
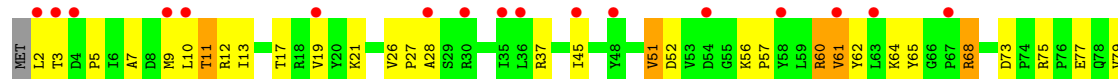
- Molecule 38: 30S ribosomal protein S7



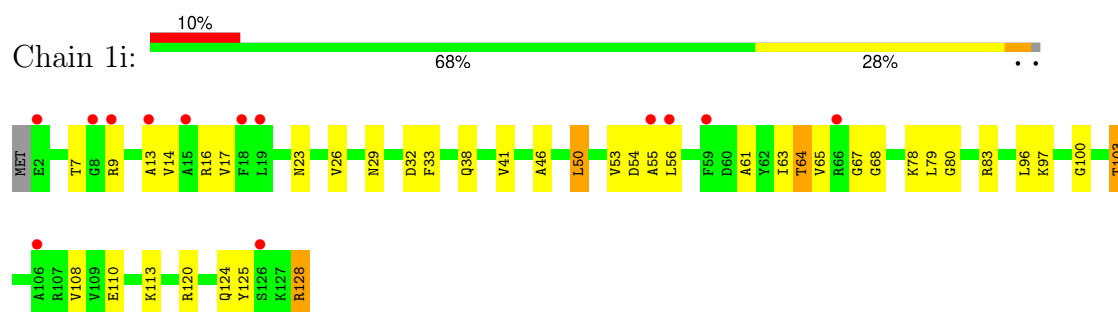
- Molecule 39: 30S ribosomal protein S8



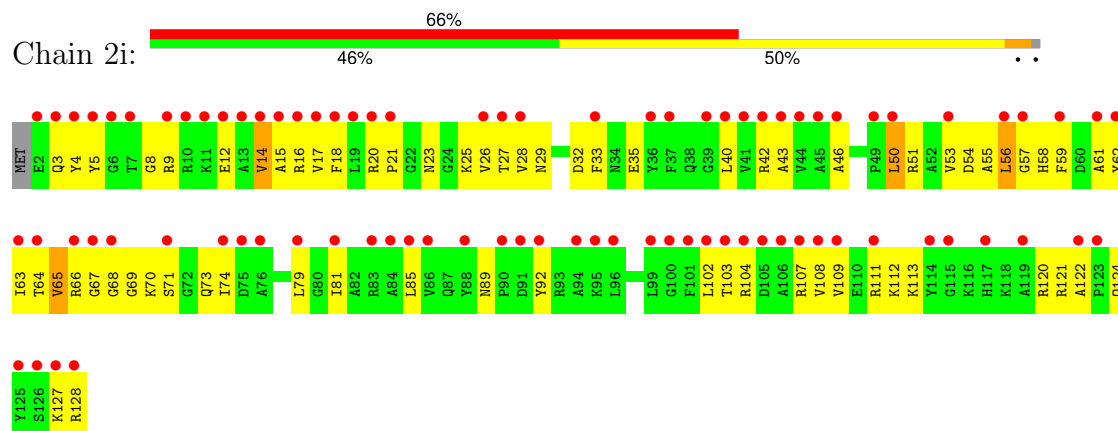
- Molecule 39: 30S ribosomal protein S8



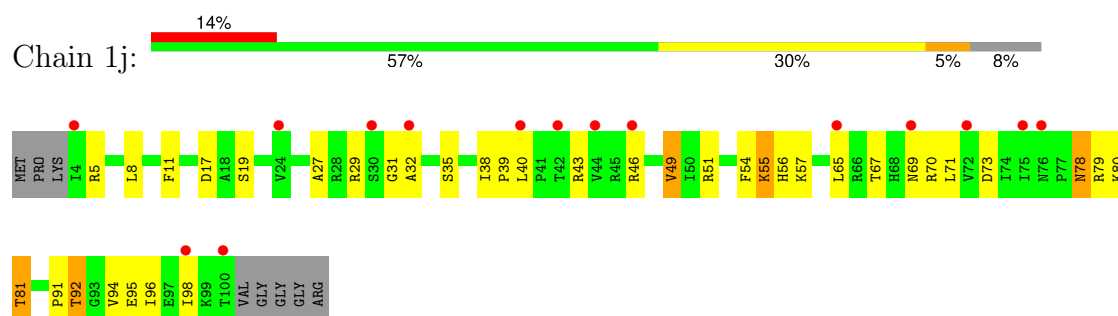
- Molecule 40: 30S ribosomal protein S9



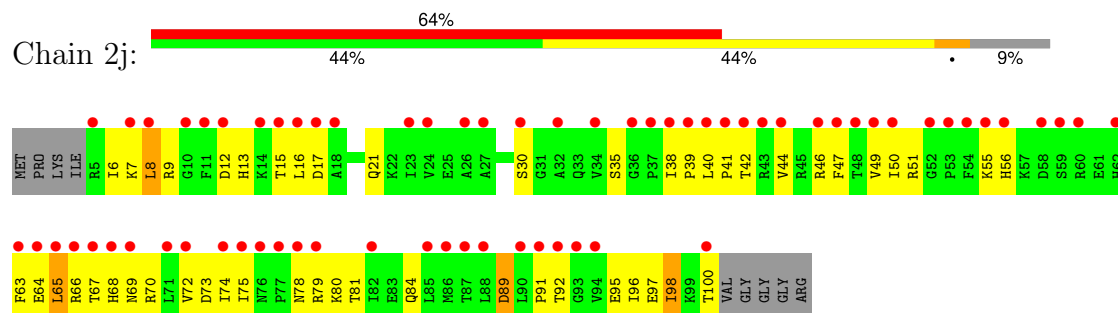
