



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:55 AM UTC

PDB ID : 6XQE / pdb_00006xqe
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with sarecycline, UAA-mRNA, and deacylated P-site tRNA at 3.00Å resolution
Authors : Batool, Z.; Lomakin, I.B.; Bunick, C.G.; Polikanov, Y.S.
Deposited on : 2020-07-09
Resolution : 3.00 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

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

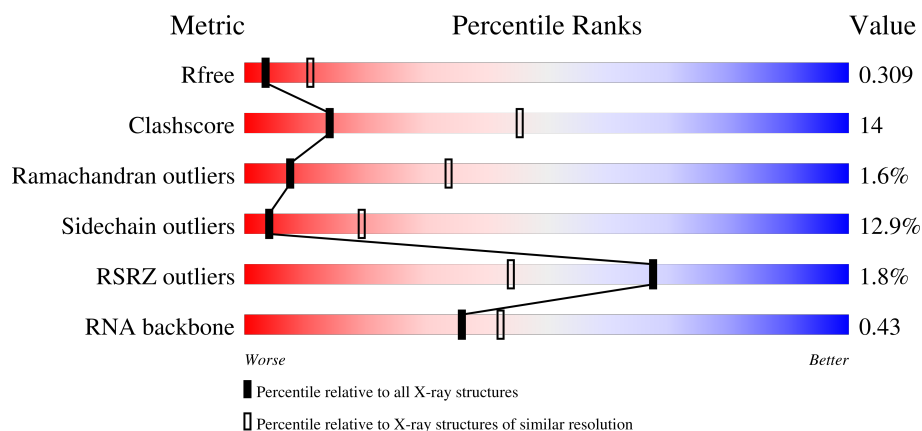
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



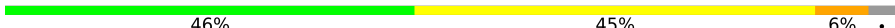
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	45% 44% 10% .
1	2A	2915	42% 44% 10% .
2	1B	121	55% 41% ..
2	2B	121	33% 51% 15% .

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

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

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Mol	Chain	Length	Quality of chain
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	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
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	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	

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
55	MG	1A	3793	-	-	-	X
59	SF4	1d	302	-	-	X	-
59	SF4	2d	303	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292071 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	122	Total	C	N	O	S	0	0	0
			951	587	197	165	2			
44	2m	121	Total	C	N	O	S	0	0	0
			943	581	196	164	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	10	Total	C	N	O	P	0	0	0
			217	98	44	65	10			
53	2v	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
54	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	1040	Total	Mg	0	0
			1040	1040		
55	1B	36	Total	Mg	0	0
			36	36		
55	1D	10	Total	Mg	0	0
			10	10		
55	1E	14	Total	Mg	0	0
			14	14		
55	1F	13	Total	Mg	0	0
			13	13		
55	1G	4	Total	Mg	0	0
			4	4		
55	1H	2	Total	Mg	0	0
			2	2		
55	1I	1	Total	Mg	0	0
			1	1		
55	1N	5	Total	Mg	0	0
			5	5		
55	1O	5	Total	Mg	0	0
			5	5		
55	1P	6	Total	Mg	0	0
			6	6		
55	1Q	5	Total	Mg	0	0
			5	5		
55	1R	7	Total	Mg	0	0
			7	7		
55	1S	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1T	2	Total 2	Mg 2	0	0
55	1U	8	Total 8	Mg 8	0	0
55	1V	4	Total 4	Mg 4	0	0
55	1W	9	Total 9	Mg 9	0	0
55	1X	4	Total 4	Mg 4	0	0
55	1Y	2	Total 2	Mg 2	0	0
55	1Z	3	Total 3	Mg 3	0	0
55	10	7	Total 7	Mg 7	0	0
55	11	3	Total 3	Mg 3	0	0
55	12	2	Total 2	Mg 2	0	0
55	13	5	Total 5	Mg 5	0	0
55	14	1	Total 1	Mg 1	0	0
55	15	4	Total 4	Mg 4	0	0
55	16	3	Total 3	Mg 3	0	0
55	17	7	Total 7	Mg 7	0	0
55	18	6	Total 6	Mg 6	0	0
55	19	2	Total 2	Mg 2	0	0
55	1a	212	Total 212	Mg 212	0	0
55	1b	1	Total 1	Mg 1	0	0
55	1d	1	Total 1	Mg 1	0	0
55	1e	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1f	2	Total 2	Mg 2	0	0
55	1l	3	Total 3	Mg 3	0	0
55	1n	3	Total 3	Mg 3	0	0
55	1t	1	Total 1	Mg 1	0	0
55	1v	5	Total 5	Mg 5	0	0
55	1x	13	Total 13	Mg 13	0	0
55	2A	850	Total 850	Mg 850	0	0
55	2B	20	Total 20	Mg 20	0	0
55	2D	8	Total 8	Mg 8	0	0
55	2E	5	Total 5	Mg 5	0	0
55	2F	6	Total 6	Mg 6	0	0
55	2G	1	Total 1	Mg 1	0	0
55	2O	1	Total 1	Mg 1	0	0
55	2P	4	Total 4	Mg 4	0	0
55	2Q	4	Total 4	Mg 4	0	0
55	2R	1	Total 1	Mg 1	0	0
55	2T	4	Total 4	Mg 4	0	0
55	2U	2	Total 2	Mg 2	0	0
55	2V	1	Total 1	Mg 1	0	0
55	2W	1	Total 1	Mg 1	0	0
55	2X	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2Y	2	Total 2	Mg 2	0	0
55	2Z	2	Total 2	Mg 2	0	0
55	21	6	Total 6	Mg 6	0	0
55	23	3	Total 3	Mg 3	0	0
55	25	4	Total 4	Mg 4	0	0
55	26	1	Total 1	Mg 1	0	0
55	27	2	Total 2	Mg 2	0	0
55	28	3	Total 3	Mg 3	0	0
55	2a	216	Total 216	Mg 216	0	0
55	2d	2	Total 2	Mg 2	0	0
55	2e	2	Total 2	Mg 2	0	0
55	2f	2	Total 2	Mg 2	0	0
55	2g	1	Total 1	Mg 1	0	0
55	2i	1	Total 1	Mg 1	0	0
55	2j	2	Total 2	Mg 2	0	0
55	2k	1	Total 1	Mg 1	0	0
55	2l	2	Total 2	Mg 2	0	0
55	2n	1	Total 1	Mg 1	0	0
55	2q	2	Total 2	Mg 2	0	0
55	2r	1	Total 1	Mg 1	0	0
55	2t	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2x	7	Total	Mg	0	0
			7	7		

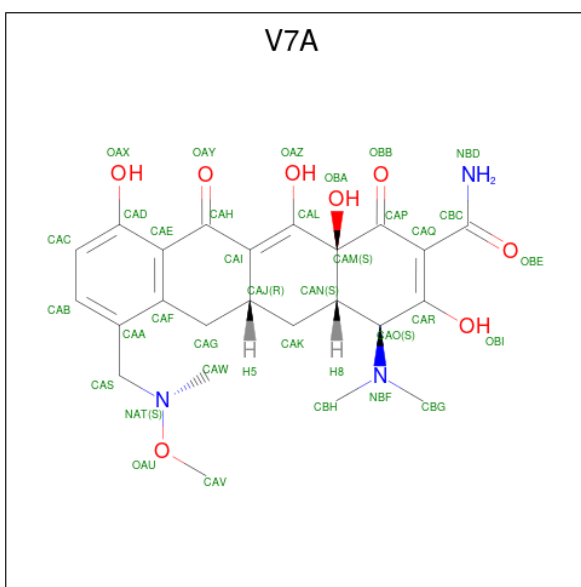
- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1	Total	K	0	0
			1	1		
56	2A	1	Total	K	0	0
			1	1		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

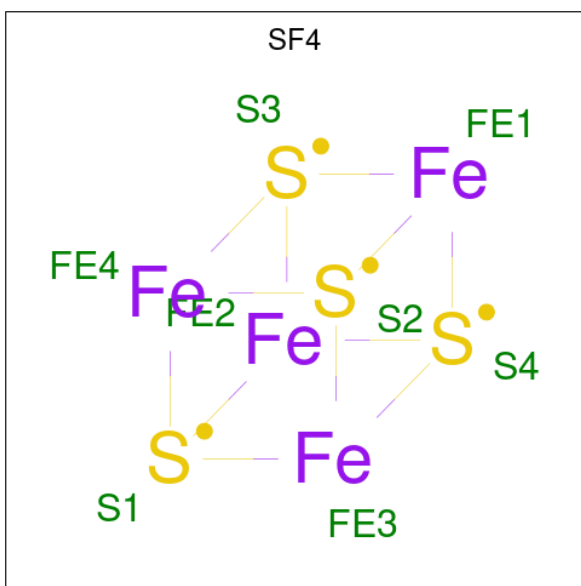
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	1n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		

- Molecule 58 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1a	1	Total	C	N	O	0	0
			35	24	3	8		
58	2a	1	Total	C	N	O	0	0
			35	24	3	8		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1402	Total 1402	O 1402	0	0
60	1B	54	Total 54	O 54	0	0
60	1D	21	Total 21	O 21	0	0
60	1E	18	Total 18	O 18	0	0
60	1F	9	Total 9	O 9	0	0
60	1G	4	Total 4	O 4	0	0
60	1H	1	Total 1	O 1	0	0
60	1I	1	Total 1	O 1	0	0
60	1N	5	Total 5	O 5	0	0
60	1O	8	Total 8	O 8	0	0
60	1P	18	Total 18	O 18	0	0
60	1Q	7	Total 7	O 7	0	0
60	1R	9	Total 9	O 9	0	0
60	1S	4	Total 4	O 4	0	0
60	1T	4	Total 4	O 4	0	0
60	1U	14	Total 14	O 14	0	0
60	1V	10	Total 10	O 10	0	0
60	1W	8	Total 8	O 8	0	0
60	1X	4	Total 4	O 4	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	10	11	Total 11	O 11	0	0
60	11	8	Total 8	O 8	0	0
60	12	3	Total 3	O 3	0	0
60	13	3	Total 3	O 3	0	0
60	14	1	Total 1	O 1	0	0
60	15	6	Total 6	O 6	0	0
60	16	4	Total 4	O 4	0	0
60	17	10	Total 10	O 10	0	0
60	18	8	Total 8	O 8	0	0
60	1a	211	Total 211	O 211	0	0
60	1b	1	Total 1	O 1	0	0
60	1d	2	Total 2	O 2	0	0
60	1e	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1l	4	Total 4	O 4	0	0
60	1m	1	Total 1	O 1	0	0
60	1q	2	Total 2	O 2	0	0
60	1u	2	Total 2	O 2	0	0
60	1v	3	Total 3	O 3	0	0
60	1x	11	Total 11	O 11	0	0
60	2A	680	Total 680	O 680	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2B	24	Total 24	O 24	0	0
60	2D	12	Total 12	O 12	0	0
60	2E	13	Total 13	O 13	0	0
60	2F	10	Total 10	O 10	0	0
60	2I	1	Total 1	O 1	0	0
60	2O	2	Total 2	O 2	0	0
60	2P	4	Total 4	O 4	0	0
60	2Q	2	Total 2	O 2	0	0
60	2R	3	Total 3	O 3	0	0
60	2T	4	Total 4	O 4	0	0
60	2U	1	Total 1	O 1	0	0
60	2W	2	Total 2	O 2	0	0
60	2X	2	Total 2	O 2	0	0
60	2Y	1	Total 1	O 1	0	0
60	2Z	3	Total 3	O 3	0	0
60	2I	10	Total 10	O 10	0	0
60	23	1	Total 1	O 1	0	0
60	27	1	Total 1	O 1	0	0
60	28	2	Total 2	O 2	0	0
60	29	1	Total 1	O 1	0	0
60	2a	173	Total 173	O 173	0	0

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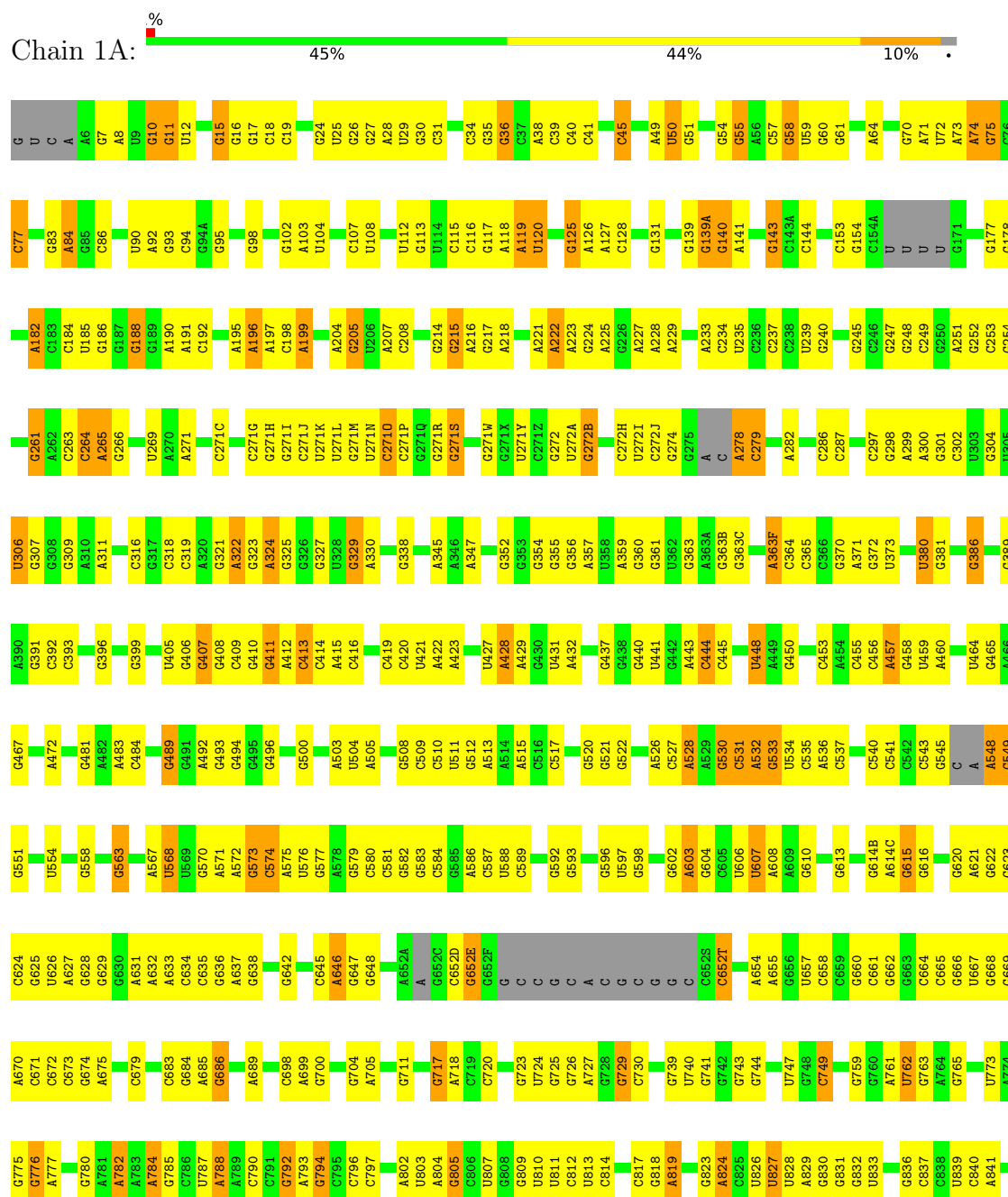
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2e	2	Total	O	0	0
			2	2		
60	2g	1	Total	O	0	0
			1	1		
60	2i	1	Total	O	0	0
			1	1		
60	2j	4	Total	O	0	0
			4	4		
60	2l	3	Total	O	0	0
			3	3		
60	2n	1	Total	O	0	0
			1	1		
60	2t	3	Total	O	0	0
			3	3		
60	2v	1	Total	O	0	0
			1	1		
60	2x	5	Total	O	0	0
			5	5		

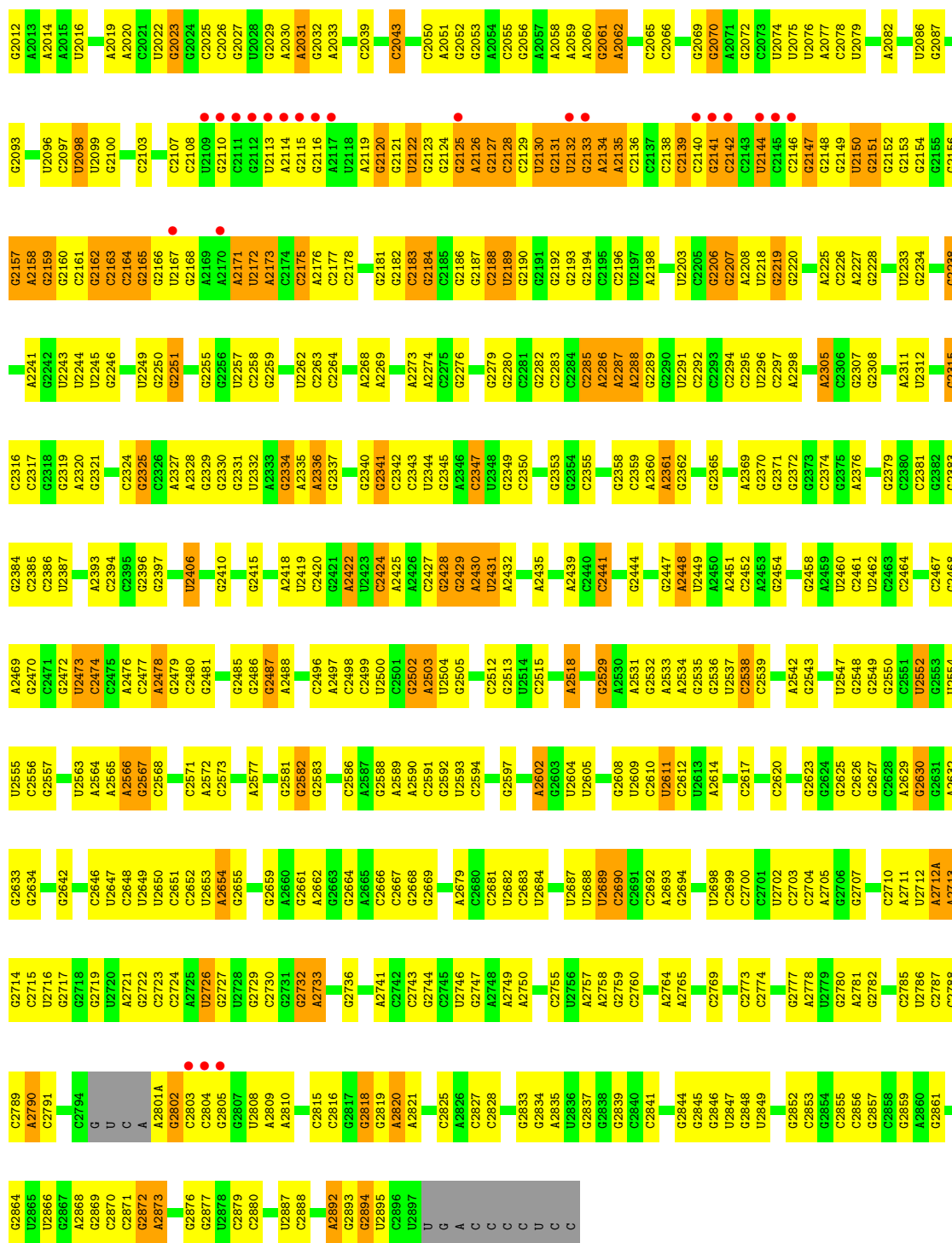
3 Residue-property plots

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

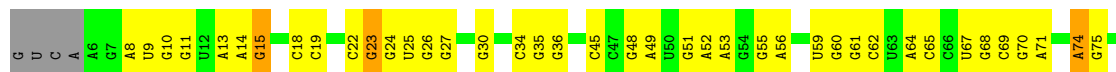
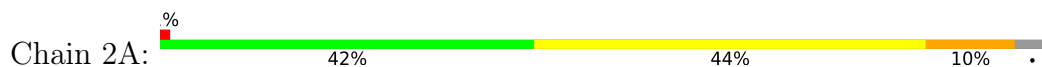
• Molecule 1: 23S Ribosomal RNA