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

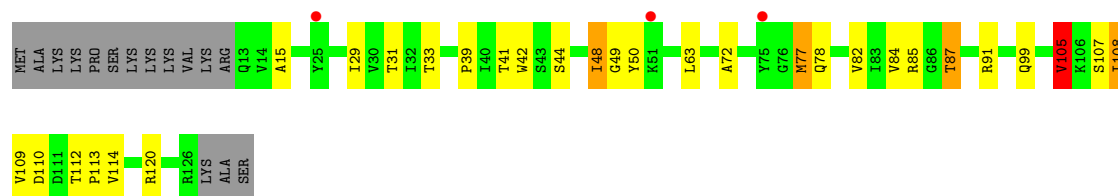


- Molecule 41: 30S ribosomal protein S10

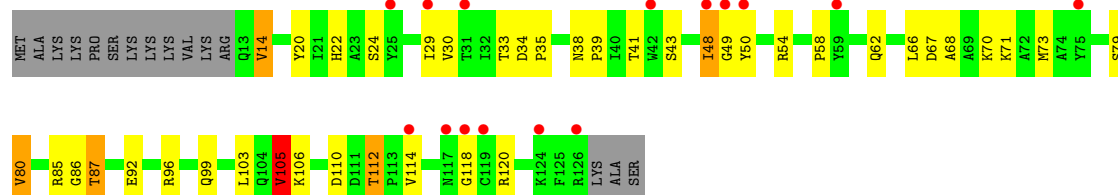


- Molecule 42: 30S ribosomal protein S11

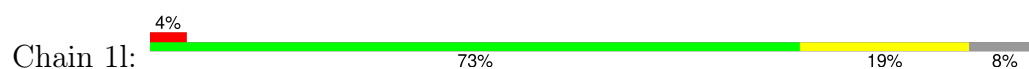




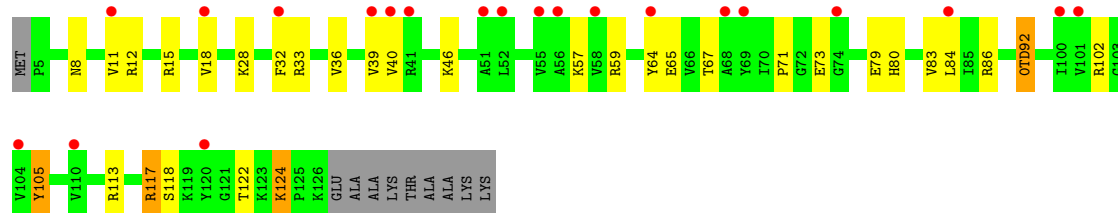
- Molecule 42: 30S ribosomal protein S11