G1929	G1842	U1766	G1685	C1557	G1484	U1396	G1309	G1237	C1153	A1077	G1011	G928	G848
G1930	C1843	C1767	G1666	A1558	G1485	G1400	G1310	G1238	C1154	U1078	U1012	G928	A849
U1931	C1844	U1768	G1667	A1559	A1486	G1401	G1311	G1239	G1155	C1079	C1013	G932	G852
G1932	G1845	G1769	A1668	C1565	G1487	C1402	U1312	G1240	A1156	U1082	G1016	G938	
G1933	G1846	G1770	A1669	C1566	A1490	G1405	U1313	G1241	C1157				C857
G1935	A1847	A1773	G1670	A1567	C1493	U1406	U1316	G1248	C1158	A1085	A1020	G942	U858
A1936	A1848		U1671	G1568	U1497	C1407	A1317	U1249	U1159	A1086	A1021	U943	C859
A1937	G1849	U1778	G1674	A1572	C1498	U1408	U1318	G1250	G1087	G1087	G1022	U944	U860
A1938	A1850	U1779	C1675	A1573	U1499	A1412	G1319	G1251	U1164	G1088	U1023	A945	A861
U1939	U1851	U1780	A1676	U1574	G1500	G1413	C1320	G1252	U1165	G1089	G1024	G946	C862
U1940		G1781	A1676	U1575	C1501	G1416	A1321	A1253	U1167	U1090	G1025	G947	A863
C1941	G1858	G1782	U1680	A1579	G1504	G1417		A1254	C1168	C1092	U1026		U868
C1942	A1859	A1783	G1681	U1580	C1505	C1418	G1324	U1256	G1169	G1093	A1027	C955	C869
U1943	G1860	U1784	G1682	G1581	C1506	A1419	G1325	U1257	G1170	U1094	A1028	G956	A870
U1944	G1861	A1785	C1683	C1584	U1507	G1420	A1331	C1258	G1171	U1095	A1029	U958	U871
G1945	G1862	G1786	C1684	A1586	A1508	A1421	G1332	G1259	G1173	A1096	G1030	A959	A872
	G1863	A1787	C1685	A1587	C1509			G1260	A1174		U1033	A960	G873
U1951	U1864	C1788		C1588	C1509	G1424	A1336	G1261	U1175	U1101		C961	
A1952	G1865	A1789	U1688	C1589	C1509	G1425	A1337	G1262	U1176	C1102	G1036	G962	G879
A1953	C1866	C1790	U1689	G1595	A1509B	G1426	G1337	A1262	A1177	A1103	U1039	U963	G880
U1954	A1876	G1791	G1696	A1596	G1510	G1428	G1338	U1263	C1178	C1104	G1040	C964	G881
U1955	A1877	G1792	G1697	A1597	C1511	G1429	G1343	G1264	C1179	U1105	G1041	G965	G882
	G1878	G1793		U1603	U1512	G1428	A1342	A1265	C1180	G1107	G1042	G966	G883
C1958	C1879	U1794	C1604	C1604	C1513	G1429	G1343	G1266	G1183	G1108	G1043	C967	C884
		C1795	A1700	A1701	U1514	G1430	G1344	U1267	G1184	U1109	G1044	C970	C885
		U1796	G1702	C1607	U1515	U1431		A1268	C1185	G1110	A1045	C971	C886
C1962	C1882	U1797	G1702	A1608	U1516	U1431	U1352	G1270	G1186	A1111	A1046	G972	A887
U1963	G1883	U1798	G1703	A1609	U1517	A1439	G1355	G1271	G1187	G1112	G1047	A973	C889
G1964	A1884	U1798	G1703	A1609	U1518	G1440	G1355	A1272	U1188	U1113	A1048	G974	A890
C1965	A1885	G1799	U1706	A1610	U1519	G1441	G1355	U1273	A1189	G1114	G1049	C975	G892
A1966	U1706	C1800	U1706	A1610	G1520	G1442	A1359	A1274	C1201	G1115	A1050	C976	C893
C1967	A1889	G1801	C1710	A1614	U1523	G1443	A1360	A1275	G1202	C1116	C1052	A984	C894
G1968	A1890	A1802	C1711	C1615	G1524	A1445	G1361	A1276	G1203		C1053	G987	U895
A1969	G1891	A1803	C1712	A1616	U1525	C1445A	G1364	A1276	G1209	G1119	A1054	A988	A896
U1970	C1892	C1712	G1712	G1617	G1526		A1365	G1279	G1209	G1125	G1055	A989	C897
A1971		U1720	U1720	A1618	G1527	G1448	G1365	G1281	A1210	G1129	G1056	A990	C904
G1972	G1899	G1807	G1721	G1626	A1528	A1449	C1370	G1281	U1211	U1130	A1057	C991	U905
C1973	A1900	U1808	G1721	G1626	A1529	G1450	G1371	G1281	G1212	G1131	G1058	C992	C906
C1974		A1809	A1722	G1626	A1530	G1450A	C1371	G1281	G1213	U1132	U1059	G993	U907
		G1814	A1741	C1636	C1532	G1451	C1372	A1286	A1214	U1133	U	C994	
		A1815	G1742	C1639	U	U	A1373	A1287	G1215	C1135	G1062	C995	A910
		G1816	C1743	U1639	A	A	G1374	U1288	G1220	G1136	C1064	A996	A911
		G1817	A1641	A1641	C	C	C1375	C1289	G1223	G1137	U1065	G997	C914
		U1820	C1745A	G1647	G1537	G1456	G1376	G1290	A1220	G1138	U1066		C915
		A1825	G1746	G1647	G1541	G1466	G1377	C1291	G1223	G1139	A1067	A1000	
		G1826	G1747	G1648	G1542	G1467	A1378	U1292	G1224	G1140	A1068	A1001	
		C1827	A1749	G1650	A1542	C1468	G1379	U1293	G1226	U1141	G1069	G1002	
		G1828	G1756	G1651	A1545	A1471		C1297	A1226	U1142	A1070	G1003	A918
		A1829	U1757	A1655	C1546	A1472	A1384	C1298	G1229	U142A	A1070	C1004	
		C1832	G1758	C1656	C1547	A1473	G1385	G1299	G1229	A142A	G1071	C1005	U922
		U1833	A1759	C1657	C1548	A1477	C1386	U1300	G1230	G1143	G1072	C1006	C923
		G1834	A1760	C1658	C1549	G1478	C1387	A1301	G1231	A1144	C1073	C1007	C924
		G1835	U1659	C1659	C1550	G1479	G1388	C1304	G1232	C1145	A1074	C1007	C925
		C1836	G1660	C1660	C1551	G1480	G1389	C1305	G1235	G1149	C1075	A1009	A926
		U1837	G1661	A1554	A1554	U1481	U1394	C1305	G1236	C1150	C1076	A1010	G927
		C1838	C1765			G1482	A1395	A1308					



• Molecule 1: 23S Ribosomal RNA



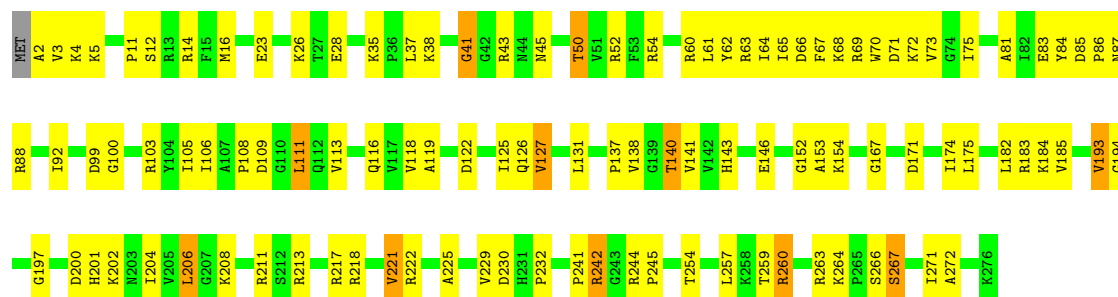
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U	G1031	C964	C888	G623		G666	U614	G545	A479	A371	G298	C253	G79
A	A1032	C965	C889	A824	A752	U667	U614A	C	A480	G372	A299		G80
A	U1033	G966	A890	C825	A752	U668	U614B	A	A481		A300	A256	G81
U		C967	C892	U826	C753	G669	A614C	A	A482	G379	G301	A257	G82
A		G968	C893	U827	C754	A670	U615	G549	A483	U380	G302	G258	G83
G	G1038	U969	C894	U828	C755	C671	U616	G551	A484	U383	U303	G259	A84
C	G1039	U970	U965	A829		C672	C618	G552	C485	U384			G85
U	C1040	C971	A896	G830	G759	C673	A621		C486	A262	G307	A262	
C	G1042	G972	A897	G831	A761	U674		U557	G308	C263	G308	C264	G89
C	C1043	A973	C898	G832	A761	A675		G558	C263	C264	G309	C264	U90
G		G974	A899	U833	U762	A676	U626	G559	A310	A265	A196	A265	A92
A		C975	A900		U763		U627	G560	A311	G266	A197	G266	G93
A		G975A	A901	G836	G763	C679	G628	G561	G312	C267	C198	C267	C94
G								G562	C313	U268	A199	G268	G94
G								G563	A314	U269	U200	G269	G95
G								A567	G315		C201		
U								U568	C316	U271E	U202	U271E	G98
U								U569	G317	C271F	C203	C271F	
U								G570	C318	C271G	A204		G102
U								A571	C319	G271H	G205		A103
U								A572	A320	G271I	U206		U104
U								G573	G321	C271J	A207		C105
U								A574	A322	U271K	C208		C106
U								G575	G323	U271L	C209		
U								C574	A324	G271M	C210		G113
U								A575	G325	U271N	C211		U114
U								U576			G212		C115
U								G577	G329	G271Q	A213		A118
U								A578	A330	G271R	G214		A119
U								G579	A331	G271S	G215		U120
U								C580	A332	C271T	A216		G121
U								C581	G333	G271U	G217		G122
U								G582	C334	G271V	A222		G123
U								G583	C335		G224		G124
U								A586	G338	U271Y	A225		G125
U								C587	U339	C271Z	G226		A126
U								U588	A340	U272A	A127		A127
U								C589	G341	G272B	A228		
U								A590	G342	G272C	A229		G131
U								C591	C343	G272D			
U								G592	G346	G272E	G232		G136
U								U593	A347		A233		G143
U								C595	G348	G276	C234		C143
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U								U599	G356		C237		
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U								C601	U284	U284	A241		U157
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U								G604	U	U	U243		U
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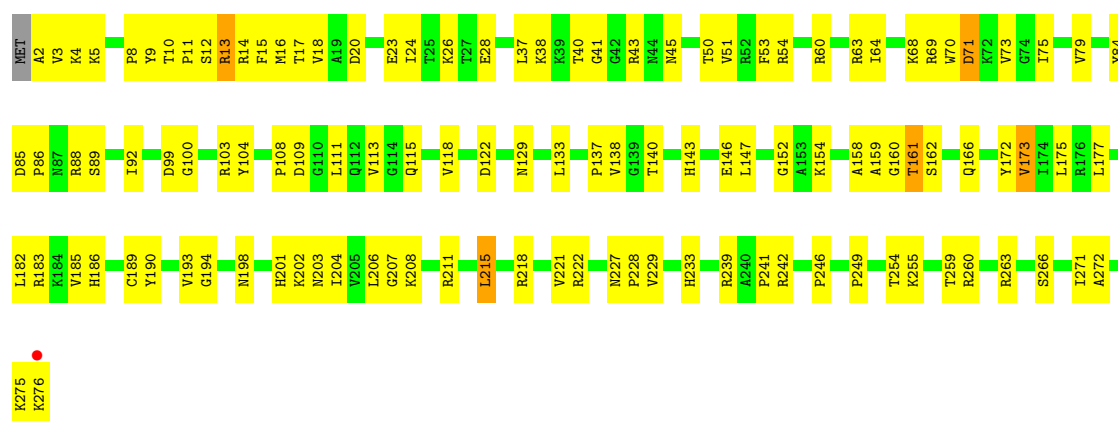
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  60% 36%



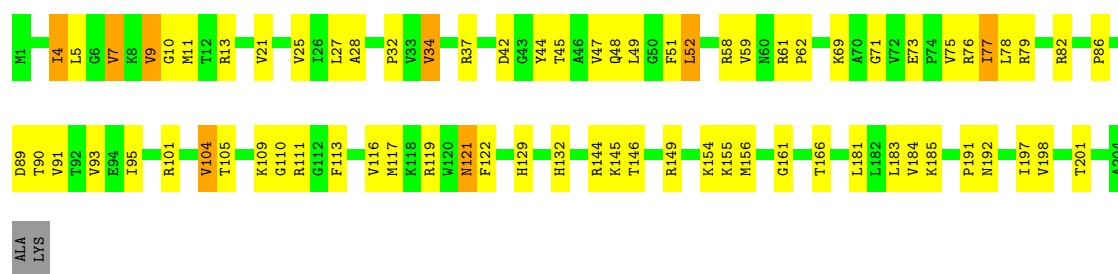
- Molecule 3: 50S ribosomal protein L2

Chain 2D:  57% 41%



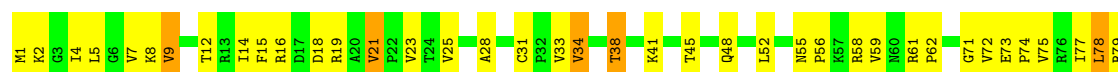
- Molecule 4: 50S ribosomal protein L3

Chain 1E:  64% 32%

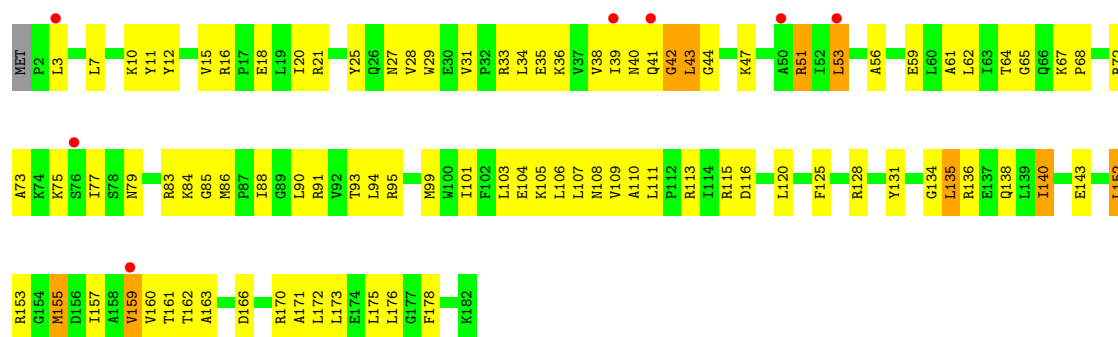


- Molecule 4: 50S ribosomal protein L3

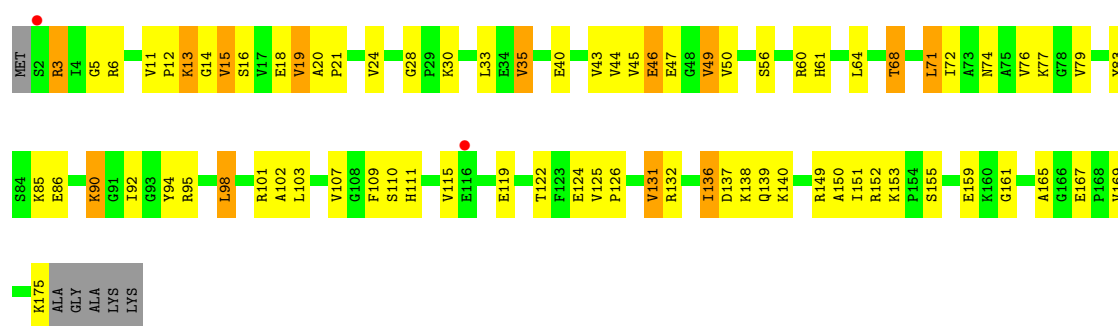
Chain 2E:  54% 40%



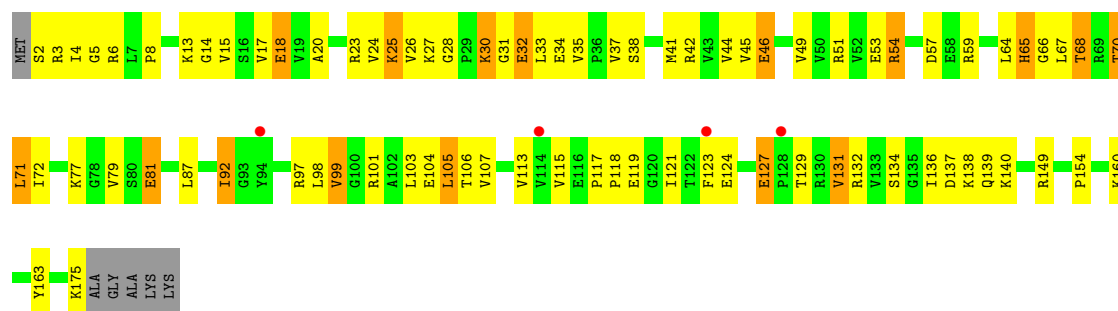




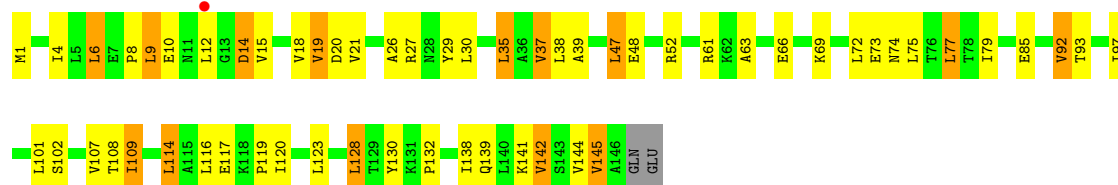
• Molecule 7: 50S ribosomal protein L6



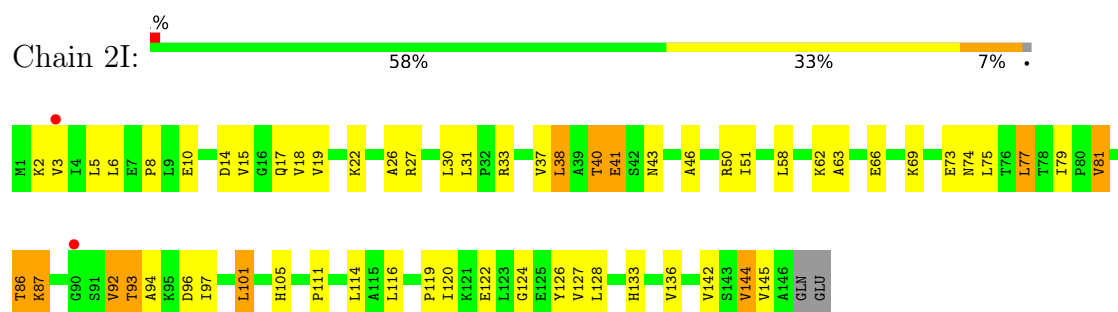
• Molecule 7: 50S ribosomal protein L6



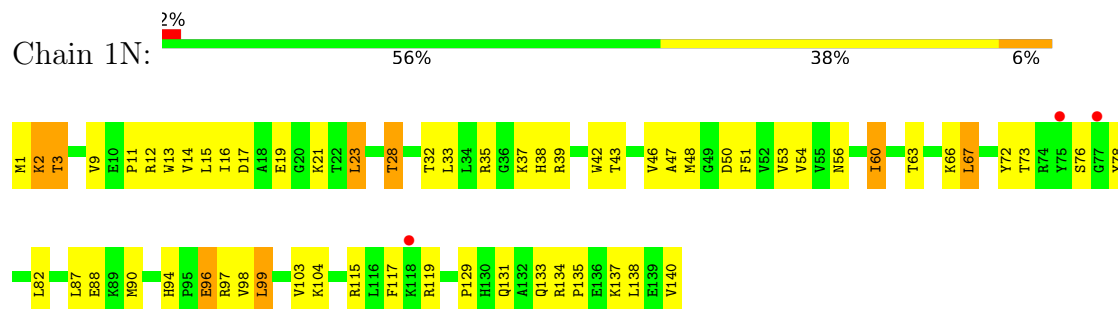
• Molecule 8: 50S ribosomal protein L9



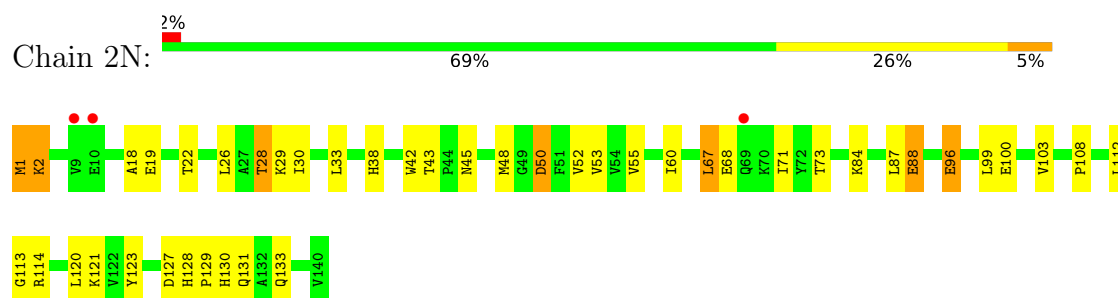
• Molecule 8: 50S ribosomal protein L9



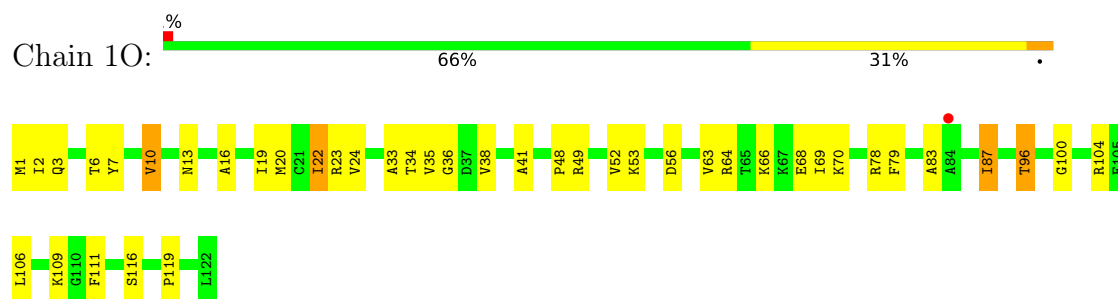
- Molecule 9: 50S ribosomal protein L13



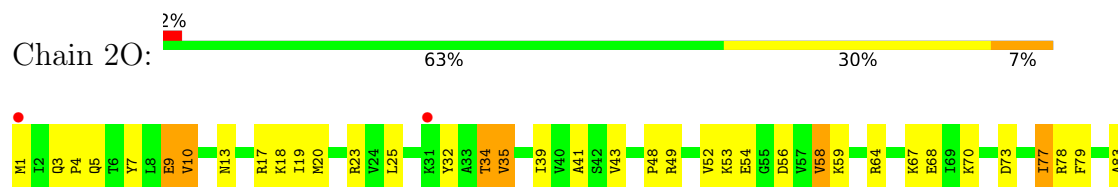
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14





- Molecule 11: 50S ribosomal protein L15



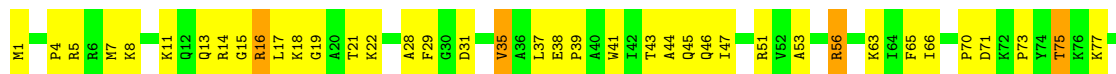
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

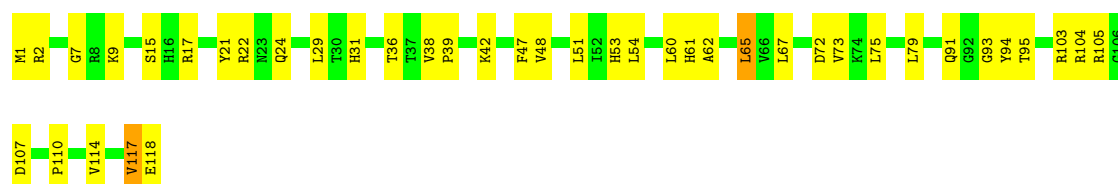


- Molecule 12: 50S ribosomal protein L16

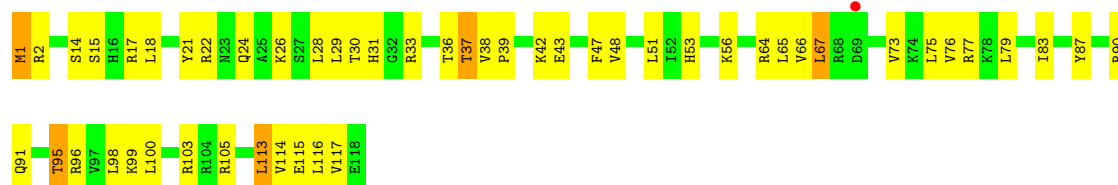


- Molecule 13: 50S ribosomal protein L17





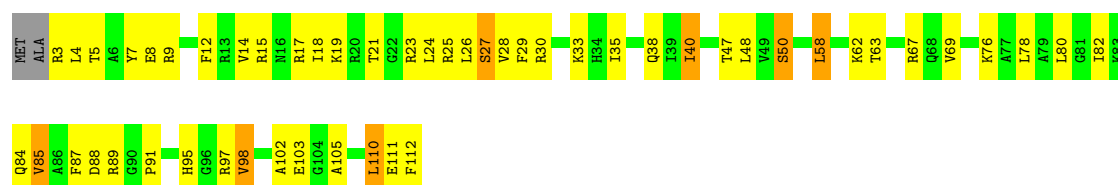
- Molecule 13: 50S ribosomal protein L17



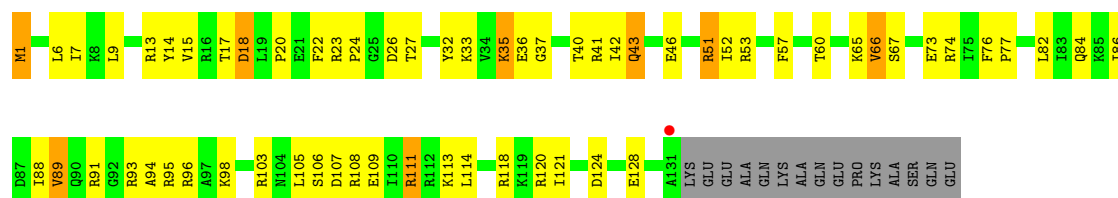
- Molecule 14: 50S ribosomal protein L18



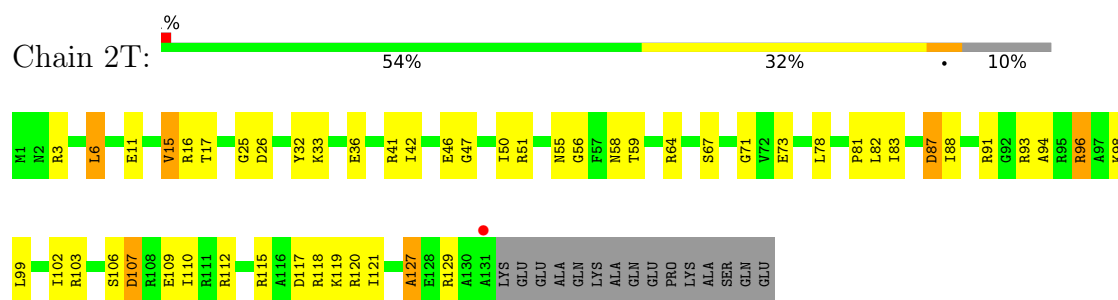
- Molecule 14: 50S ribosomal protein L18



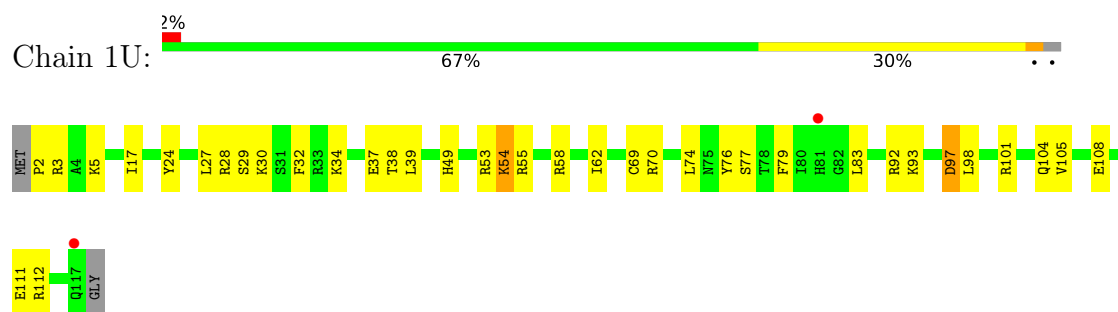
- Molecule 15: 50S ribosomal protein L19



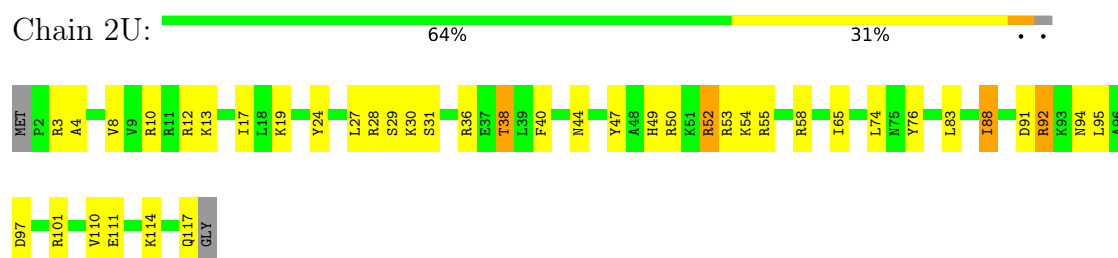
- Molecule 15: 50S ribosomal protein L19



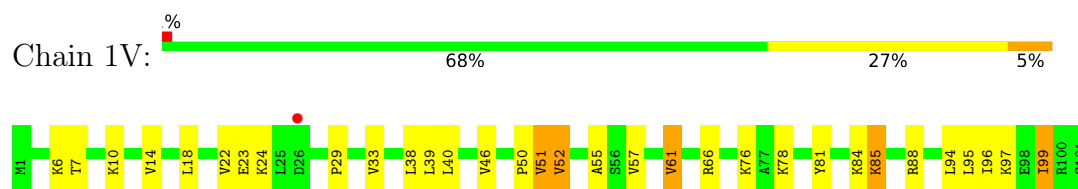
- Molecule 16: 50S ribosomal protein L20



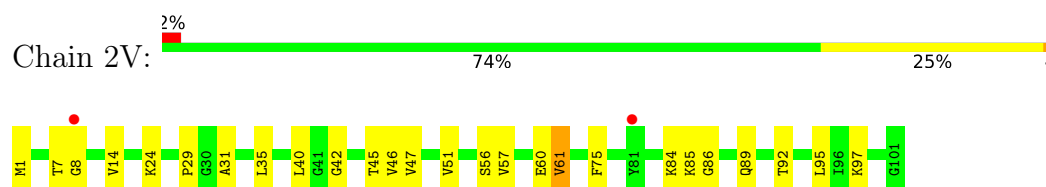
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



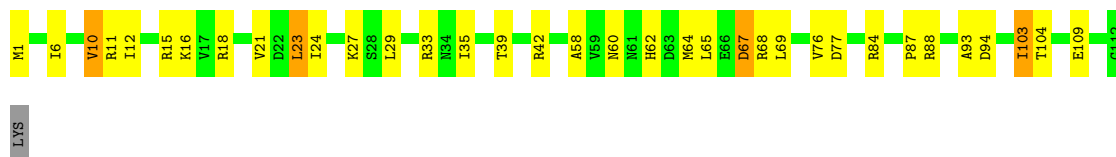
- Molecule 18: 50S ribosomal protein L22





- Molecule 18: 50S ribosomal protein L22

Chain 2W: 68% 27%



- Molecule 19: 50S ribosomal protein L23

Chain 1X: 71% 25%



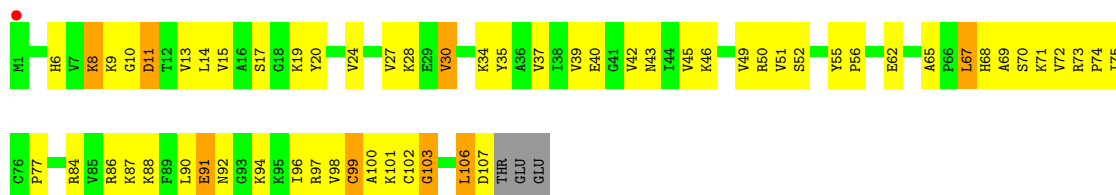
- Molecule 19: 50S ribosomal protein L23

Chain 2X: 67% 31%



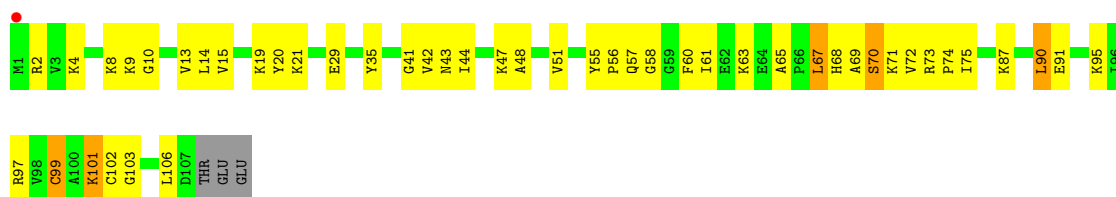
- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 43% 47% 7%

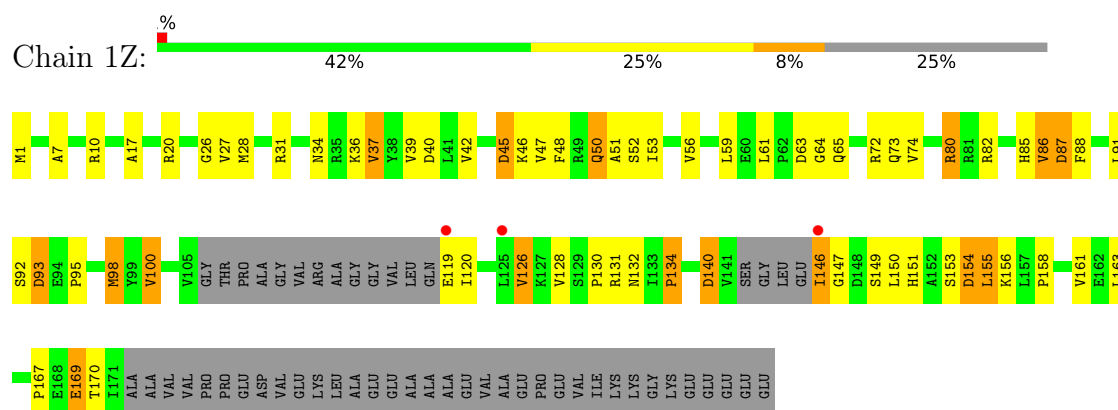


- Molecule 20: 50S ribosomal protein L24

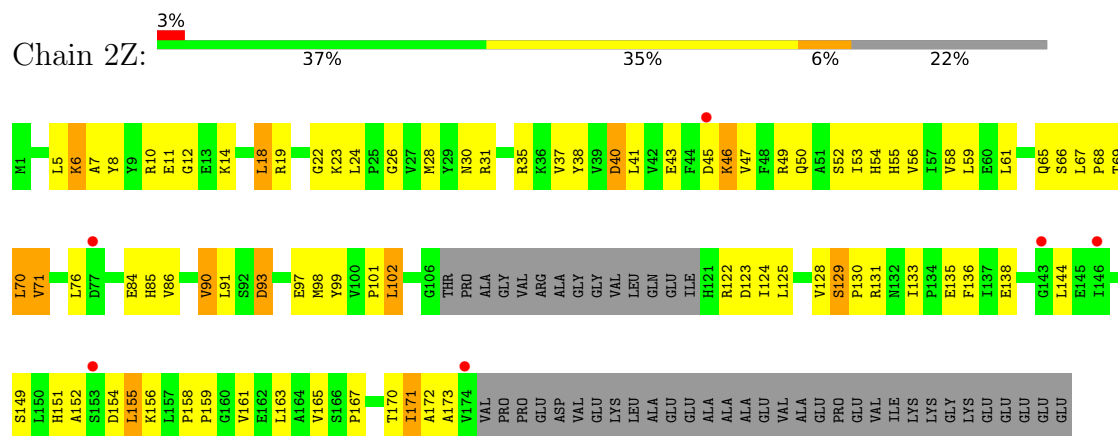
Chain 2Y: 55% 38% 5%



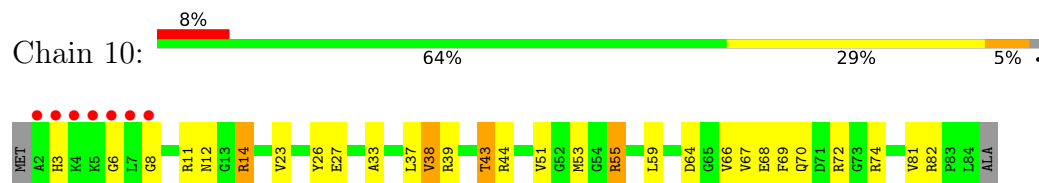
- Molecule 21: 50S ribosomal protein L25



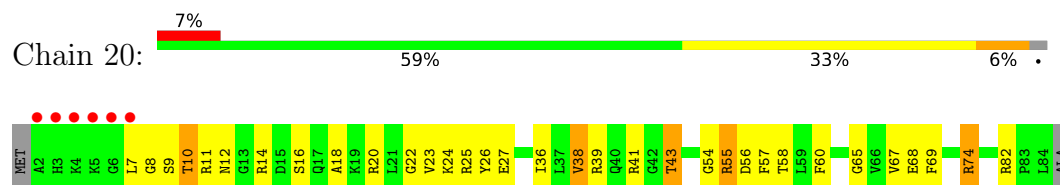
- Molecule 21: 50S ribosomal protein L25



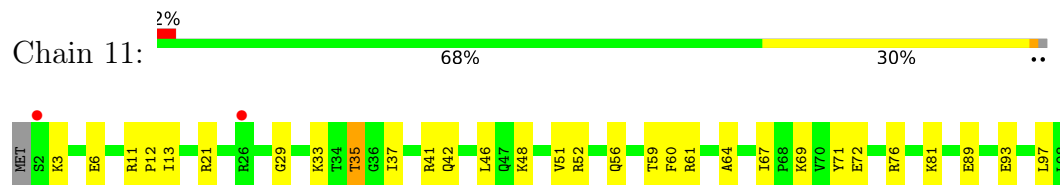
- Molecule 22: 50S ribosomal protein L27



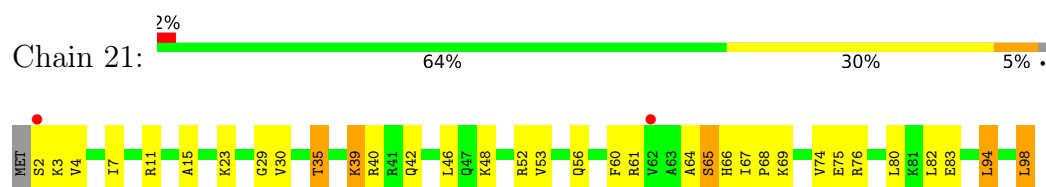
- Molecule 22: 50S ribosomal protein L27



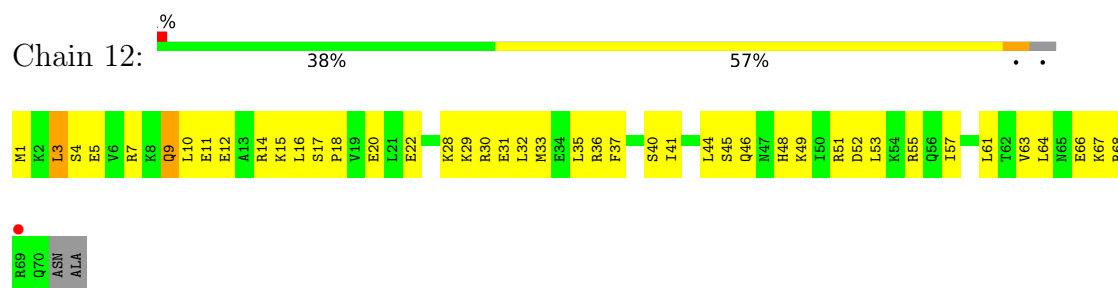
- Molecule 23: 50S ribosomal protein L28



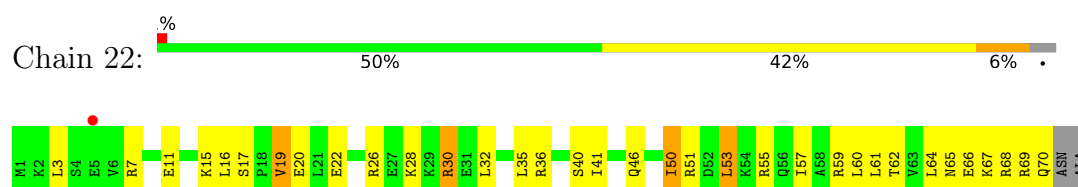
- Molecule 23: 50S ribosomal protein L28



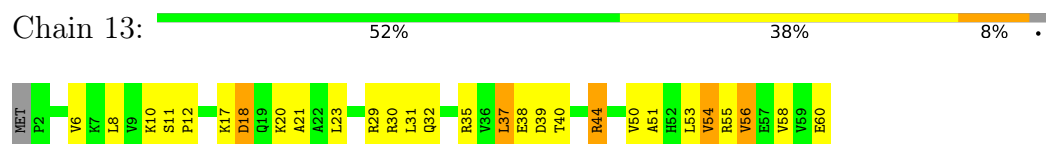
• Molecule 24: 50S ribosomal protein L29



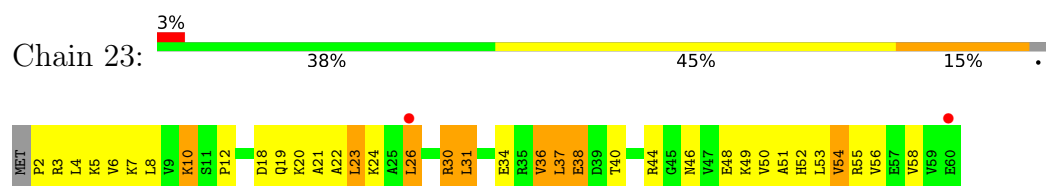
• Molecule 24: 50S ribosomal protein L29