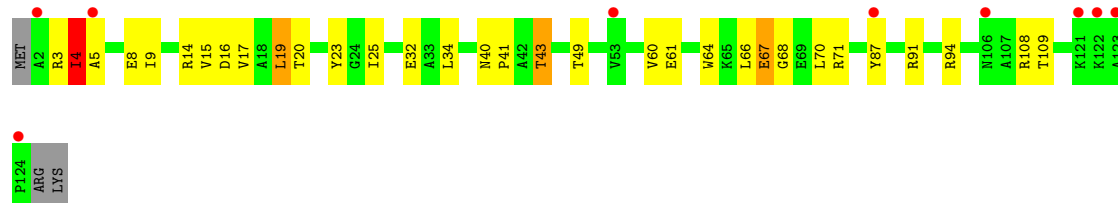
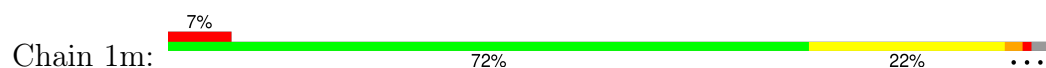
- Molecule 43: 30S ribosomal protein S12



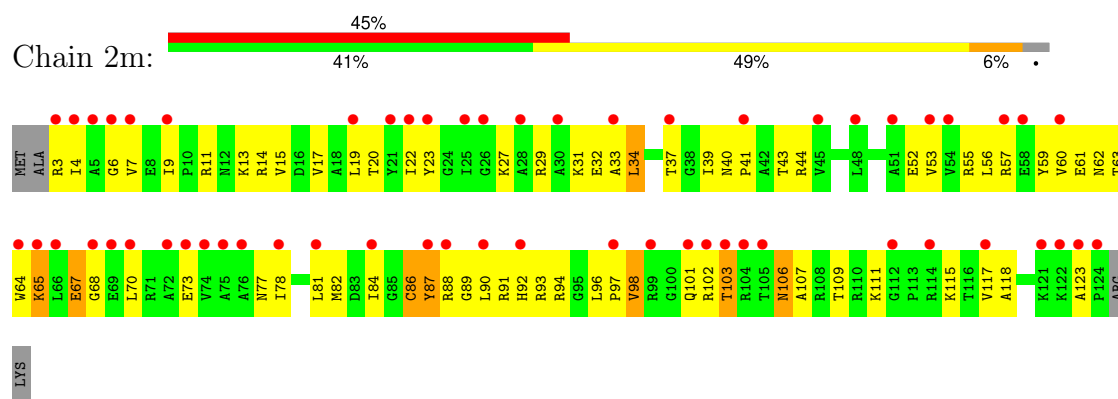
- Molecule 43: 30S ribosomal protein S12



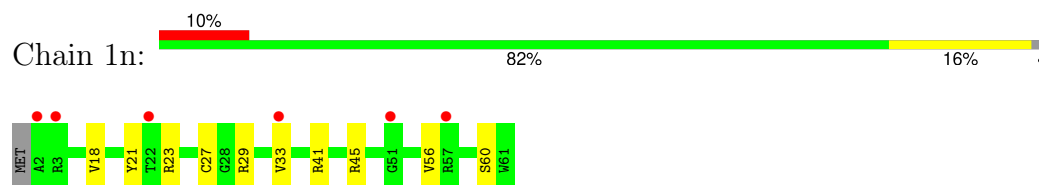
- Molecule 44: 30S ribosomal protein S13



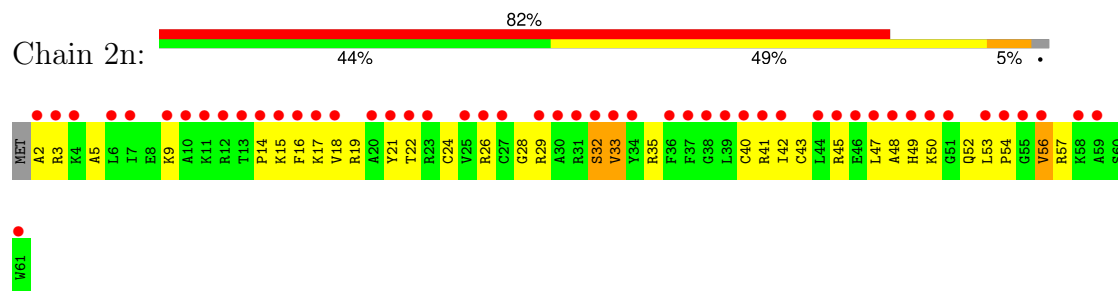
- Molecule 44: 30S ribosomal protein S13