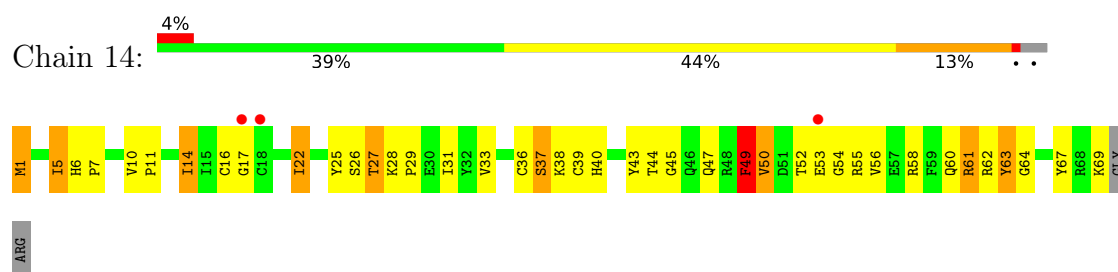
• Molecule 25: 50S ribosomal protein L30



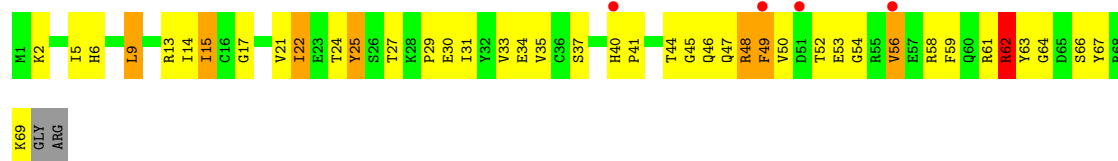
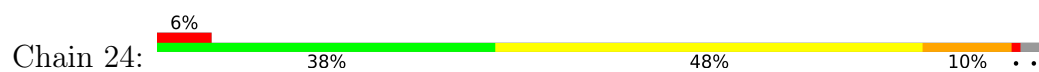
• Molecule 25: 50S ribosomal protein L30



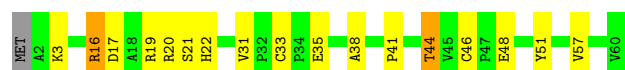
• Molecule 26: 50S ribosomal protein L31



• Molecule 26: 50S ribosomal protein L31



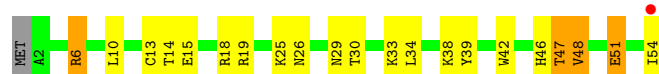
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



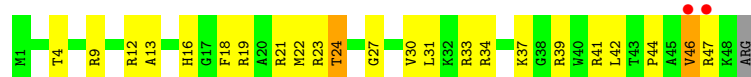
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

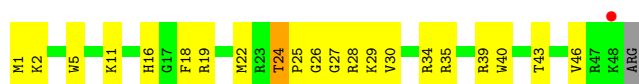


- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

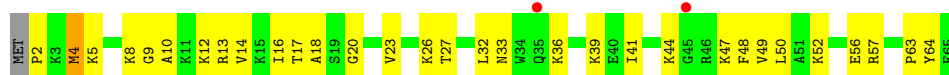




- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



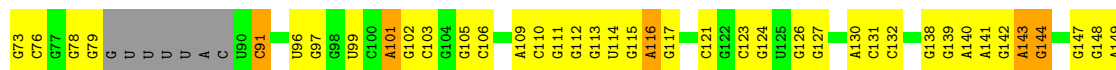
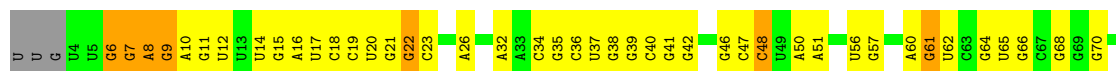
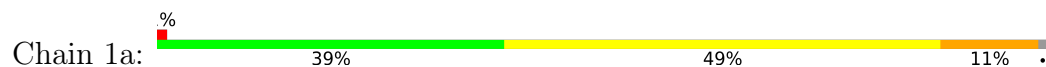
- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36



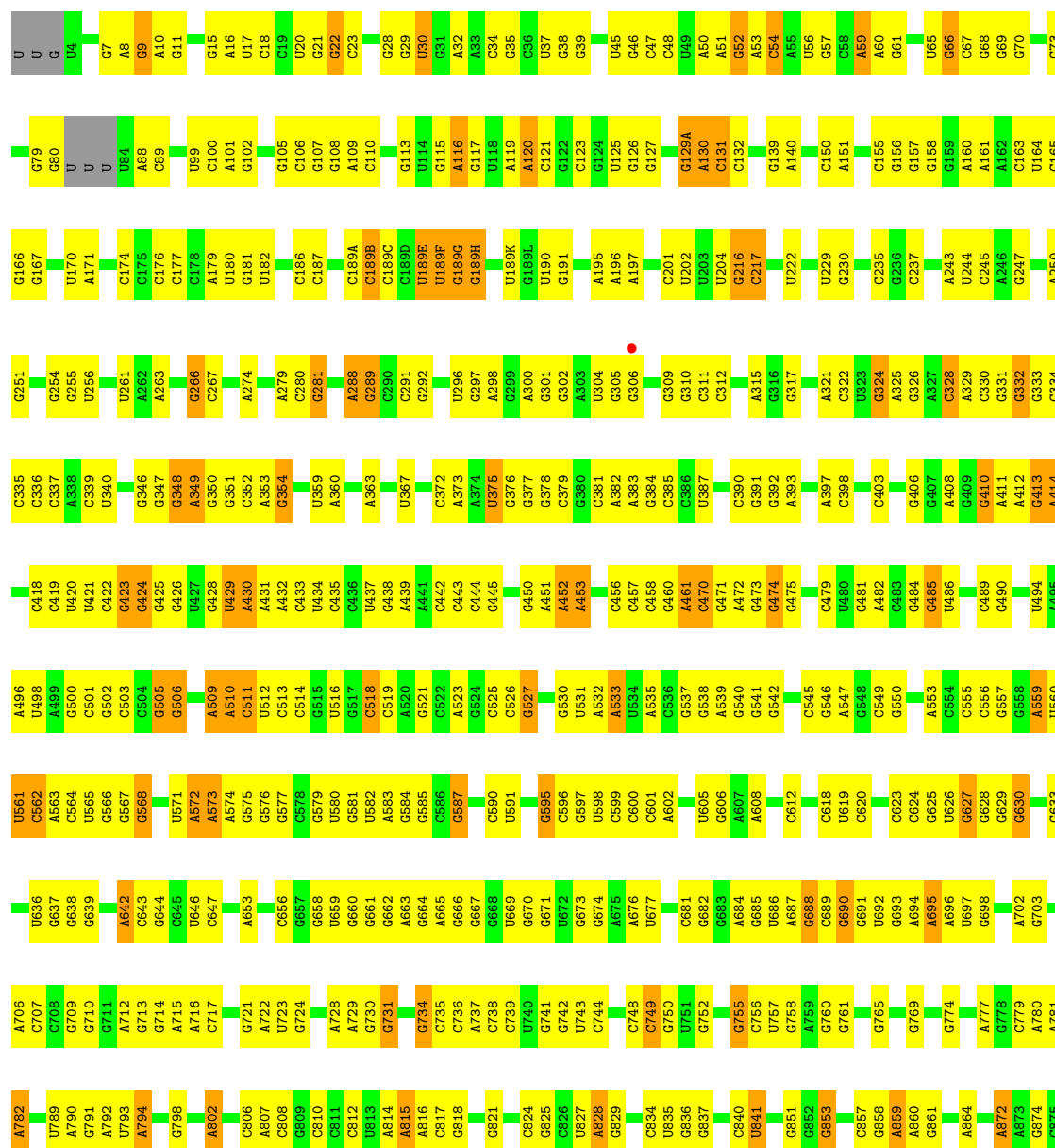
- Molecule 32: 16S Ribosomal RNA



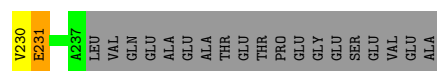




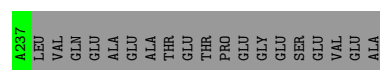
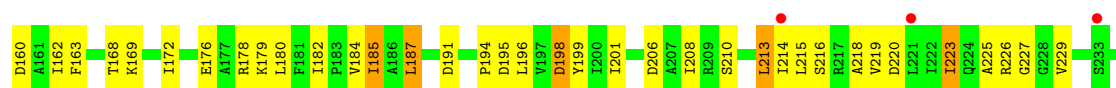
Molecule 32: 16S Ribosomal RNA



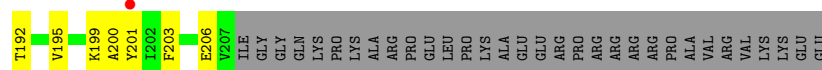
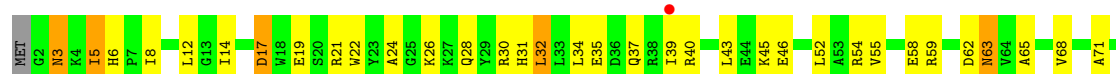




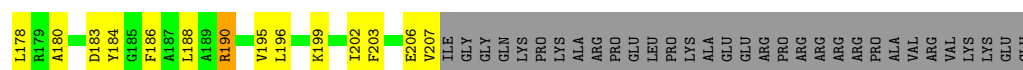
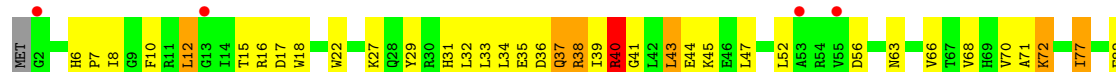
- Molecule 33: 30S ribosomal protein S2



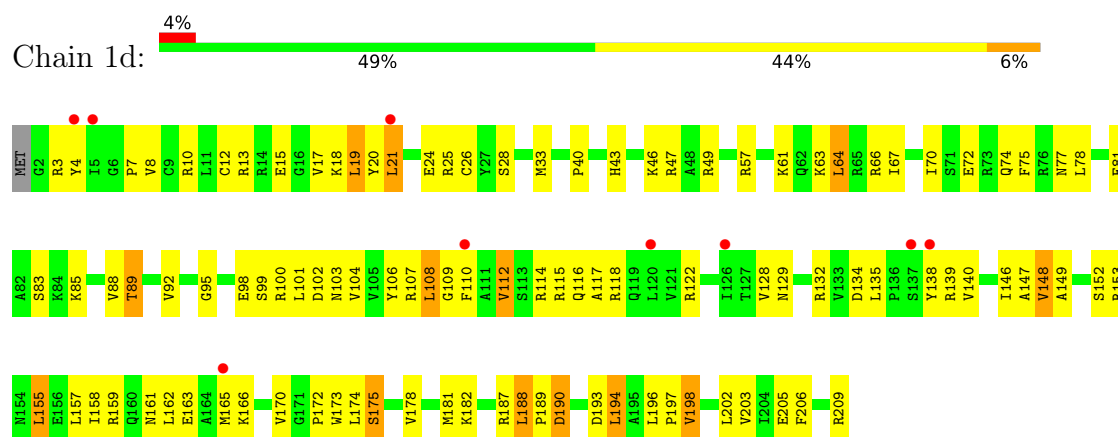
- Molecule 34: 30S ribosomal protein S3



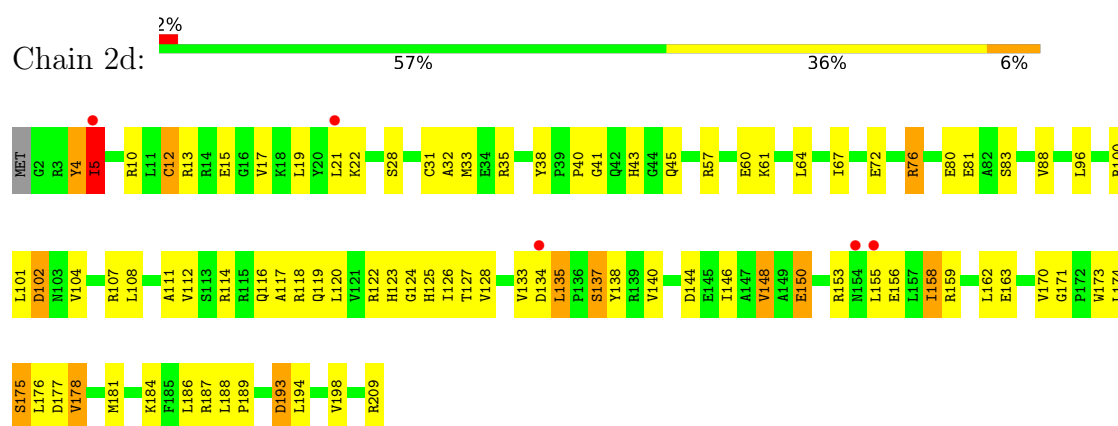
- Molecule 34: 30S ribosomal protein S3



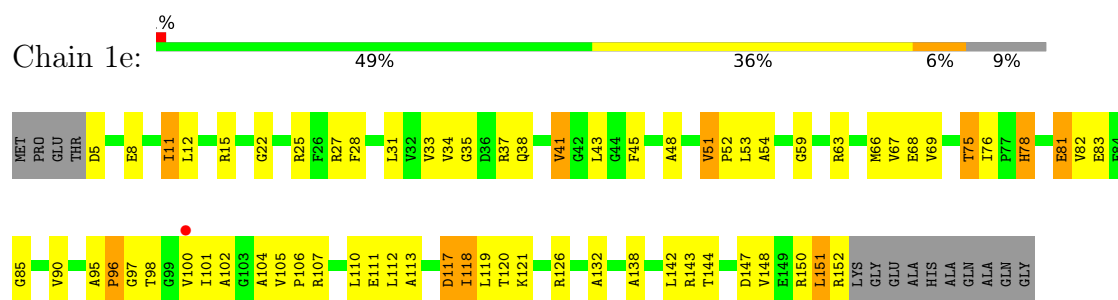
- Molecule 35: 30S ribosomal protein S4



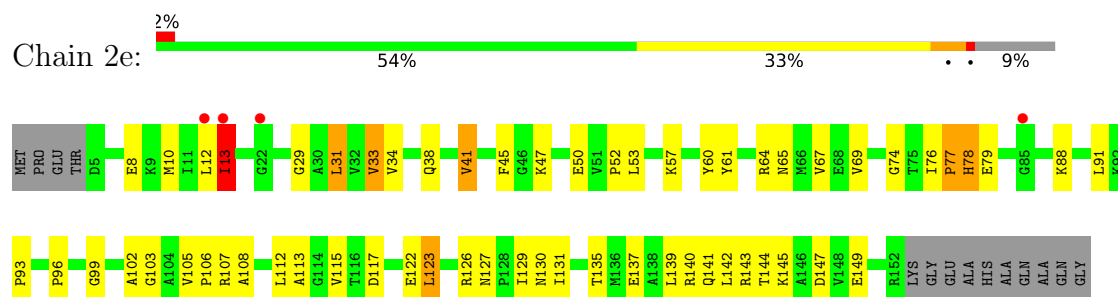
• Molecule 35: 30S ribosomal protein S4



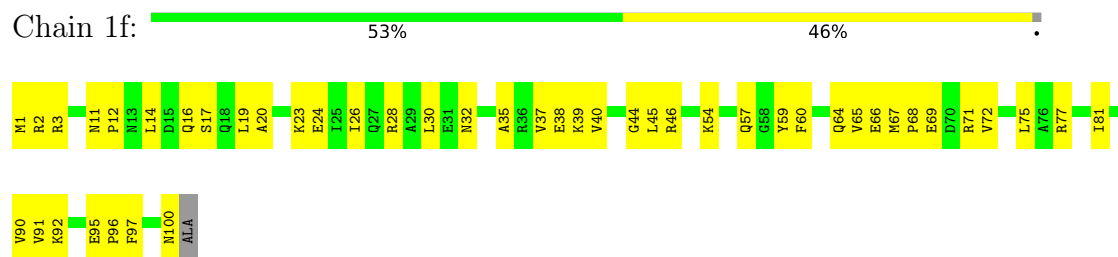
• Molecule 36: 30S ribosomal protein S5



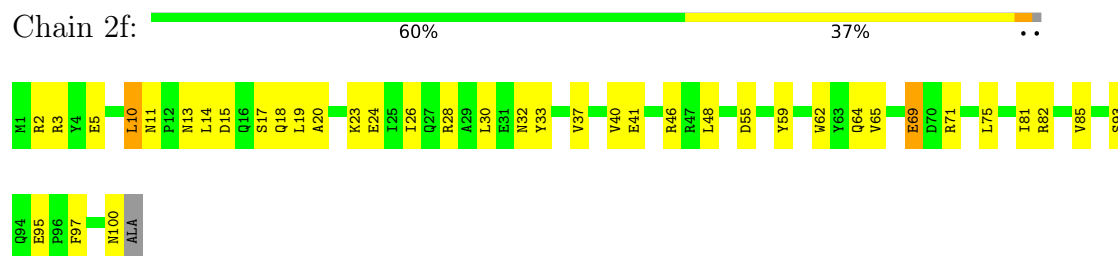
• Molecule 36: 30S ribosomal protein S5



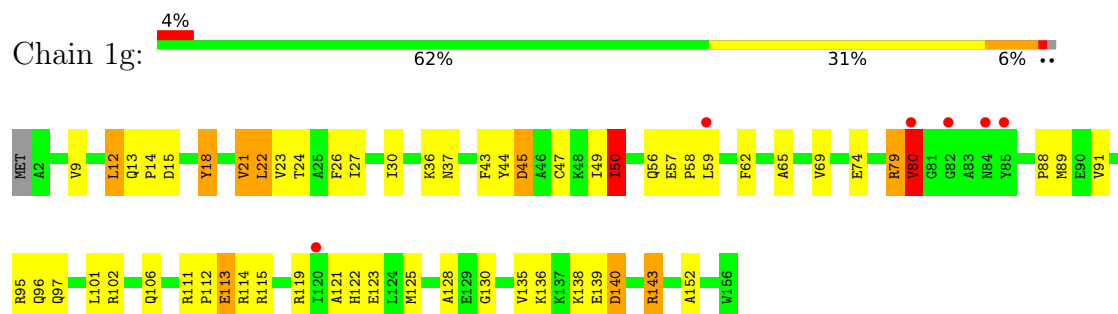
• Molecule 37: 30S ribosomal protein S6



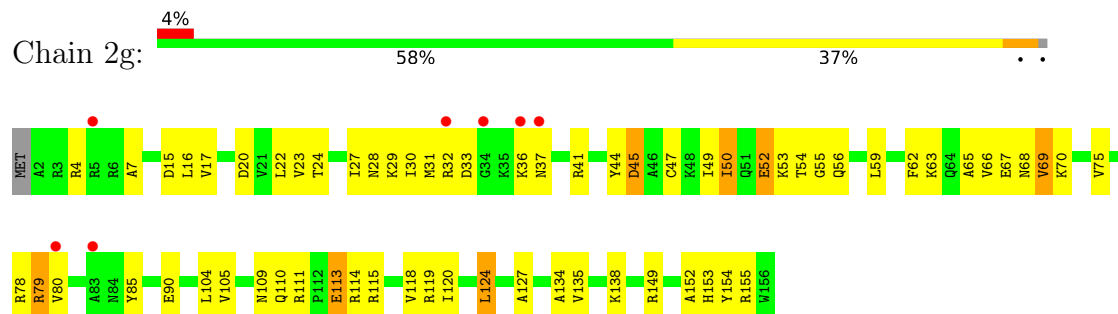
• Molecule 37: 30S ribosomal protein S6



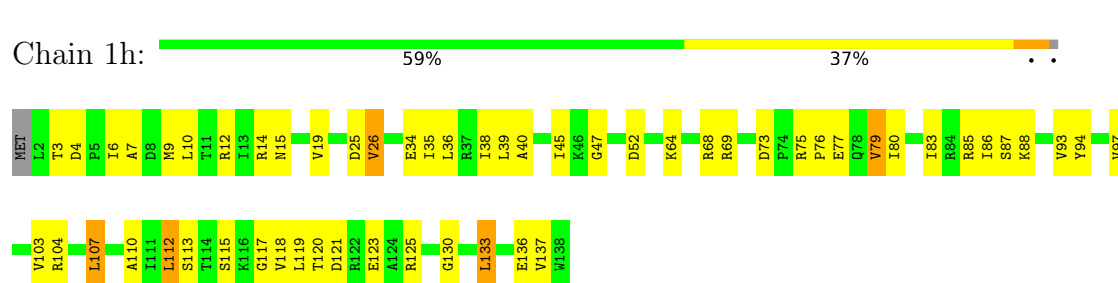
• Molecule 38: 30S ribosomal protein S7



• Molecule 38: 30S ribosomal protein S7

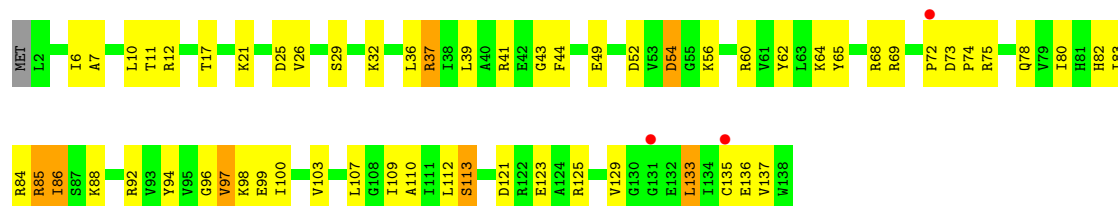


• Molecule 39: 30S ribosomal protein S8



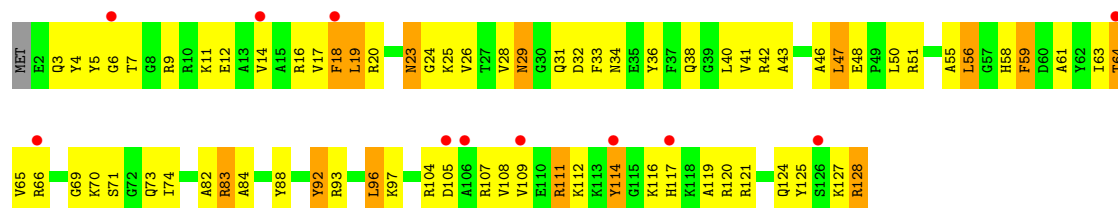
- Molecule 39: 30S ribosomal protein S8

Chain 2h: 



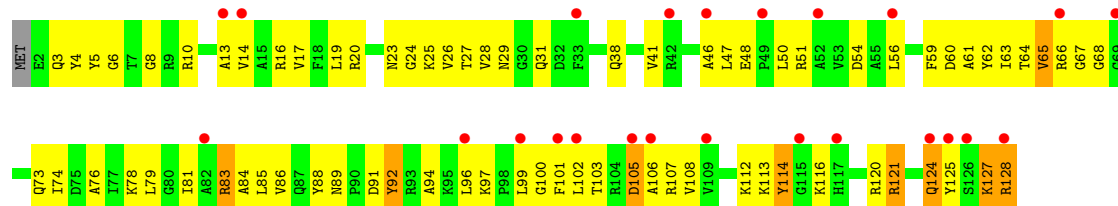
- Molecule 40: 30S ribosomal protein S9

Chain 1i: 



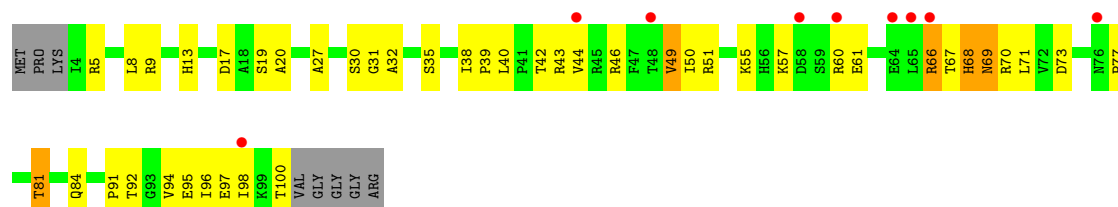
- Molecule 40: 30S ribosomal protein S9

Chain 2i: 



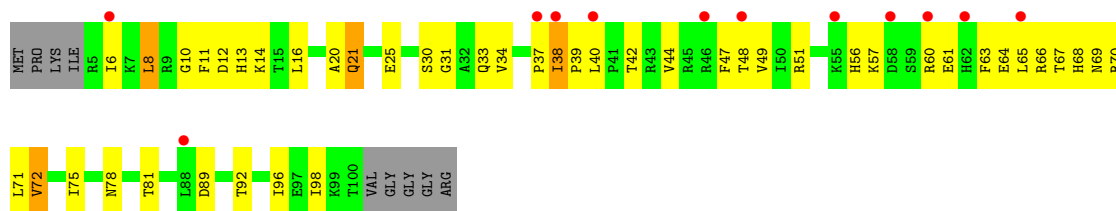
- Molecule 41: 30S ribosomal protein S10

Chain 1j: 

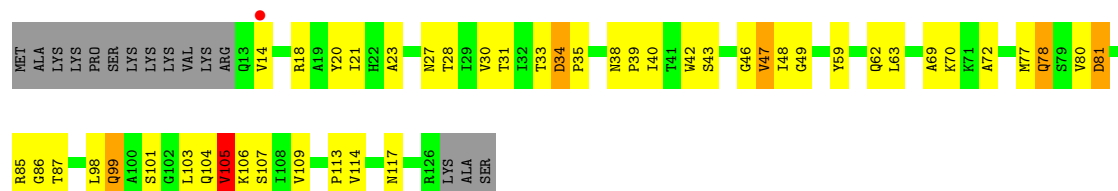


- Molecule 41: 30S ribosomal protein S10

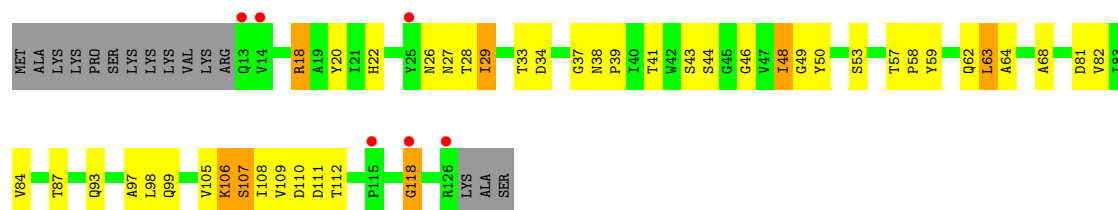
Chain 2j: 



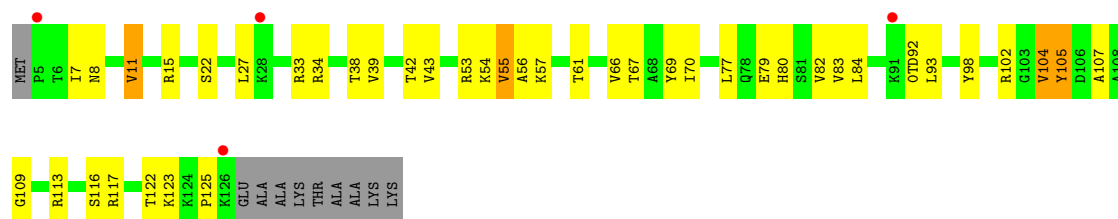
• Molecule 42: 30S ribosomal protein S11



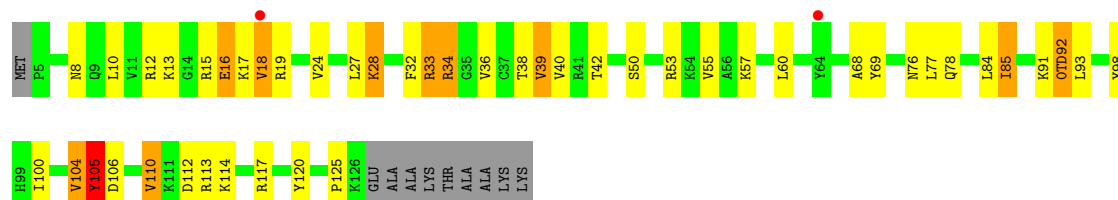
• Molecule 42: 30S ribosomal protein S11



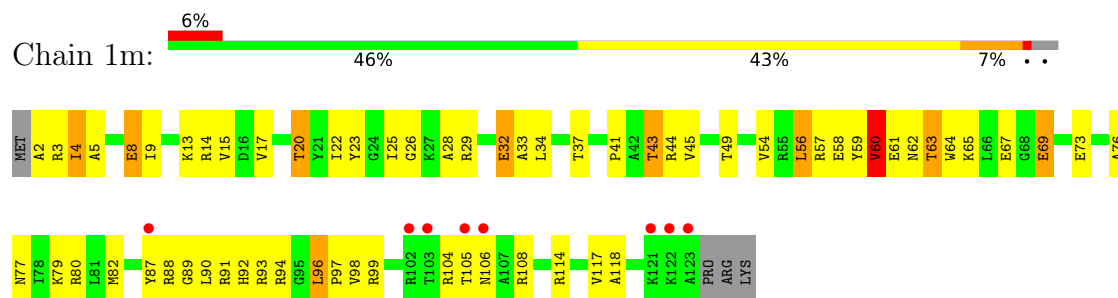
• Molecule 43: 30S ribosomal protein S12



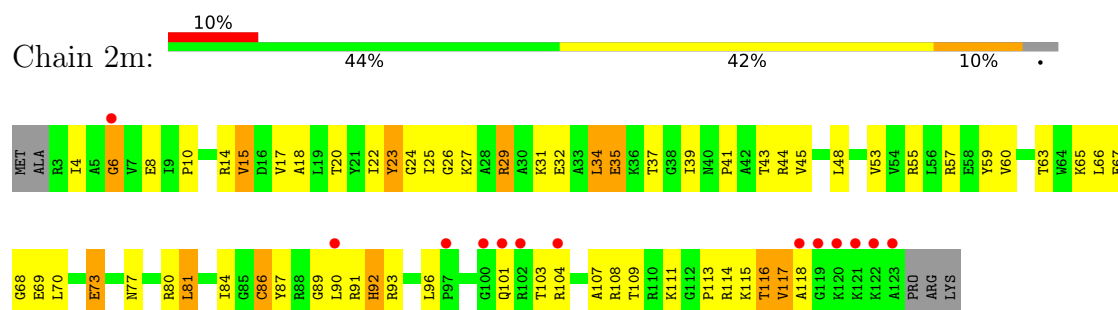
• Molecule 43: 30S ribosomal protein S12



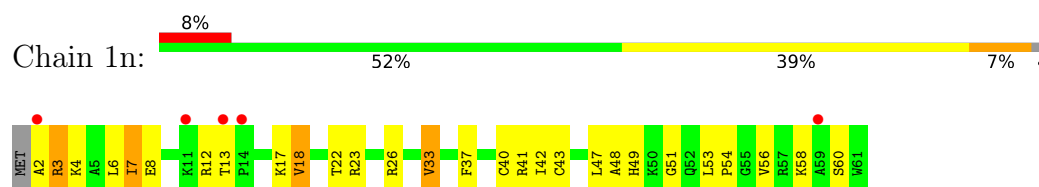
- Molecule 44: 30S ribosomal protein S13



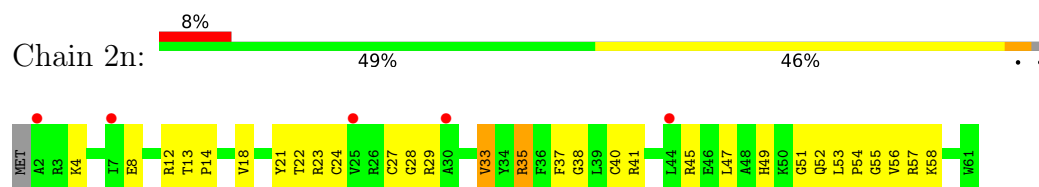
- Molecule 44: 30S ribosomal protein S13



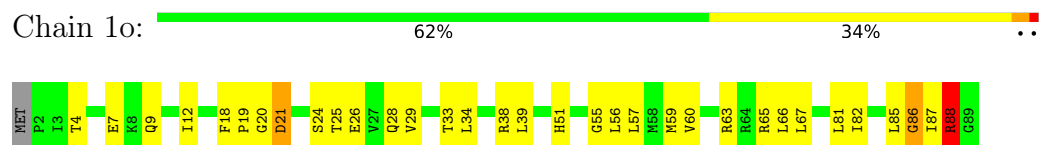
- Molecule 45: 30S ribosomal protein S14 type Z



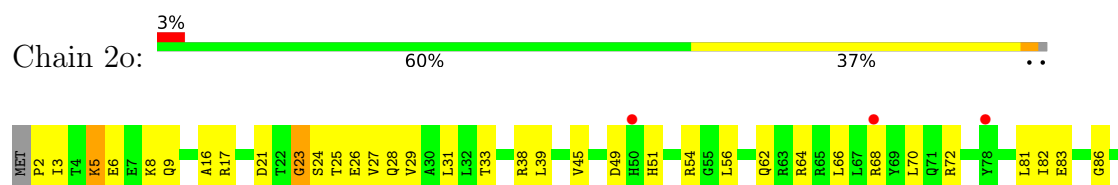
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



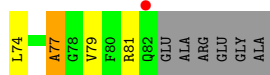
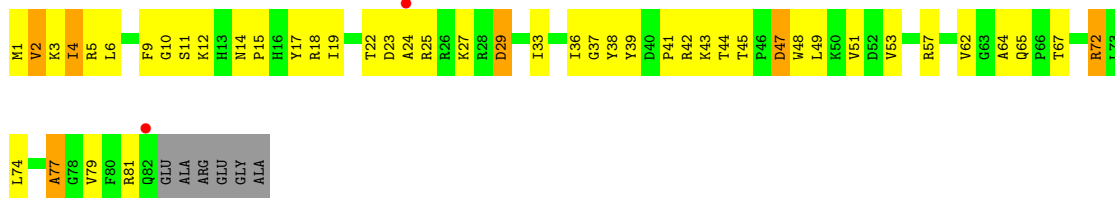
- Molecule 46: 30S ribosomal protein S15



659

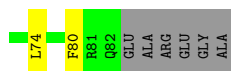
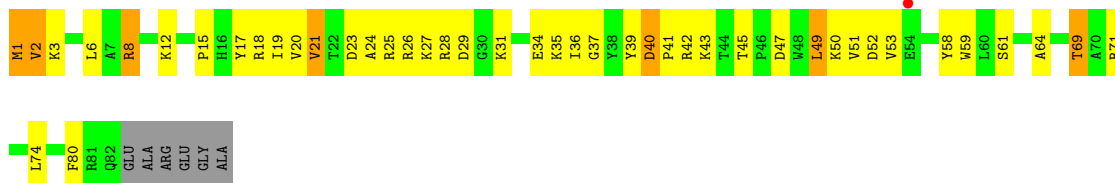
- Molecule 47: 30S ribosomal protein S16

Chain 1p: 



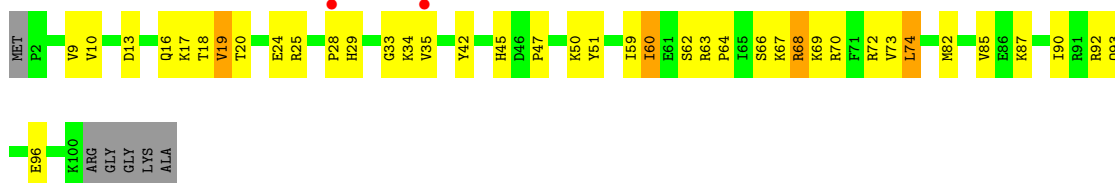
- Molecule 47: 30S ribosomal protein S16

Chain 2p: 



- Molecule 48: 30S ribosomal protein S17

Chain 1q: 



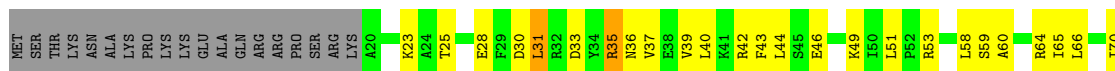
- Molecule 48: 30S ribosomal protein S17

Chain 2q: 



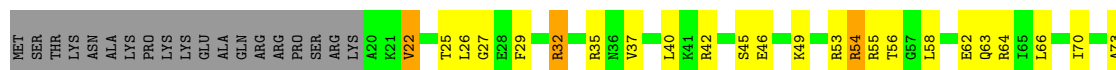
- Molecule 49: 30S ribosomal protein S18

Chain 1r: 

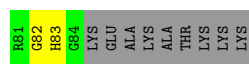
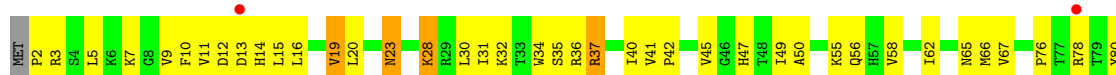
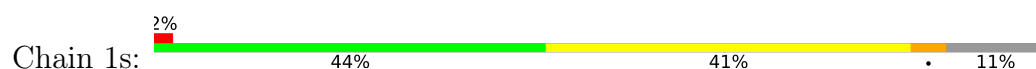




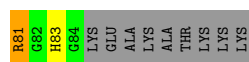
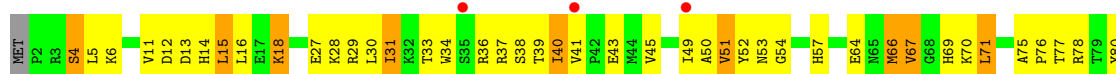
- Molecule 49: 30S ribosomal protein S18



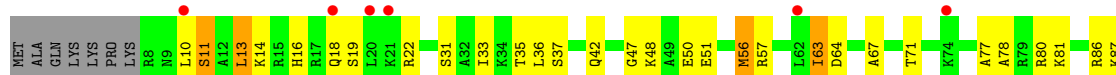
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20

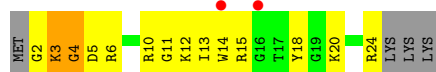


- Molecule 51: 30S ribosomal protein S20

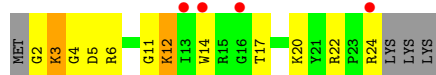




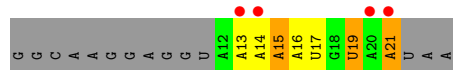
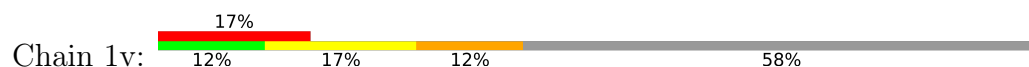
- Molecule 52: 30S ribosomal protein Thx



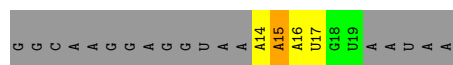
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