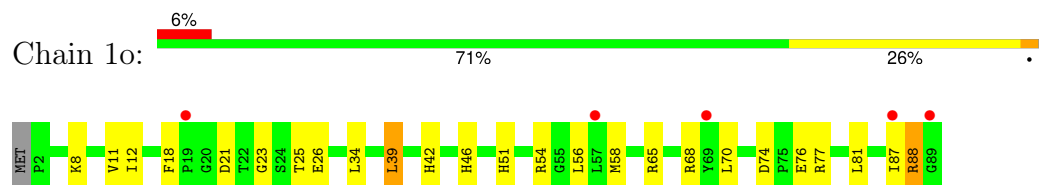
- Molecule 45: 30S ribosomal protein S14 type Z



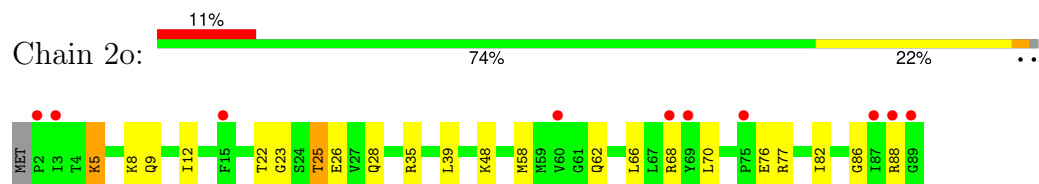
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

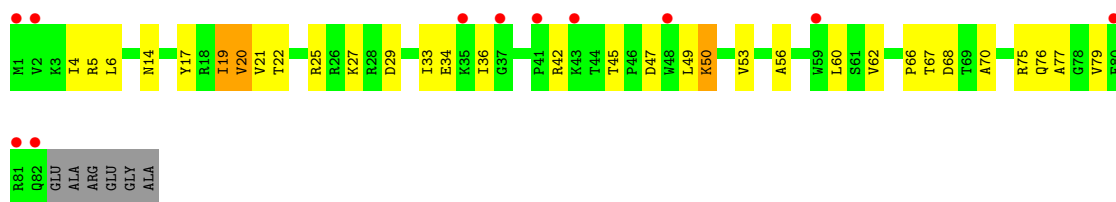


- Molecule 46: 30S ribosomal protein S15

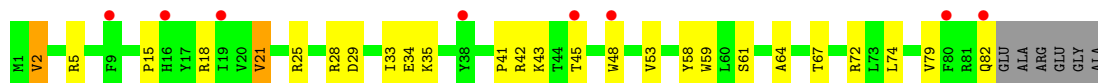


- Molecule 47: 30S ribosomal protein S16





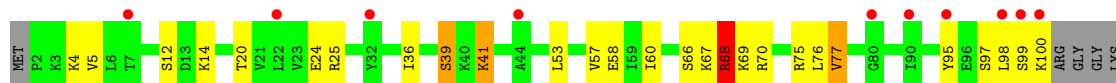
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

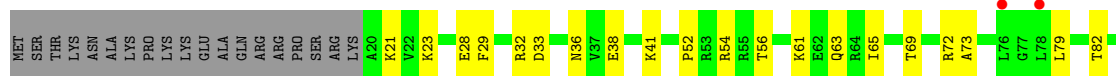


- Molecule 48: 30S ribosomal protein S17



ALA

- Molecule 49: 30S ribosomal protein S18



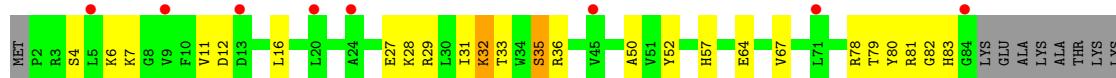
V66
R67
LYS

- Molecule 49: 30S ribosomal protein S18

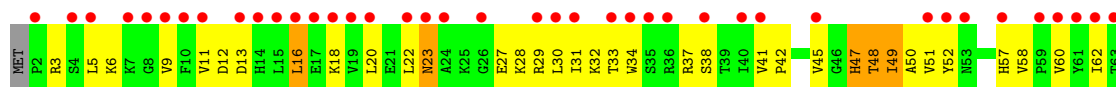




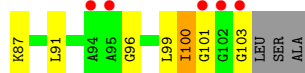
- Molecule 50: 30S ribosomal protein S19