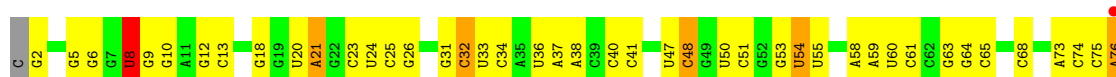
- Molecule 53: mRNA



- Molecule 54: P-site tRNA



- Molecule 54: P-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	209.13Å 448.15Å 621.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.77 – 3.00 86.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.77-3.00) 98.9 (86.77-3.00)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.246 , 0.311 0.246 , 0.309	Depositor DCC
R_{free} test set	57107 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	292071	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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, 2MG, 2MA, M2G, 5MC, K, 4OC, V7A, OMG, MG, UR3, 2MU, SF4, 7MG, 0TD, 5MU, ZN, 4SU, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.26	0/69009	0.44	0/107712
1	2A	0.23	0/67293	0.42	1/105034 (0.0%)
2	1B	0.22	0/2882	0.42	0/4494
2	2B	0.20	0/2879	0.39	0/4487
3	1D	0.27	0/2186	0.53	1/2944 (0.0%)
3	2D	0.23	0/2186	0.50	1/2944 (0.0%)
4	1E	0.24	0/1592	0.48	0/2149
4	2E	0.22	0/1592	0.44	0/2149
5	1F	0.28	0/1619	0.49	0/2193
5	2F	0.22	0/1615	0.48	2/2188 (0.1%)
6	1G	0.21	0/1448	0.48	0/1957
6	2G	0.19	0/1453	0.43	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.20	0/1356	0.39	0/1834
8	1I	0.20	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.43	0/1475
9	1N	0.23	0/1144	0.46	0/1543
9	2N	0.20	0/1144	0.44	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.23	0/943	0.46	0/1269
11	1P	0.24	0/1152	0.54	0/1533
11	2P	0.22	0/1152	0.49	0/1533
12	1Q	0.25	0/1143	0.49	0/1527
12	2Q	0.22	0/1143	0.45	0/1527
13	1R	0.25	0/982	0.50	0/1312
13	2R	0.22	0/982	0.46	0/1312
14	1S	0.24	0/883	0.49	0/1176
14	2S	0.21	0/880	0.43	0/1172
15	1T	0.23	0/1105	0.49	0/1477
15	2T	0.22	0/1097	0.46	0/1468
16	1U	0.25	0/977	0.44	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.40	0/1301
17	1V	0.23	0/782	0.44	0/1049
17	2V	0.19	0/782	0.41	0/1049
18	1W	0.25	0/897	0.45	0/1205
18	2W	0.22	0/897	0.41	0/1205
19	1X	0.26	0/764	0.49	0/1025
19	2X	0.22	0/764	0.45	0/1025
20	1Y	0.24	0/819	0.44	0/1095
20	2Y	0.21	0/819	0.45	0/1095
21	1Z	0.22	0/1267	0.45	0/1717
21	2Z	0.23	0/1299	0.49	0/1763
22	10	0.25	0/662	0.54	0/881
22	20	0.23	0/662	0.46	0/881
23	11	0.25	0/762	0.47	0/1014
23	21	0.23	0/762	0.47	0/1014
24	12	0.27	0/590	0.49	0/781
24	22	0.21	0/590	0.41	0/781
25	13	0.25	0/474	0.49	0/635
25	23	0.20	0/469	0.40	0/630
26	14	0.24	0/565	0.49	0/761
26	24	0.23	0/545	0.57	0/737
27	15	0.23	0/469	0.45	0/635
27	25	0.23	0/469	0.45	0/635
28	16	0.28	0/460	0.52	0/613
28	26	0.24	0/456	0.46	0/608
29	17	0.30	0/426	0.50	0/561
29	27	0.26	0/426	0.51	0/561
30	18	0.28	0/525	0.48	0/691
30	28	0.24	0/525	0.45	0/691
31	19	0.23	0/310	0.44	0/407
31	29	0.22	0/310	0.46	0/407
32	1a	0.21	0/35795	0.40	0/55864
32	2a	0.20	0/35886	0.40	0/56005
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.22	0/1860	0.53	1/2518 (0.0%)
34	1c	0.21	0/1572	0.42	0/2126
34	2c	0.23	0/1566	0.48	0/2119
35	1d	0.22	0/1685	0.47	0/2262
35	2d	0.20	0/1704	0.47	0/2284
36	1e	0.22	0/1145	0.48	0/1543
36	2e	0.23	0/1149	0.48	0/1548
37	1f	0.22	0/823	0.43	0/1115
37	2f	0.21	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.22	0/1250	0.48	1/1679 (0.1%)
38	2g	0.21	0/1254	0.47	0/1683
39	1h	0.19	0/1108	0.43	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.21	0/1002	0.50	0/1346
40	2i	0.21	0/997	0.46	0/1343
41	1j	0.21	0/722	0.44	0/982
41	2j	0.24	0/727	0.49	0/988
42	1k	0.19	0/844	0.41	0/1145
42	2k	0.19	0/848	0.40	0/1149
43	1l	0.21	0/937	0.47	0/1260
43	2l	0.22	0/937	0.49	0/1260
44	1m	0.21	0/961	0.49	0/1290
44	2m	0.24	0/953	0.49	0/1279
45	1n	0.22	0/501	0.42	0/664
45	2n	0.20	0/501	0.49	1/664 (0.2%)
46	1o	0.19	0/739	0.43	0/985
46	2o	0.19	0/739	0.40	0/985
47	1p	0.23	0/697	0.48	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.20	0/836	0.45	0/1117
48	2q	0.19	0/836	0.44	0/1117
49	1r	0.20	0/560	0.41	0/746
49	2r	0.19	0/560	0.37	0/746
50	1s	0.21	0/667	0.45	0/900
50	2s	0.23	0/661	0.56	0/893
51	1t	0.21	0/730	0.49	0/965
51	2t	0.22	0/729	0.51	0/965
52	1u	0.22	0/203	0.51	0/266
52	2u	0.21	0/203	0.47	0/266
53	1v	0.25	0/244	0.41	0/378
53	2v	0.28	0/126	0.45	0/195
54	1x	0.26	0/1725	0.41	0/2689
54	2x	0.25	0/1725	0.41	0/2689
All	All	0.23	0/310069	0.43	8/463831 (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
20	1Y	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1D	41	GLY	N-CA-C	-6.09	107.26	115.36
5	2F	21	ALA	CA-C-N	5.71	131.98	121.70
5	2F	21	ALA	C-N-CA	5.71	131.98	121.70
33	2b	87	ARG	N-CA-C	-5.41	106.75	113.19
38	1g	50	ILE	N-CA-C	-5.39	107.22	112.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	1Y	52	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31184	1170	0
1	2A	60322	0	30423	1110	0
2	1B	2577	0	1305	47	0
2	2B	2575	0	1303	57	0
3	1D	2136	0	2218	88	0
3	2D	2136	0	2218	86	0
4	1E	1559	0	1618	53	0
4	2E	1559	0	1618	58	0
5	1F	1584	0	1624	65	0
5	2F	1580	0	1619	75	0
6	1G	1423	0	1436	55	0
6	2G	1428	0	1438	73	0
7	1H	1330	0	1407	37	0
7	2H	1330	0	1407	47	0
8	1I	1097	0	1140	39	0
8	2I	1064	0	1082	37	0
9	1N	1117	0	1184	35	0
9	2N	1117	0	1184	26	0
10	1O	933	0	995	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	2O	933	0	996	36	0
11	1P	1135	0	1212	44	0
11	2P	1135	0	1212	55	0
12	1Q	1122	0	1179	33	0
12	2Q	1122	0	1179	46	0
13	1R	968	0	1031	22	0
13	2R	968	0	1033	37	0
14	1S	873	0	926	40	0
14	2S	870	0	923	43	0
15	1T	1091	0	1151	38	0
15	2T	1083	0	1136	40	0
16	1U	959	0	1019	29	0
16	2U	959	0	1019	33	0
17	1V	771	0	829	17	0
17	2V	771	0	830	15	0
18	1W	886	0	940	24	0
18	2W	886	0	940	23	0
19	1X	750	0	814	18	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	38	0
20	2Y	806	0	881	32	0
21	1Z	1240	0	1240	45	0
21	2Z	1271	0	1273	56	0
22	10	653	0	674	22	0
22	20	653	0	674	28	0
23	11	755	0	826	21	0
23	21	755	0	826	20	0
24	12	588	0	643	31	0
24	22	588	0	643	24	0
25	13	469	0	518	15	0
25	23	464	0	514	24	0
26	14	552	0	533	30	0
26	24	532	0	503	31	0
27	15	455	0	465	9	0
27	25	455	0	465	18	0
28	16	453	0	472	16	0
28	26	449	0	469	16	0
29	17	418	0	467	17	0
29	27	418	0	467	14	0
30	18	517	0	582	27	0
30	28	517	0	582	22	0
31	19	307	0	335	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	29	307	0	335	11	0
32	1a	32246	0	16295	716	0
32	2a	32327	0	16339	717	0
33	1b	1846	0	1867	80	0
33	2b	1825	0	1828	84	0
34	1c	1548	0	1535	46	0
34	2c	1542	0	1517	69	0
35	1d	1655	0	1672	75	0
35	2d	1674	0	1714	60	0
36	1e	1129	0	1185	52	0
36	2e	1133	0	1191	37	0
37	1f	810	0	804	32	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	37	0
38	2g	1235	0	1249	52	0
39	1h	1088	0	1126	35	0
39	2h	1088	0	1126	45	0
40	1i	983	0	986	63	0
40	2i	978	0	966	60	0
41	1j	709	0	650	42	0
41	2j	714	0	672	36	0
42	1k	829	0	825	30	0
42	2k	833	0	836	34	0
43	1l	932	0	981	31	0
43	2l	932	0	981	36	0
44	1m	951	0	995	51	0
44	2m	943	0	981	52	0
45	1n	492	0	529	27	0
45	2n	492	0	529	26	0
46	1o	728	0	760	18	0
46	2o	728	0	760	24	0
47	1p	681	0	697	30	0
47	2p	677	0	686	30	0
48	1q	823	0	891	28	0
48	2q	823	0	891	22	0
49	1r	555	0	618	22	0
49	2r	555	0	618	24	0
50	1s	652	0	662	31	0
50	2s	646	0	644	40	0
51	1t	728	0	798	23	0
51	2t	727	0	796	31	0
52	1u	199	0	208	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	2u	199	0	208	11	0
53	1v	217	0	109	7	0
53	2v	113	0	54	5	0
54	1x	1625	0	829	18	0
54	2x	1625	0	828	27	0
55	10	7	0	0	0	0
55	11	3	0	0	0	0
55	12	2	0	0	0	0
55	13	5	0	0	0	0
55	14	1	0	0	0	0
55	15	4	0	0	0	0
55	16	3	0	0	0	0
55	17	7	0	0	0	0
55	18	6	0	0	0	0
55	19	2	0	0	0	0
55	1A	1040	0	0	1	0
55	1B	36	0	0	0	0
55	1D	10	0	0	0	0
55	1E	14	0	0	0	0
55	1F	13	0	0	0	0
55	1G	4	0	0	0	0
55	1H	2	0	0	0	0
55	1I	1	0	0	0	0
55	1N	5	0	0	0	0
55	1O	5	0	0	0	0
55	1P	6	0	0	0	0
55	1Q	5	0	0	0	0
55	1R	7	0	0	0	0
55	1S	3	0	0	0	0
55	1T	2	0	0	0	0
55	1U	8	0	0	0	0
55	1V	4	0	0	0	0
55	1W	9	0	0	0	0
55	1X	4	0	0	0	0
55	1Y	2	0	0	0	0
55	1Z	3	0	0	0	0
55	1a	212	0	0	0	0
55	1b	1	0	0	0	0
55	1d	1	0	0	0	0
55	1e	1	0	0	0	0
55	1f	2	0	0	0	0
55	1l	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1n	3	0	0	0	0
55	1t	1	0	0	0	0
55	1v	5	0	0	0	0
55	1x	13	0	0	0	0
55	21	6	0	0	0	0
55	23	3	0	0	0	0
55	25	4	0	0	0	0
55	26	1	0	0	0	0
55	27	2	0	0	0	0
55	28	3	0	0	0	0
55	2A	850	0	0	0	0
55	2B	20	0	0	0	0
55	2D	8	0	0	0	0
55	2E	5	0	0	0	0
55	2F	6	0	0	0	0
55	2G	1	0	0	0	0
55	2O	1	0	0	0	0
55	2P	4	0	0	0	0
55	2Q	4	0	0	0	0
55	2R	1	0	0	0	0
55	2T	4	0	0	0	0
55	2U	2	0	0	0	0
55	2V	1	0	0	0	0
55	2W	1	0	0	0	0
55	2X	1	0	0	0	0
55	2Y	2	0	0	0	0
55	2Z	2	0	0	0	0
55	2a	216	0	0	0	0
55	2d	2	0	0	0	0
55	2e	2	0	0	0	0
55	2f	2	0	0	0	0
55	2g	1	0	0	0	0
55	2i	1	0	0	0	0
55	2j	2	0	0	0	0
55	2k	1	0	0	0	0
55	2l	2	0	0	0	0
55	2n	1	0	0	0	0
55	2q	2	0	0	0	0
55	2r	1	0	0	0	0
55	2t	1	0	0	0	0
55	2x	7	0	0	0	0
56	1A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2A	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1a	35	0	0	3	0
58	2a	35	0	0	3	0
59	1d	8	0	0	3	0
59	2d	8	0	0	3	0
60	10	11	0	0	0	0
60	11	8	0	0	0	0
60	12	3	0	0	0	0
60	13	3	0	0	0	0
60	14	1	0	0	0	0
60	15	6	0	0	0	0
60	16	4	0	0	0	0
60	17	10	0	0	2	0
60	18	8	0	0	2	0
60	1A	1402	0	0	154	0
60	1B	54	0	0	5	0
60	1D	21	0	0	3	0
60	1E	18	0	0	2	0
60	1F	9	0	0	0	0
60	1G	4	0	0	0	0
60	1H	1	0	0	0	0
60	1I	1	0	0	0	0
60	1N	5	0	0	0	0
60	1O	8	0	0	1	0
60	1P	18	0	0	1	0
60	1Q	7	0	0	1	0
60	1R	9	0	0	1	0
60	1S	4	0	0	1	0
60	1T	4	0	0	0	0
60	1U	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1V	10	0	0	0	0
60	1W	8	0	0	0	0
60	1X	4	0	0	0	0
60	1Y	4	0	0	1	0
60	1Z	1	0	0	0	0
60	1a	211	0	0	14	0
60	1b	1	0	0	0	0
60	1d	2	0	0	0	0
60	1e	1	0	0	0	0
60	1i	1	0	0	0	0
60	1l	4	0	0	0	0
60	1m	1	0	0	0	0
60	1q	2	0	0	0	0
60	1u	2	0	0	1	0
60	1v	3	0	0	0	0
60	1x	11	0	0	0	0
60	21	10	0	0	0	0
60	23	1	0	0	0	0
60	27	1	0	0	0	0
60	28	2	0	0	0	0
60	29	1	0	0	0	0
60	2A	680	0	0	70	0
60	2B	24	0	0	1	0
60	2D	12	0	0	4	0
60	2E	13	0	0	2	0
60	2F	10	0	0	1	0
60	2I	1	0	0	0	0
60	2O	2	0	0	0	0
60	2P	4	0	0	0	0
60	2Q	2	0	0	0	0
60	2R	3	0	0	0	0
60	2T	4	0	0	0	0
60	2U	1	0	0	0	0
60	2W	2	0	0	0	0
60	2X	2	0	0	0	0
60	2Y	1	0	0	0	0
60	2Z	3	0	0	0	0
60	2a	173	0	0	19	0
60	2e	2	0	0	0	0
60	2g	1	0	0	0	0
60	2i	1	0	0	0	0
60	2j	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2l	3	0	0	0	0
60	2n	1	0	0	0	0
60	2t	3	0	0	0	0
60	2v	1	0	0	1	0
60	2x	5	0	0	2	0
All	All	292071	0	193336	6489	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 14.

The worst 5 of 6489 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	1.24	1.32
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.37	1.06
1:2A:2101:G:H1	1:2A:2188:C:N4	1.55	1.04
1:1A:1082:U:O4	1:1A:1086:A:N1	1.89	1.04
1:1A:2128:C:N4	1:1A:2160:G:H1	1.60	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	249 (91%)	24 (9%)	0	100	100
3	2D	273/276 (99%)	245 (90%)	26 (10%)	2 (1%)	18	53
4	1E	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	12	45
4	2E	202/206 (98%)	179 (89%)	19 (9%)	4 (2%)	6	28
5	1F	201/210 (96%)	177 (88%)	21 (10%)	3 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2F	201/210 (96%)	175 (87%)	19 (10%)	7 (4%)	3	16
6	1G	179/182 (98%)	156 (87%)	19 (11%)	4 (2%)	5	26
6	2G	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	11	43
7	1H	172/180 (96%)	155 (90%)	12 (7%)	5 (3%)	3	20
7	2H	172/180 (96%)	150 (87%)	18 (10%)	4 (2%)	5	25
8	1I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	18	53
8	2I	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	36
9	1N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	18	53
9	2N	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	9	36
10	1O	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
10	2O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	50
11	1P	147/150 (98%)	122 (83%)	20 (14%)	5 (3%)	3	17
11	2P	147/150 (98%)	128 (87%)	17 (12%)	2 (1%)	9	36
12	1Q	139/141 (99%)	123 (88%)	15 (11%)	1 (1%)	18	53
12	2Q	139/141 (99%)	125 (90%)	10 (7%)	4 (3%)	3	20
13	1R	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	7	32
13	2R	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
14	1S	108/112 (96%)	94 (87%)	14 (13%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	48
15	1T	129/146 (88%)	109 (84%)	18 (14%)	2 (2%)	7	34
15	2T	129/146 (88%)	114 (88%)	14 (11%)	1 (1%)	16	50
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
17	1V	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	12	45
17	2V	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
18	1W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	14	48
18	2W	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	14	48
19	1X	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
19	2X	93/96 (97%)	80 (86%)	12 (13%)	1 (1%)	11	43
20	1Y	105/110 (96%)	92 (88%)	12 (11%)	1 (1%)	12	45
20	2Y	105/110 (96%)	93 (89%)	8 (8%)	4 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1Z	148/206 (72%)	120 (81%)	23 (16%)	5 (3%)	3	17
21	2Z	156/206 (76%)	118 (76%)	35 (22%)	3 (2%)	6	30
22	10	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	40
22	20	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
23	11	95/98 (97%)	88 (93%)	7 (7%)	0	100	100
23	21	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	3	18
24	12	68/72 (94%)	61 (90%)	7 (10%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	4
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2	12
27	15	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	6	31
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
28	26	51/54 (94%)	43 (84%)	8 (16%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
33	1b	229/256 (90%)	186 (81%)	36 (16%)	7 (3%)	3	19
33	2b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	16
34	1c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	8	35
34	2c	204/239 (85%)	171 (84%)	29 (14%)	4 (2%)	6	28
35	1d	206/209 (99%)	173 (84%)	31 (15%)	2 (1%)	12	45
35	2d	206/209 (99%)	185 (90%)	17 (8%)	4 (2%)	6	30
36	1e	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	4	22
36	2e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	27
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
38	1g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	6	28
38	2g	153/156 (98%)	132 (86%)	18 (12%)	3 (2%)	6	28
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18	53
40	1i	125/128 (98%)	102 (82%)	20 (16%)	3 (2%)	4	24
40	2i	125/128 (98%)	106 (85%)	15 (12%)	4 (3%)	3	18
41	1j	95/105 (90%)	78 (82%)	15 (16%)	2 (2%)	5	27
41	2j	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	3	18
42	1k	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	4	22
42	2k	112/129 (87%)	95 (85%)	13 (12%)	4 (4%)	2	16
43	1l	119/132 (90%)	103 (87%)	14 (12%)	2 (2%)	7	32
43	2l	119/132 (90%)	99 (83%)	19 (16%)	1 (1%)	16	50
44	1m	120/126 (95%)	96 (80%)	19 (16%)	5 (4%)	2	13
44	2m	119/126 (94%)	99 (83%)	17 (14%)	3 (2%)	4	23
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	32
46	1o	86/89 (97%)	77 (90%)	6 (7%)	3 (4%)	3	16
46	2o	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	10	40
47	1p	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	4	23
47	2p	80/88 (91%)	64 (80%)	15 (19%)	1 (1%)	9	38
48	1q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	12	45
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12	45
49	1r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	35
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	65 (80%)	15 (18%)	1 (1%)	10	40
50	2s	81/93 (87%)	60 (74%)	21 (26%)	0	100	100
51	1t	94/106 (89%)	78 (83%)	13 (14%)	3 (3%)	3	18
51	2t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5	27
52	1u	21/27 (78%)	13 (62%)	6 (29%)	2 (10%)	0	2
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11368/12128 (94%)	9944 (88%)	1244 (11%)	180 (2%)	7 34

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	92	ILE
11	1P	45	LEU
33	1b	17	PHE
33	1b	33	TYR

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%)	188 (87%)	27 (13%)	4 20
3	2D	215/218 (99%)	197 (92%)	18 (8%)	10 37
4	1E	164/166 (99%)	142 (87%)	22 (13%)	4 18
4	2E	164/166 (99%)	142 (87%)	22 (13%)	4 18
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5 22
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5 22
6	1G	143/156 (92%)	124 (87%)	19 (13%)	4 18
6	2G	143/156 (92%)	124 (87%)	19 (13%)	4 18
7	1H	144/148 (97%)	121 (84%)	23 (16%)	2 12
7	2H	144/148 (97%)	116 (81%)	28 (19%)	1 8
8	1I	113/124 (91%)	93 (82%)	20 (18%)	2 10
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2 11
9	1N	118/119 (99%)	101 (86%)	17 (14%)	3 15
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6 25
10	1O	100/100 (100%)	93 (93%)	7 (7%)	14 44
10	2O	100/100 (100%)	87 (87%)	13 (13%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	1P	115/116 (99%)	102 (89%)	13 (11%)	5	24
11	2P	115/116 (99%)	102 (89%)	13 (11%)	5	24
12	1Q	111/111 (100%)	97 (87%)	14 (13%)	4	20
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	38
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	30
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	19
14	1S	86/88 (98%)	68 (79%)	18 (21%)	1	7
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	22
15	1T	115/127 (91%)	100 (87%)	15 (13%)	4	19
15	2T	113/127 (89%)	103 (91%)	10 (9%)	9	35
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	67
16	2U	93/94 (99%)	84 (90%)	9 (10%)	8	30
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4	20
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	35
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	46
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	46
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	47
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	47
20	1Y	85/91 (93%)	71 (84%)	14 (16%)	2	12
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	10	37
21	1Z	135/179 (75%)	112 (83%)	23 (17%)	2	11
21	2Z	137/179 (76%)	114 (83%)	23 (17%)	2	11
22	10	65/67 (97%)	57 (88%)	8 (12%)	4	21
22	20	65/67 (97%)	58 (89%)	7 (11%)	6	26
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	48
23	21	80/83 (96%)	70 (88%)	10 (12%)	4	20
24	12	65/67 (97%)	55 (85%)	10 (15%)	2	13
24	22	65/67 (97%)	53 (82%)	12 (18%)	1	9
25	13	51/52 (98%)	40 (78%)	11 (22%)	1	6
25	23	50/52 (96%)	35 (70%)	15 (30%)	0	1
26	14	59/63 (94%)	44 (75%)	15 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	24	53/63 (84%)	40 (76%)	13 (24%)	1	4
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	22
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	62
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	30
28	26	50/52 (96%)	36 (72%)	14 (28%)	0	2
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	21
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	30
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	64
30	28	54/55 (98%)	49 (91%)	5 (9%)	8	32
31	19	34/34 (100%)	31 (91%)	3 (9%)	9	35
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	50
33	1b	192/220 (87%)	157 (82%)	35 (18%)	2	9
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	18
34	1c	142/188 (76%)	121 (85%)	21 (15%)	3	15
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	19
35	1d	169/181 (93%)	141 (83%)	28 (17%)	2	12
35	2d	173/181 (96%)	147 (85%)	26 (15%)	3	14
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	27
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	24
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	31
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	27
38	1g	119/127 (94%)	98 (82%)	21 (18%)	2	10
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	16
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	35
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	35
40	1i	90/99 (91%)	75 (83%)	15 (17%)	2	12
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	13
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2	12
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	23
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	21
42	2k	83/99 (84%)	73 (88%)	10 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8	32
43	2l	96/108 (89%)	81 (84%)	15 (16%)	2	13
44	1m	92/101 (91%)	79 (86%)	13 (14%)	3	16
44	2m	91/101 (90%)	75 (82%)	16 (18%)	2	10
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2	12
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	29
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	40
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	34
47	1p	69/74 (93%)	55 (80%)	14 (20%)	1	7
47	2p	68/74 (92%)	56 (82%)	12 (18%)	2	10
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	42
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	48
49	1r	59/77 (77%)	50 (85%)	9 (15%)	3	14
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	36
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	35
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	8
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	24
51	2t	70/82 (85%)	58 (83%)	12 (17%)	2	11
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	52
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	25
All	All	9301/10064 (92%)	8105 (87%)	1196 (13%)	4	19