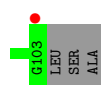
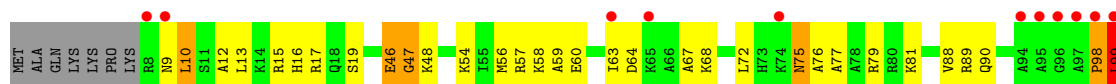
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

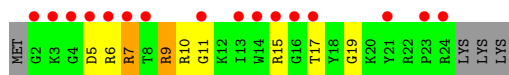


- Molecule 52: 30S ribosomal protein Thx





- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



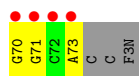
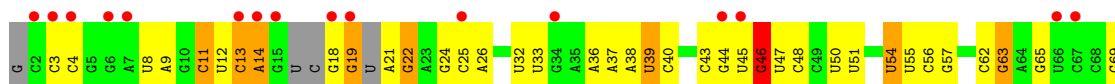
- Molecule 53: mRNA



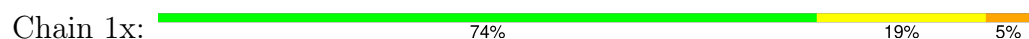
- Molecule 54: A-site tRNA



- 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: MA6, SF4, OMC, PSU, 7MG, OMU, MIA, UR3, 0TD, 4SU, MG, 2MA, 4OC, M2G, 31H, 5MC, OMG, K, 6IF, ZN, 5MU, 2MG