5 of 1196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	25	6	VAL
47	2p	1	MET
33	2b	7	VAL
26	24	69	LYS
37	2f	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
33	2b	40	HIS
41	2j	21	GLN
34	2c	37	GLN
35	2d	116	GLN
46	2o	28	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	554 (19%)	21 (0%)
1	2A	2791/2915 (95%)	578 (20%)	21 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1497/1521 (98%)	304 (20%)	0
32	2a	1501/1521 (98%)	337 (22%)	0
53	1v	9/24 (37%)	5 (55%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	9 (12%)	0
54	2x	75/77 (97%)	9 (12%)	0
All	All	9054/9316 (97%)	1838 (20%)	43 (0%)

5 of 1838 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	15	G
1	1A	34	C
1	1A	36	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	669	G
1	2A	1240	U
1	2A	752	A
1	2A	900	A
1	2A	1530	C

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

56 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$
32	5MC	2a	967	32	19,22,23	1.68	3 (15%)	26,32,35	1.23	4 (15%)
32	2MG	2a	1207	55,32	23,26,27	1.24	4 (17%)	33,38,41	2.11	7 (21%)
32	PSU	1a	516	55,32	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
54	PSU	1x	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.95	4 (19%)
32	7MG	1a	527	55,32	23,26,27	1.33	3 (13%)	27,39,42	2.59	7 (25%)
54	5MU	2x	54	54	19,22,23	1.40	5 (26%)	27,32,35	2.15	6 (22%)
1	2MA	1A	2503	1,55	22,25,26	1.42	5 (22%)	32,37,40	2.31	10 (31%)
32	M2G	1a	966	55,32	24,27,28	1.35	4 (16%)	33,40,43	1.98	5 (15%)
1	OMG	2A	2251	1,55,54	23,26,27	1.29	3 (13%)	32,38,41	1.90	6 (18%)
32	MA6	2a	1518	32	23,26,27	1.54	5 (21%)	33,38,41	2.33	13 (39%)
43	0TD	2l	92	43	8,9,10	4.72	2 (25%)	6,11,13	6.44	3 (50%)
32	MA6	2a	1519	32	23,26,27	1.58	4 (17%)	33,38,41	2.37	13 (39%)
32	5MC	2a	1407	32	19,22,23	1.68	3 (15%)	26,32,35	1.27	4 (15%)
1	PSU	1A	2605	1	18,21,22	1.39	2 (11%)	21,30,33	2.13	3 (14%)
1	5MC	1A	1962	1	19,22,23	1.58	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	21,30,33	1.96	3 (14%)
1	5MU	2A	1915	1,55	19,22,23	1.54	6 (31%)	27,32,35	2.11	7 (25%)
32	7MG	2a	527	55,32	23,26,27	1.37	4 (17%)	27,39,42	2.53	8 (29%)
32	UR3	2a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.65	4 (15%)
54	4SU	2x	8	54	18,21,22	2.12	6 (33%)	25,30,33	1.67	6 (24%)
1	5MU	1A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.18	6 (22%)
54	PSU	2x	55	54	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
1	4OC	1A	1920	1	19,22,24	0.82	0	25,31,35	1.09	3 (12%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.00	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.22	3 (11%)
32	MA6	1a	1519	32	23,26,27	1.57	5 (21%)	33,38,41	2.26	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1962	1,55	19,22,23	1.66	3 (15%)	26,32,35	1.38	6 (23%)
32	5MC	1a	967	32	19,22,23	1.46	3 (15%)	26,32,35	1.14	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.36	3 (16%)	21,30,33	2.14	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.84	3 (11%)
1	5MC	1A	1942	1	19,22,23	1.46	3 (15%)	26,32,35	1.16	3 (11%)
1	5MC	2A	1942	1,55	19,22,23	1.78	3 (15%)	26,32,35	1.29	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.55	6 (31%)	27,32,35	2.27	7 (25%)
1	4OC	2A	1920	1	19,22,24	0.80	0	25,31,35	1.08	1 (4%)
1	2MA	2A	2503	1,55	22,25,26	1.51	4 (18%)	32,37,40	2.24	8 (25%)
1	2MU	2A	2552	1,55	19,22,24	1.30	2 (10%)	25,31,36	1.91	6 (24%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	2.04	4 (19%)
54	4SU	1x	8	54	18,21,22	2.19	5 (27%)	25,30,33	1.49	4 (16%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
54	5MC	2x	32	54	19,22,23	1.75	3 (15%)	26,32,35	1.24	3 (11%)
32	5MC	2a	1400	54,32	19,22,23	1.90	3 (15%)	26,32,35	1.36	4 (15%)
32	5MC	2a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.22	3 (11%)
1	2MU	1A	2552	1,55	19,22,24	1.27	3 (15%)	25,31,36	1.96	5 (20%)
32	4OC	1a	1402	32	20,23,24	0.79	0	25,32,35	0.90	0
1	5MU	1A	1915	1	19,22,23	1.40	5 (26%)	27,32,35	2.20	7 (25%)
1	OMG	1A	2251	1,55,54	23,26,27	1.30	3 (13%)	32,38,41	2.18	7 (21%)
54	5MU	1x	54	54	19,22,23	1.40	6 (31%)	27,32,35	1.68	5 (18%)
32	2MG	1a	1207	32	23,26,27	1.26	4 (17%)	33,38,41	2.22	6 (18%)
32	MA6	1a	1518	32	23,26,27	1.44	5 (21%)	33,38,41	2.34	13 (39%)
32	5MC	1a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.11	3 (11%)
32	PSU	2a	516	32	18,21,22	1.40	2 (11%)	21,30,33	1.90	4 (19%)
32	5MC	1a	1407	32	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
43	0TD	1l	92	43	8,9,10	4.33	1 (12%)	6,11,13	2.26	3 (50%)
32	4OC	2a	1402	32	20,23,24	0.79	0	25,32,35	1.05	2 (8%)
32	M2G	2a	966	55,32	24,27,28	1.32	3 (12%)	33,40,43	1.92	5 (15%)
54	5MC	1x	32	54	19,22,23	1.60	3 (15%)	26,32,35	1.26	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	55,32	-	1/9/27/28	0/3/3/3
32	PSU	1a	516	55,32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	55,32	-	2/7/37/38	0/3/3/3
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,55	-	2/7/25/26	0/3/3/3
32	M2G	1a	966	55,32	-	1/11/29/30	0/3/3/3
1	OMG	2A	2251	1,55,54	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	3/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
1	5MU	2A	1915	1,55	-	1/7/25/26	0/2/2/2
32	7MG	2a	527	55,32	-	2/7/37/38	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	2/9/27/30	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	5MC	2A	1962	1,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
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	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1,55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
1	2MA	2A	2503	1,55	-	2/7/25/26	0/3/3/3
1	2MU	2A	2552	1,55	-	2/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	54,32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,55	-	0/9/27/28	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,54	-	0/9/27/28	0/3/3/3
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	M2G	2a	966	55,32	-	0/11/29/30	0/3/3/3
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.79	1.69	1.82
43	1l	92	0TD	CB-SB	-11.86	1.70	1.82
32	2a	1400	5MC	C5-C4	7.01	1.49	1.44
1	2A	1942	5MC	C5-C4	6.48	1.49	1.44
32	1a	1404	5MC	C5-C4	6.45	1.49	1.44

The worst 5 of 281 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-15.22	75.00	102.36
32	1a	527	7MG	N9-C4-N3	8.73	138.25	125.46
32	2a	527	7MG	N9-C4-N3	8.13	137.37	125.46
1	2A	2503	2MA	C5-C4-N3	-7.94	118.82	127.18
1	1A	2503	2MA	C5-C4-N3	-7.36	119.43	127.18

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C9
43	1l	92	0TD	CA-CB-SB-CSB
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

33 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	967	5MC	2	0
32	2a	1207	2MG	3	0
54	1x	55	PSU	1	0
54	2x	54	5MU	1	0
1	1A	2503	2MA	5	0
32	2a	1518	MA6	2	0
43	2l	92	0TD	2	0
32	2a	1519	MA6	3	0
1	2A	1911	PSU	1	0
32	2a	527	7MG	1	0
32	2a	1498	UR3	2	0
54	2x	8	4SU	2	0
1	1A	1939	5MU	1	0
1	1A	1920	4OC	1	0
32	1a	1519	MA6	1	0
32	1a	967	5MC	1	0
1	1A	1917	PSU	2	0
32	1a	1498	UR3	1	0
1	2A	1942	5MC	1	0
1	2A	1939	5MU	2	0
1	2A	1920	4OC	2	0
1	2A	2503	2MA	1	0
1	2A	2552	2MU	2	0
54	1x	8	4SU	1	0
54	2x	32	5MC	1	0
32	2a	1400	5MC	1	0
32	2a	1404	5MC	2	0
1	1A	2552	2MU	1	0
32	1a	1402	4OC	3	0
1	1A	2251	OMG	1	0
32	1a	1207	2MG	2	0
32	1a	1518	MA6	5	0
32	2a	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2656 ligands modelled in this entry, 2652 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	$\# Z > 2$
59	SF4	1d	302	35	0,12,12	-	-	-		
58	V7A	2a	1817	55	37,38,38	4.07	12 (32%)	43,60,60	1.74	9 (20%)
59	SF4	2d	303	35	0,12,12	-	-	-		
58	V7A	1a	3213	55	37,38,38	4.04	12 (32%)	43,60,60	1.70	9 (20%)

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
59	SF4	1d	302	35	-	-	0/6/5/5
58	V7A	2a	1817	55	-	3/13/72/72	0/4/4/4
59	SF4	2d	303	35	-	-	0/6/5/5
58	V7A	1a	3213	55	-	4/13/72/72	0/4/4/4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2a	1817	V7A	CAM-CAL	-13.28	1.40	1.52
58	1a	3213	V7A	CAM-CAL	-12.63	1.41	1.52
58	1a	3213	V7A	CAM-CAP	-11.56	1.39	1.55
58	2a	1817	V7A	CAM-CAP	-11.01	1.40	1.55
58	1a	3213	V7A	CAJ-CAI	-11.00	1.40	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2a	1817	V7A	CAJ-CAK-CAN	-4.75	102.28	110.38
58	1a	3213	V7A	OBI-CAR-CAQ	-4.02	116.20	122.93
58	2a	1817	V7A	CBG-NBF-CAO	-3.79	105.47	114.10
58	1a	3213	V7A	CBG-NBF-CAO	-3.77	105.53	114.10
58	1a	3213	V7A	CAJ-CAK-CAN	-3.71	104.06	110.38

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1a	3213	V7A	CAN-CAO-NBF-CBH
58	1a	3213	V7A	CAW-NAT-OAU-CAV
58	2a	1817	V7A	CAN-CAO-NBF-CBH
58	2a	1817	V7A	CAW-NAT-OAU-CAV
58	1a	3213	V7A	CAA-CAS-NAT-CAW

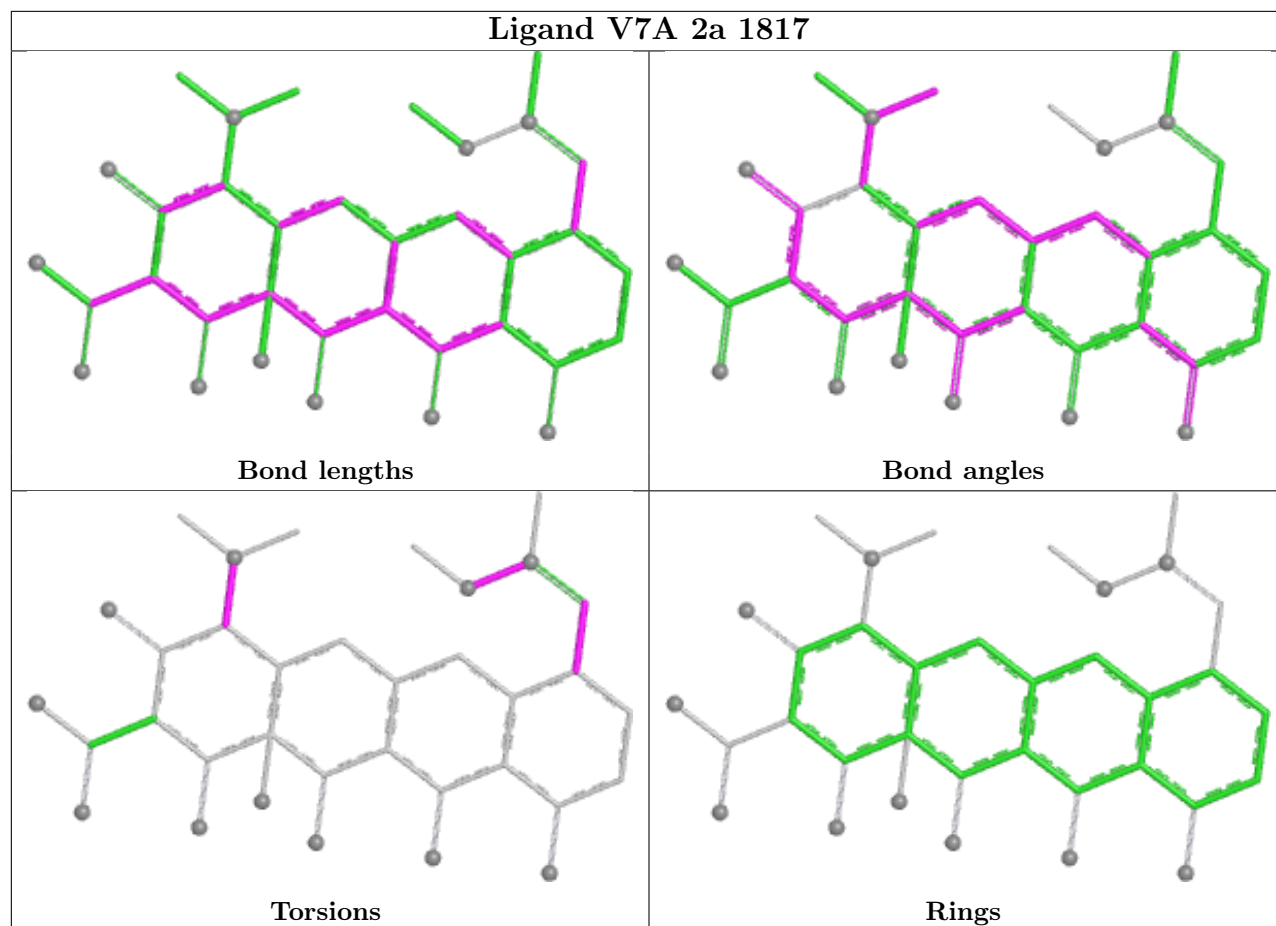
There are no ring outliers.

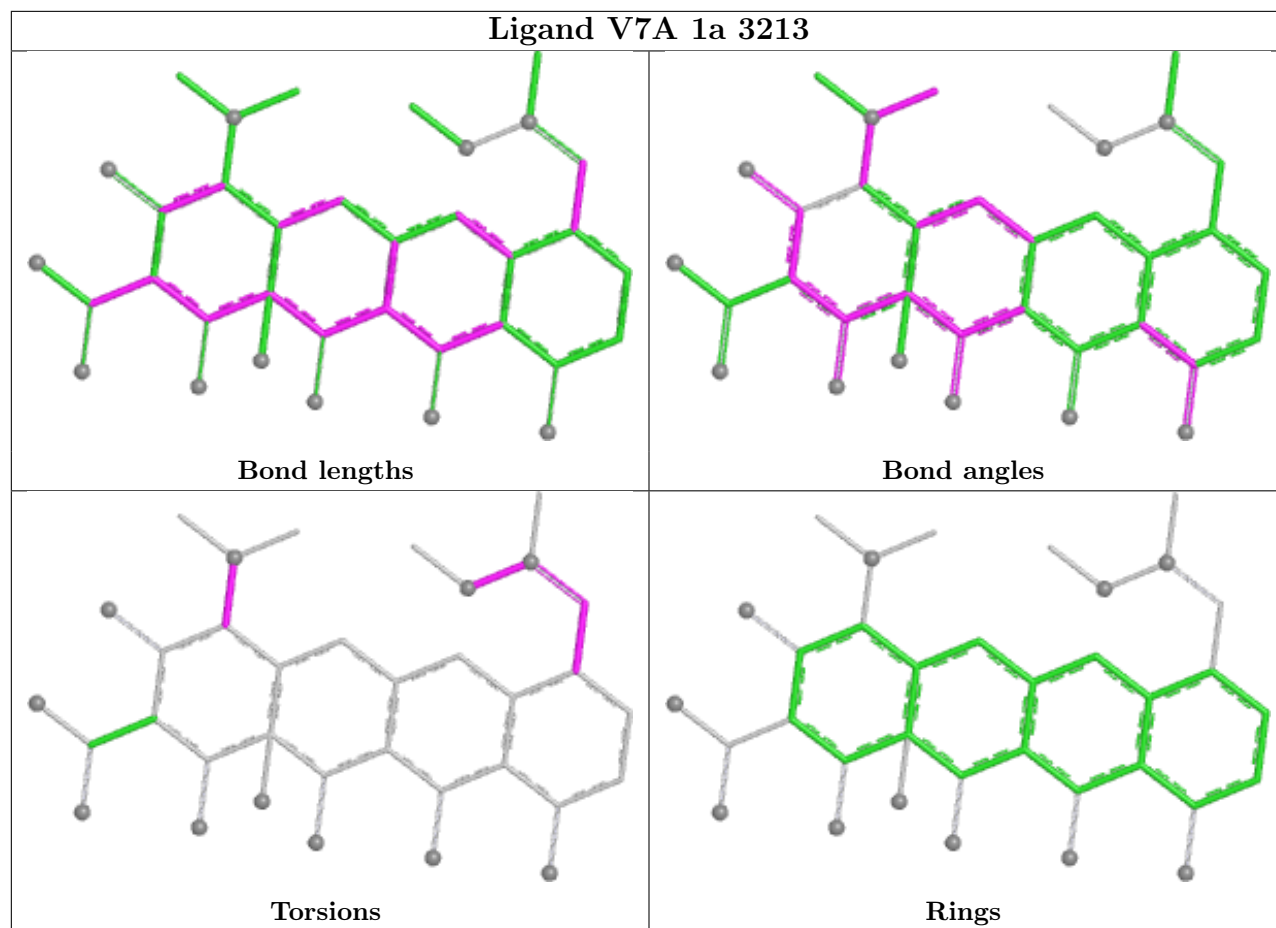
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1d	302	SF4	3	0
58	2a	1817	V7A	3	0
59	2d	303	SF4	3	0
58	1a	3213	V7A	3	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 V7A 2a 1817