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
56	7MG	2y	46	56	23,26,27	1.34	2 (8%)	27,39,42	2.71	7 (25%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.10	2 (7%)
54	MIA	2w	37	54	24,27,32	1.99	5 (20%)	32,39,47	2.50	10 (31%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.20	6 (22%)
56	5MU	1y	54	56	19,22,23	1.46	4 (21%)	27,32,35	1.58	5 (18%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.79	3 (11%)
56	PSU	1y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.31	9 (27%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
56	MIA	2y	37	56	21,24,32	1.61	3 (14%)	30,35,47	2.09	10 (33%)
55	31H	1x	76	55,57	31,34,35	1.15	3 (9%)	35,47,50	2.05	12 (34%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.11	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	1x	8	55	18,21,22	2.05	6 (33%)	25,30,33	1.33	3 (12%)
32	PSU	1a	516	32	18,21,22	1.44	2 (11%)	21,30,33	1.98	4 (19%)
1	5MC	1A	1942	1,57	19,22,23	1.43	3 (15%)	26,32,35	1.20	2 (7%)
54	4SU	1w	8	54	18,21,22	1.82	5 (27%)	25,30,33	2.02	4 (16%)
56	PSU	2y	32	56	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.16	4 (19%)
54	7MG	1w	46	54	23,26,27	1.39	2 (8%)	27,39,42	2.55	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.95	3 (14%)
55	5MC	1x	32	55	19,22,23	1.84	3 (15%)	26,32,35	1.24	3 (11%)
56	7MG	1y	46	56	23,26,27	1.33	4 (17%)	27,39,42	2.64	7 (25%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.95	3 (14%)
56	PSU	2y	55	56	18,21,22	1.34	3 (16%)	21,30,33	2.00	4 (19%)
54	4SU	2w	8	54	18,21,22	1.66	3 (16%)	25,30,33	2.15	5 (20%)
1	5MC	2A	1962	1	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
1	PSU	1A	2605	1,57	18,21,22	1.43	4 (22%)	21,30,33	2.02	4 (19%)
56	MIA	1y	37	56	21,24,32	1.61	3 (14%)	30,35,47	2.02	9 (30%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.20	3 (14%)
56	4SU	2y	8	56	18,21,22	1.70	4 (22%)	25,30,33	2.17	5 (20%)
1	OMG	2A	2251	1,55	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
1	2MA	1A	2503	1,57	22,25,26	1.54	4 (18%)	32,37,40	2.29	8 (25%)
55	31H	2x	76	55,57	31,34,35	1.18	3 (9%)	35,47,50	2.06	12 (34%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.18	3 (11%)
1	5MC	1A	1962	1,57	19,22,23	1.65	3 (15%)	26,32,35	1.14	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.84	0
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.04	2 (8%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.05	9 (27%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.07	2 (8%)
32	4OC	2a	1402	32,57	20,23,24	0.79	0	25,32,35	1.14	3 (12%)
54	PSU	1w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.16	4 (19%)
43	0TD	1l	92	43	8,9,10	4.51	1 (12%)	6,11,13	5.91	2 (33%)
55	5MU	2x	54	55	19,22,23	1.45	5 (26%)	27,32,35	2.15	6 (22%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.90	3 (14%)
1	OMG	1A	2251	1,55,57	23,26,27	1.26	3 (13%)	32,38,41	1.95	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.89	5 (15%)
43	0TD	2l	92	43	8,9,10	4.57	1 (12%)	6,11,13	5.09	3 (50%)
56	5MU	2y	54	56	19,22,23	1.51	4 (21%)	27,32,35	1.98	8 (29%)
1	2MA	2A	2503	1,57	22,25,26	1.49	4 (18%)	32,37,40	2.34	8 (25%)
1	PSU	1A	1917	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	3 (14%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.80	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.09	5 (23%)
32	5MC	1a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.13	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.69	3 (15%)	26,32,35	1.18	2 (7%)
32	M2G	2a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.97	6 (18%)
56	4SU	1y	8	56	18,21,22	1.81	5 (27%)	25,30,33	2.11	4 (16%)
1	5MU	1A	1939	1	19,22,23	1.45	5 (26%)	27,32,35	2.12	7 (25%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.26	4 (15%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.13	3 (11%)
54	7MG	2w	46	54	23,26,27	1.36	2 (8%)	27,39,42	2.51	8 (29%)
54	PSU	1w	55	54	18,21,22	1.45	2 (11%)	21,30,33	2.03	4 (19%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
32	7MG	1a	527	32,57	23,26,27	1.46	4 (17%)	27,39,42	2.54	7 (25%)
56	PSU	1y	39	56	18,21,22	1.42	2 (11%)	21,30,33	1.89	3 (14%)
55	4SU	2x	8	55	18,21,22	1.99	5 (27%)	25,30,33	1.49	5 (20%)
54	PSU	1w	32	54,57	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.08	9 (27%)
54	5MU	1w	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.97	6 (22%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.05	6 (22%)
1	OMU	1A	2552	1,57	19,22,23	1.23	3 (15%)	25,31,34	1.81	5 (20%)
1	OMU	2A	2552	1,57	19,22,23	1.29	3 (15%)	25,31,34	1.99	6 (24%)
1	5MU	2A	1939	1,57	19,22,23	1.42	5 (26%)	27,32,35	2.27	6 (22%)
32	5MC	2a	1407	32	19,22,23	1.69	3 (15%)	26,32,35	1.22	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.16	3 (11%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.71	12 (31%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	2.06	9 (27%)
32	7MG	2a	527	32,57	23,26,27	1.33	4 (17%)	27,39,42	2.62	7 (25%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.14	9 (27%)
56	PSU	2y	39	56	18,21,22	1.35	2 (11%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	2605	1	18,21,22	1.31	3 (16%)	21,30,33	2.02	4 (19%)
54	5MU	2w	54	54	19,22,23	1.44	5 (26%)	27,32,35	1.76	6 (22%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
55	5MU	1x	54	55	19,22,23	1.42	6 (31%)	27,32,35	1.82	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	0/7/25/34	0/3/3/3
55	31H	1x	76	55,57	-	4/22/40/41	0/3/3/3
32	2MG	2a	1207	32	-	4/9/27/28	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,57	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
56	7MG	1y	46	56	-	4/7/37/38	0/3/3/3
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	4/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	0/7/25/34	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
1	2MA	1A	2503	1,57	-	2/7/25/26	0/3/3/3
55	31H	2x	76	55,57	-	3/22/40/41	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	4OC	2a	1402	32,57	-	2/9/29/30	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/9/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	4/7/12/14	-
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	1/7/37/38	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	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

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Mol	Chain	Res	Type	Atoms
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
56	2y	46	7MG	1	0
32	2a	967	5MC	2	0
1	1A	1915	5MU	1	0
56	1y	54	5MU	1	0
55	1x	8	4SU	2	0
56	2y	55	PSU	9	0
1	1A	2503	2MA	1	0
55	2x	76	31H	1	0
56	1y	55	PSU	2	0
32	2a	1404	5MC	1	0
32	1a	967	5MC	1	0
32	1a	1402	4OC	1	0
32	2a	1518	MA6	3	0
32	2a	1402	4OC	2	0
54	2w	39	PSU	2	0
1	1A	2251	OMG	1	0
43	2l	92	0TD	1	0
1	2A	2503	2MA	2	0
56	1y	8	4SU	2	0
1	1A	1939	5MU	1	0
55	2x	32	5MC	1	0
54	2w	46	7MG	1	0
54	1w	55	PSU	1	0
56	1y	39	PSU	1	0
55	2x	8	4SU	1	0
32	2a	1519	MA6	3	0
1	2A	1915	5MU	1	0
1	2A	2552	OMU	2	0
32	1a	1518	MA6	1	0
32	1a	1519	MA6	1	0
56	2y	39	PSU	2	0
54	2w	54	5MU	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
58	6IF	2A	3731	-	30,34,34	0.77	0	30,49,49	1.08	3 (10%)
60	SF4	1d	302	35	0,12,12	-	-	-		
60	SF4	2d	302	35	0,12,12	-	-	-		
58	6IF	1A	4109	-	30,34,34	1.02	1 (3%)	30,49,49	1.18	3 (10%)

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
58	6IF	2A	3731	-	-	2/22/65/65	0/3/3/3
60	SF4	1d	302	35	-	-	0/6/5/5
60	SF4	2d	302	35	-	-	0/6/5/5
58	6IF	1A	4109	-	-	4/22/65/65	0/3/3/3

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

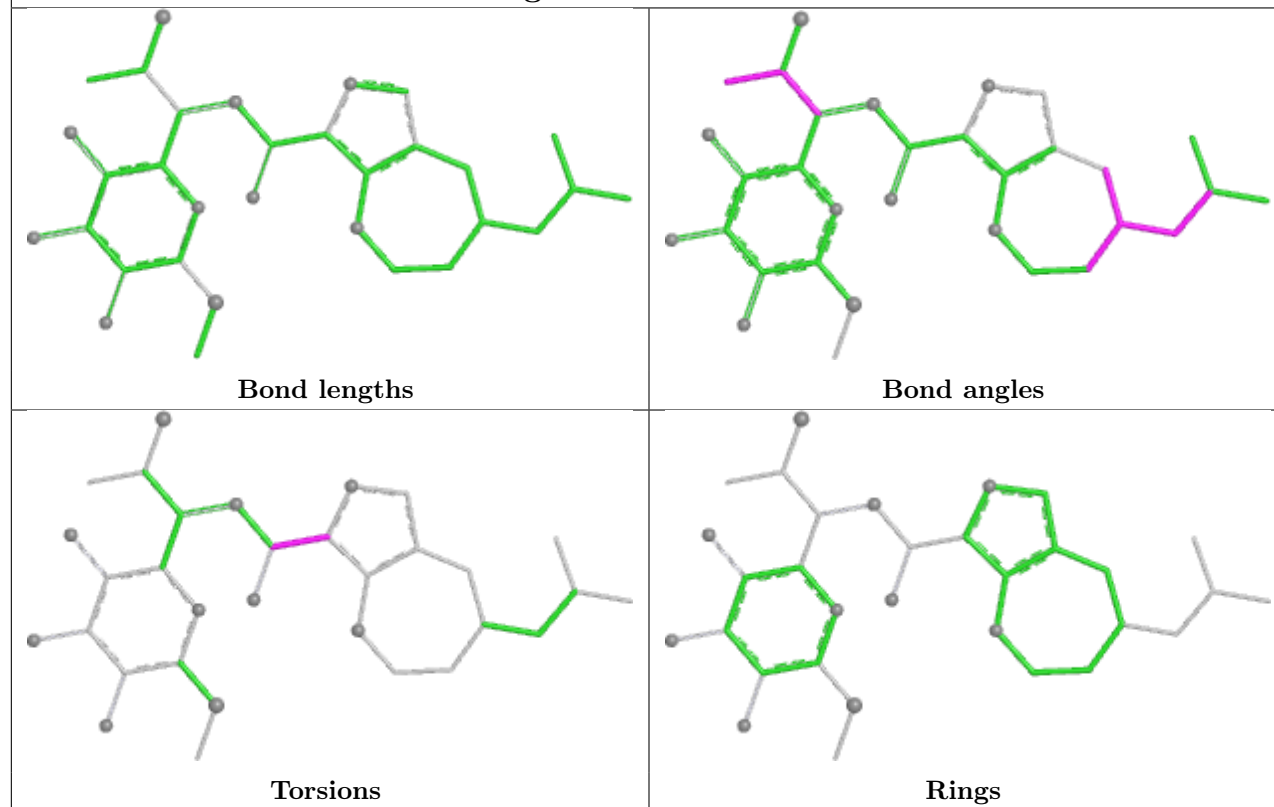
There are no ring outliers.

2 monomers are involved in 3 short contacts:

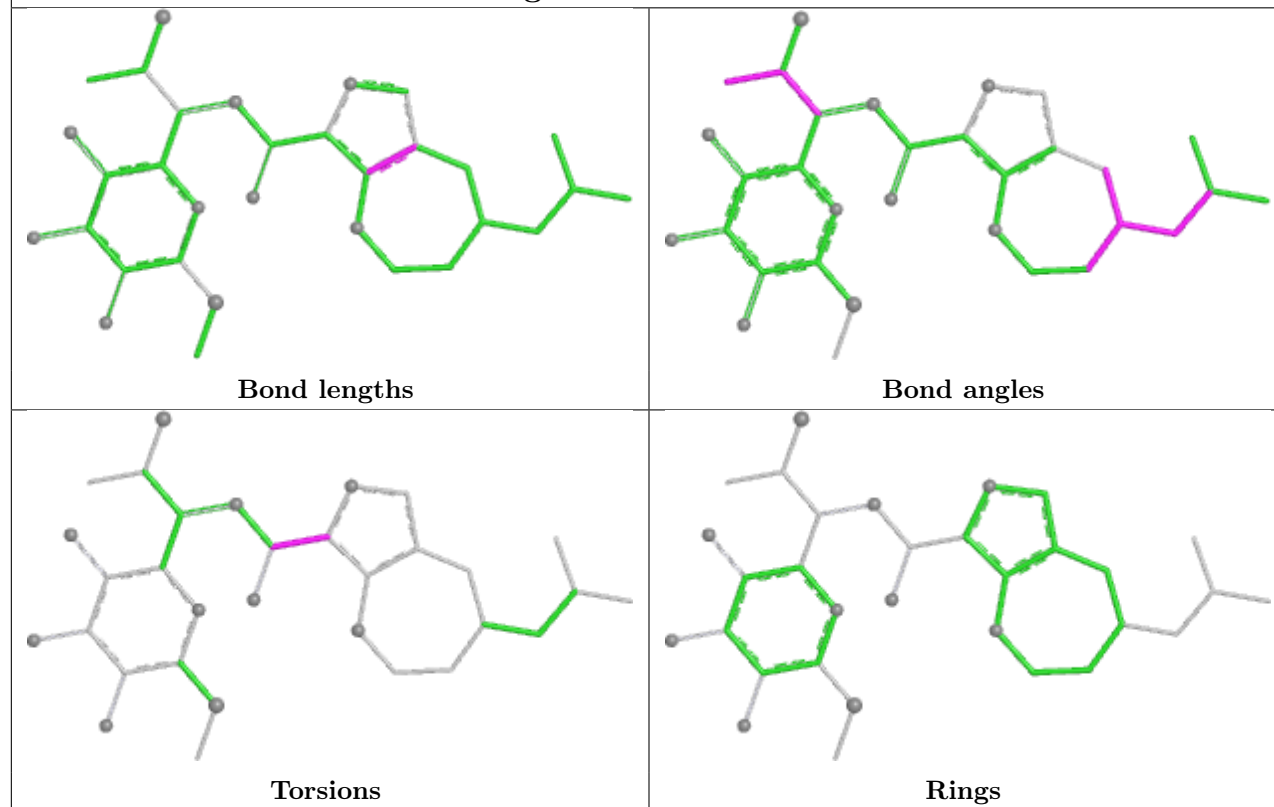
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2d	302	SF4	1	0
58	1A	4109	6IF	2	0

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.

Ligand 6IF 2A 3731



Ligand 6IF 1A 4109



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	1I	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	1I	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.