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%)	-0.40	31 (1%) 78 57	11, 36, 96, 112	0
1	2A	2789/2915 (95%)	-0.19	37 (1%) 75 53	21, 49, 90, 116	0
2	1B	120/121 (99%)	-0.40	0 100 100	27, 51, 64, 85	0
2	2B	120/121 (99%)	0.11	0 100 100	49, 68, 83, 95	0
3	1D	275/276 (99%)	-0.21	0 100 100	14, 31, 47, 61	0
3	2D	275/276 (99%)	-0.01	1 (0%) 88 76	22, 42, 58, 84	0
4	1E	204/206 (99%)	-0.03	0 100 100	18, 43, 63, 78	0
4	2E	204/206 (99%)	0.05	1 (0%) 87 72	24, 50, 66, 77	0
5	1F	203/210 (96%)	-0.07	0 100 100	16, 40, 64, 82	0
5	2F	203/210 (96%)	0.15	0 100 100	27, 57, 73, 79	0
6	1G	181/182 (99%)	0.36	5 (2%) 55 32	37, 53, 70, 83	0
6	2G	181/182 (99%)	0.74	7 (3%) 43 24	53, 68, 82, 88	0
7	1H	174/180 (96%)	0.12	2 (1%) 78 57	33, 51, 64, 71	0
7	2H	174/180 (96%)	0.56	4 (2%) 61 38	50, 75, 84, 88	0
8	1I	146/148 (98%)	0.18	1 (0%) 84 66	40, 64, 75, 81	0
8	2I	146/148 (98%)	0.27	2 (1%) 73 51	42, 68, 80, 87	0
9	1N	140/140 (100%)	0.06	3 (2%) 63 40	22, 42, 60, 68	0
9	2N	140/140 (100%)	0.32	3 (2%) 63 40	35, 58, 75, 82	0
10	1O	122/122 (100%)	-0.15	1 (0%) 82 64	23, 37, 55, 65	0
10	2O	122/122 (100%)	0.00	2 (1%) 70 47	30, 44, 60, 71	0
11	1P	149/150 (99%)	0.18	3 (2%) 65 41	17, 43, 65, 72	0
11	2P	149/150 (99%)	0.37	2 (1%) 75 53	30, 59, 74, 85	0
12	1Q	141/141 (100%)	0.10	2 (1%) 73 51	25, 41, 53, 61	0
12	2Q	141/141 (100%)	0.35	1 (0%) 84 66	38, 52, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.09	0 100 100	22, 39, 53, 62	0
13	2R	118/118 (100%)	0.18	1 (0%) 82 64	31, 44, 57, 67	0
14	1S	110/112 (98%)	0.06	2 (1%) 67 44	33, 45, 57, 65	0
14	2S	110/112 (98%)	0.28	0 100 100	48, 60, 71, 79	0
15	1T	131/146 (89%)	0.01	1 (0%) 82 64	27, 48, 67, 79	0
15	2T	131/146 (89%)	0.02	1 (0%) 82 64	36, 49, 67, 79	0
16	1U	116/118 (98%)	0.05	2 (1%) 69 45	22, 37, 56, 63	0
16	2U	116/118 (98%)	0.21	0 100 100	37, 54, 66, 82	0
17	1V	101/101 (100%)	-0.08	1 (0%) 79 59	22, 48, 61, 69	0
17	2V	101/101 (100%)	0.26	2 (1%) 65 41	39, 63, 73, 80	0
18	1W	112/113 (99%)	-0.18	0 100 100	22, 37, 56, 88	0
18	2W	112/113 (99%)	0.03	0 100 100	29, 44, 60, 78	0
19	1X	95/96 (98%)	-0.14	0 100 100	21, 34, 50, 73	0
19	2X	95/96 (98%)	0.16	1 (1%) 78 57	34, 50, 65, 74	0
20	1Y	107/110 (97%)	0.05	1 (0%) 81 61	31, 47, 64, 71	0
20	2Y	107/110 (97%)	0.47	1 (0%) 81 61	49, 64, 77, 84	0
21	1Z	154/206 (74%)	0.25	3 (1%) 66 43	38, 56, 70, 85	0
21	2Z	160/206 (77%)	0.61	6 (3%) 44 24	50, 66, 85, 96	0
22	10	83/85 (97%)	0.24	7 (8%) 17 9	26, 34, 68, 92	0
22	20	83/85 (97%)	0.64	6 (7%) 21 11	37, 51, 73, 87	0
23	11	97/98 (98%)	0.40	2 (2%) 63 40	17, 39, 63, 67	0
23	21	97/98 (98%)	0.23	2 (2%) 63 40	27, 50, 67, 75	0
24	12	70/72 (97%)	0.02	1 (1%) 73 51	26, 41, 56, 62	0
24	22	70/72 (97%)	0.27	1 (1%) 73 51	43, 59, 71, 77	0
25	13	59/60 (98%)	-0.23	0 100 100	27, 39, 59, 63	0
25	23	59/60 (98%)	0.42	2 (3%) 48 27	47, 56, 72, 75	0
26	14	69/71 (97%)	0.54	3 (4%) 40 21	53, 74, 87, 101	0
26	24	69/71 (97%)	0.79	4 (5%) 29 15	61, 82, 95, 102	0
27	15	59/60 (98%)	0.07	0 100 100	23, 44, 75, 81	0
27	25	59/60 (98%)	0.34	1 (1%) 69 45	28, 48, 77, 89	0
28	16	53/54 (98%)	-0.21	1 (1%) 66 43	30, 39, 51, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	-0.02	0 100 100	40, 48, 59, 61	0
29	17	48/49 (97%)	-0.08	2 (4%) 40 22	16, 24, 49, 53	0
29	27	48/49 (97%)	0.09	1 (2%) 63 40	26, 33, 51, 67	0
30	18	64/65 (98%)	-0.08	1 (1%) 70 47	23, 30, 39, 58	0
30	28	64/65 (98%)	0.45	2 (3%) 51 30	35, 45, 56, 73	0
31	19	37/37 (100%)	0.05	0 100 100	31, 44, 54, 65	0
31	29	37/37 (100%)	0.48	2 (5%) 31 16	46, 61, 74, 76	0
32	1a	1488/1521 (97%)	0.04	11 (0%) 84 66	27, 65, 93, 112	0
32	2a	1491/1521 (98%)	0.08	13 (0%) 81 61	43, 69, 93, 110	0
33	1b	231/256 (90%)	0.37	3 (1%) 75 53	55, 73, 86, 101	0
33	2b	231/256 (90%)	0.55	6 (2%) 57 34	61, 79, 86, 93	0
34	1c	206/239 (86%)	0.37	3 (1%) 72 49	51, 66, 79, 90	0
34	2c	206/239 (86%)	0.53	6 (2%) 53 31	60, 76, 84, 91	0
35	1d	208/209 (99%)	0.50	9 (4%) 40 21	49, 67, 79, 85	0
35	2d	208/209 (99%)	0.52	5 (2%) 59 36	51, 66, 75, 82	0
36	1e	148/162 (91%)	0.14	1 (0%) 84 66	43, 57, 68, 71	0
36	2e	148/162 (91%)	0.39	4 (2%) 56 33	47, 67, 77, 81	0
37	1f	100/101 (99%)	0.02	0 100 100	42, 61, 71, 75	0
37	2f	100/101 (99%)	0.04	0 100 100	53, 66, 74, 80	0
38	1g	155/156 (99%)	0.32	6 (3%) 43 24	53, 66, 83, 104	0
38	2g	155/156 (99%)	0.37	7 (4%) 38 20	63, 73, 83, 91	0
39	1h	137/138 (99%)	0.07	0 100 100	50, 61, 71, 74	0
39	2h	137/138 (99%)	0.40	3 (2%) 62 39	54, 69, 77, 84	0
40	1i	127/128 (99%)	0.80	11 (8%) 16 8	54, 69, 80, 85	0
40	2i	127/128 (99%)	1.20	24 (18%) 3 2	66, 80, 88, 94	0
41	1j	97/105 (92%)	0.80	9 (9%) 14 7	53, 68, 81, 85	0
41	2j	96/105 (91%)	1.08	12 (12%) 8 5	60, 77, 87, 97	0
42	1k	114/129 (88%)	0.26	1 (0%) 81 61	37, 60, 75, 79	0
42	2k	114/129 (88%)	0.19	6 (5%) 32 16	51, 65, 74, 81	0
43	1l	121/132 (91%)	0.18	4 (3%) 49 28	42, 52, 64, 73	0
43	2l	121/132 (91%)	0.27	2 (1%) 69 45	45, 58, 68, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	122/126 (96%)	0.73	8 (6%) 24 12	55, 70, 78, 84	0
44	2m	121/126 (96%)	0.97	13 (10%) 11 6	62, 75, 85, 92	0
45	1n	60/61 (98%)	0.85	5 (8%) 17 9	57, 66, 75, 79	0
45	2n	60/61 (98%)	0.94	5 (8%) 17 9	66, 75, 83, 88	0
46	1o	88/89 (98%)	0.40	0 100 100	43, 58, 70, 82	0
46	2o	88/89 (98%)	0.48	3 (3%) 48 27	55, 66, 75, 80	0
47	1p	82/88 (93%)	0.87	2 (2%) 59 36	50, 68, 80, 86	0
47	2p	82/88 (93%)	0.66	1 (1%) 76 55	51, 64, 71, 81	0
48	1q	99/105 (94%)	0.65	2 (2%) 65 41	47, 61, 71, 74	0
48	2q	99/105 (94%)	0.25	0 100 100	50, 62, 72, 75	0
49	1r	68/88 (77%)	0.17	0 100 100	44, 62, 72, 83	0
49	2r	68/88 (77%)	-0.01	0 100 100	51, 67, 76, 80	0
50	1s	83/93 (89%)	0.47	2 (2%) 59 36	59, 70, 80, 91	0
50	2s	83/93 (89%)	0.68	3 (3%) 46 26	67, 77, 86, 90	0
51	1t	96/106 (90%)	0.52	6 (6%) 26 13	53, 67, 78, 81	0
51	2t	96/106 (90%)	0.36	1 (1%) 79 59	45, 62, 75, 83	0
52	1u	23/27 (85%)	1.03	2 (8%) 16 8	58, 65, 72, 79	0
52	2u	23/27 (85%)	1.05	4 (17%) 4 3	65, 71, 78, 79	0
53	1v	10/24 (41%)	1.18	4 (40%) 1 1	46, 82, 94, 95	0
53	2v	6/24 (25%)	0.34	0 100 100	56, 66, 85, 85	0
54	1x	72/77 (93%)	-0.21	0 100 100	34, 52, 70, 87	0
54	2x	72/77 (93%)	0.07	1 (1%) 73 51	44, 68, 80, 93	0
All	All	20598/21444 (96%)	0.09	376 (1%) 67 44	11, 57, 84, 116	0

The worst 5 of 376 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2147	G	7.0
1	2A	2146	C	6.9
40	1i	126	SER	5.9
22	10	6	GLY	5.5
32	2a	1532	U	5.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	5MU	2x	54	21/22	0.81	0.10	70,76,87,97	0
1	5MU	2A	1915	21/22	0.83	0.12	55,72,85,88	0
54	PSU	1x	55	20/21	0.87	0.10	49,59,66,70	0
54	PSU	2x	55	20/21	0.87	0.09	64,72,80,82	0
32	2MG	2a	1207	24/25	0.88	0.09	69,74,78,93	0
32	5MC	2a	1400	21/22	0.88	0.15	60,73,79,95	0
54	4SU	2x	8	20/21	0.88	0.10	63,68,73,78	0
32	PSU	1a	516	20/21	0.88	0.10	53,70,76,77	0
32	PSU	2a	516	20/21	0.88	0.09	61,69,73,76	0
32	7MG	2a	527	24/25	0.89	0.11	47,63,71,72	0
32	2MG	1a	1207	24/25	0.89	0.10	63,68,73,79	0
1	PSU	1A	1917	20/21	0.89	0.10	48,59,63,65	0
54	5MC	2x	32	21/22	0.90	0.12	57,63,70,71	0
32	5MC	2a	967	21/22	0.90	0.13	65,71,77,81	0
1	5MU	1A	1915	21/22	0.90	0.08	53,60,70,73	0
1	PSU	2A	1911	20/21	0.91	0.08	51,55,79,79	0
43	0TD	2l	92	10/11	0.91	0.13	55,59,62,66	0
32	M2G	2a	966	25/26	0.91	0.15	65,73,80,82	0
32	4OC	2a	1402	22/23	0.92	0.10	54,61,66,69	0
54	5MU	1x	54	21/22	0.92	0.08	45,63,65,67	0
1	5MC	2A	1942	21/22	0.92	0.09	36,49,55,57	0
54	5MC	1x	32	21/22	0.93	0.11	37,52,60,64	0
1	4OC	2A	1920	21/23	0.93	0.10	44,56,61,64	0
54	4SU	1x	8	20/21	0.93	0.09	44,55,61,70	0
32	MA6	1a	1519	24/25	0.94	0.10	29,36,41,42	0
1	PSU	2A	1917	20/21	0.94	0.07	45,56,60,60	0
32	5MC	1a	967	21/22	0.94	0.11	47,57,63,65	0
1	5MU	2A	1939	21/22	0.94	0.10	30,37,45,48	0
1	PSU	1A	1911	20/21	0.94	0.08	40,51,56,57	0
1	5MC	2A	1962	21/22	0.94	0.10	31,40,49,54	0
32	5MC	1a	1400	21/22	0.94	0.10	43,50,56,59	0
32	4OC	1a	1402	22/23	0.94	0.10	35,46,53,58	0
32	5MC	1a	1404	21/22	0.94	0.09	29,38,43,47	0
32	5MC	1a	1407	21/22	0.95	0.09	32,42,49,52	0
32	5MC	2a	1404	21/22	0.95	0.08	47,58,62,62	0
32	5MC	2a	1407	21/22	0.95	0.08	41,52,56,58	0
32	UR3	2a	1498	21/22	0.95	0.10	31,51,56,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	2a	1518	24/25	0.95	0.10	44,53,61,64	0
32	MA6	2a	1519	24/25	0.95	0.13	46,53,56,65	0
32	MA6	1a	1518	24/25	0.95	0.11	27,35,38,40	0
32	M2G	1a	966	25/26	0.95	0.09	45,52,57,60	0
43	0TD	1l	92	10/11	0.95	0.08	43,49,50,55	0
1	4OC	1A	1920	21/23	0.95	0.10	27,44,55,57	0
1	PSU	2A	2605	20/21	0.95	0.10	23,31,35,36	0
1	5MU	1A	1939	21/22	0.96	0.09	19,25,29,32	0
1	OMG	2A	2251	24/25	0.96	0.07	27,33,36,37	0
1	2MA	2A	2503	23/24	0.96	0.08	20,26,36,41	0
32	UR3	1a	1498	21/22	0.96	0.08	23,37,42,47	0
32	7MG	1a	527	24/25	0.96	0.08	34,39,51,55	0
1	5MC	1A	1942	21/22	0.96	0.08	22,36,41,46	0
1	5MC	1A	1962	21/22	0.96	0.09	25,37,42,46	0
1	2MU	1A	2552	21/23	0.97	0.08	26,37,41,43	0
1	2MU	2A	2552	21/23	0.97	0.07	25,33,39,42	0
1	PSU	1A	2605	20/21	0.97	0.08	19,24,28,28	0
1	OMG	1A	2251	24/25	0.97	0.08	18,23,30,34	0
1	2MA	1A	2503	23/24	0.98	0.08	12,19,25,31	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
55	MG	1v	102	1/1	0.46	0.35	76,76,76,76	0
55	MG	1a	3172	1/1	0.56	0.22	67,67,67,67	0
55	MG	1B	229	1/1	0.60	0.11	75,75,75,75	0
55	MG	1a	3102	1/1	0.61	0.30	61,61,61,61	0
55	MG	1A	3842	1/1	0.65	0.28	28,28,28,28	0
55	MG	1A	3650	1/1	0.66	0.16	60,60,60,60	0
55	MG	1A	3952	1/1	0.66	0.13	68,68,68,68	0
55	MG	2A	3396	1/1	0.66	0.11	51,51,51,51	0
55	MG	1E	301	1/1	0.68	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	1744	1/1	0.68	0.18	72,72,72,72	0
55	MG	2A	3751	1/1	0.69	0.14	50,50,50,50	0
55	MG	1P	205	1/1	0.69	0.14	56,56,56,56	0
55	MG	2A	3115	1/1	0.70	0.18	47,47,47,47	0
55	MG	1B	218	1/1	0.70	0.12	41,41,41,41	0
55	MG	2A	3091	1/1	0.71	0.29	58,58,58,58	0
55	MG	1A	3793	1/1	0.71	0.53	48,48,48,48	0
55	MG	2A	3200	1/1	0.71	0.20	57,57,57,57	0
55	MG	1B	221	1/1	0.71	0.14	56,56,56,56	0
55	MG	2A	3577	1/1	0.71	0.13	69,69,69,69	0
55	MG	1A	3079	1/1	0.71	0.25	46,46,46,46	0
55	MG	2a	1739	1/1	0.71	0.18	83,83,83,83	0
55	MG	1A	3691	1/1	0.71	0.14	26,26,26,26	0
55	MG	2a	1810	1/1	0.71	0.10	66,66,66,66	0
55	MG	1x	102	1/1	0.72	0.26	80,80,80,80	0
55	MG	2A	3765	1/1	0.73	0.11	54,54,54,54	0
55	MG	2A	3824	1/1	0.73	0.20	53,53,53,53	0
55	MG	2a	1730	1/1	0.73	0.24	59,59,59,59	0
55	MG	1A	3680	1/1	0.73	0.16	37,37,37,37	0
55	MG	2A	3683	1/1	0.73	0.12	47,47,47,47	0
55	MG	2a	1774	1/1	0.73	0.11	29,29,29,29	0
55	MG	1a	3177	1/1	0.73	0.14	69,69,69,69	0
57	ZN	15	105	1/1	0.73	0.21	155,155,155,155	0
55	MG	1Q	205	1/1	0.74	0.18	37,37,37,37	0
55	MG	2A	3298	1/1	0.74	0.14	52,52,52,52	0
55	MG	1a	3051	1/1	0.74	0.32	78,78,78,78	0
55	MG	2A	3514	1/1	0.74	0.12	51,51,51,51	0
55	MG	1A	3749	1/1	0.74	0.27	53,53,53,53	0
55	MG	2A	3722	1/1	0.75	0.13	25,25,25,25	0
55	MG	2A	3676	1/1	0.75	0.16	65,65,65,65	0
55	MG	2B	215	1/1	0.75	0.12	60,60,60,60	0
55	MG	2A	3566	1/1	0.76	0.17	25,25,25,25	0
55	MG	2A	3361	1/1	0.76	0.14	50,50,50,50	0
55	MG	1A	3662	1/1	0.76	0.08	72,72,72,72	0
55	MG	2A	3769	1/1	0.76	0.14	69,69,69,69	0
55	MG	2A	3142	1/1	0.76	0.18	37,37,37,37	0
55	MG	2A	3707	1/1	0.76	0.12	44,44,44,44	0
55	MG	2a	1762	1/1	0.77	0.15	55,55,55,55	0
55	MG	1a	3066	1/1	0.77	0.18	62,62,62,62	0
55	MG	2a	1795	1/1	0.77	0.17	65,65,65,65	0
55	MG	1a	3149	1/1	0.77	0.10	56,56,56,56	0
55	MG	1a	3181	1/1	0.77	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
55	MG	1A	3907	1/1	0.78	0.36	61,61,61,61	0
55	MG	1A	3913	1/1	0.78	0.14	50,50,50,50	0
55	MG	1a	3191	1/1	0.78	0.10	62,62,62,62	0
55	MG	2A	3805	1/1	0.78	0.14	46,46,46,46	0
55	MG	1A	3587	1/1	0.78	0.10	37,37,37,37	0
55	MG	2A	3530	1/1	0.78	0.20	45,45,45,45	0
55	MG	1A	3957	1/1	0.78	0.19	63,63,63,63	0
55	MG	1A	3962	1/1	0.78	0.17	53,53,53,53	0
55	MG	2A	3594	1/1	0.78	0.19	37,37,37,37	0
55	MG	2A	3616	1/1	0.78	0.14	44,44,44,44	0
55	MG	1A	3722	1/1	0.78	0.18	44,44,44,44	0
55	MG	2A	3141	1/1	0.78	0.10	31,31,31,31	0
55	MG	1A	3825	1/1	0.78	0.17	52,52,52,52	0
55	MG	1A	3740	1/1	0.78	0.15	39,39,39,39	0
55	MG	2a	1721	1/1	0.79	0.17	57,57,57,57	0
55	MG	2a	1725	1/1	0.79	0.11	59,59,59,59	0
55	MG	1E	309	1/1	0.79	0.22	36,36,36,36	0
55	MG	1A	3224	1/1	0.79	0.27	48,48,48,48	0
55	MG	1A	3601	1/1	0.79	0.10	47,47,47,47	0
55	MG	2A	3787	1/1	0.79	0.17	57,57,57,57	0
55	MG	2A	3544	1/1	0.79	0.20	48,48,48,48	0
55	MG	1A	3334	1/1	0.79	0.18	51,51,51,51	0
55	MG	2B	212	1/1	0.79	0.24	60,60,60,60	0
55	MG	1A	3761	1/1	0.79	0.14	51,51,51,51	0
55	MG	2A	3619	1/1	0.80	0.14	42,42,42,42	0
55	MG	2A	3380	1/1	0.80	0.19	49,49,49,49	0
55	MG	2a	1617	1/1	0.80	0.24	46,46,46,46	0
55	MG	2a	1641	1/1	0.80	0.11	51,51,51,51	0
55	MG	2a	1717	1/1	0.80	0.16	68,68,68,68	0
55	MG	1A	3026	1/1	0.80	0.24	52,52,52,52	0
55	MG	2A	3466	1/1	0.80	0.28	45,45,45,45	0
55	MG	1A	3861	1/1	0.80	0.14	28,28,28,28	0
55	MG	2A	3728	1/1	0.80	0.18	57,57,57,57	0
55	MG	1A	3884	1/1	0.80	0.11	68,68,68,68	0
55	MG	2a	1755	1/1	0.80	0.17	44,44,44,44	0
55	MG	1A	3190	1/1	0.80	0.12	41,41,41,41	0
55	MG	1a	3048	1/1	0.80	0.11	64,64,64,64	0
55	MG	1A	3530	1/1	0.80	0.11	42,42,42,42	0
55	MG	1a	3197	1/1	0.80	0.12	61,61,61,61	0
55	MG	2a	1813	1/1	0.80	0.12	63,63,63,63	0
55	MG	1A	3943	1/1	0.80	0.18	41,41,41,41	0
55	MG	2A	3423	1/1	0.81	0.19	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1O	203	1/1	0.81	0.17	58,58,58,58	0
55	MG	1A	3965	1/1	0.81	0.12	27,27,27,27	0
55	MG	2A	3054	1/1	0.81	0.13	43,43,43,43	0
55	MG	2A	3681	1/1	0.81	0.11	50,50,50,50	0
55	MG	2A	3817	1/1	0.81	0.17	55,55,55,55	0
55	MG	2a	1746	1/1	0.81	0.19	40,40,40,40	0
55	MG	2A	3541	1/1	0.81	0.12	39,39,39,39	0
55	MG	1A	3158	1/1	0.81	0.17	58,58,58,58	0
55	MG	2A	3717	1/1	0.81	0.11	28,28,28,28	0
55	MG	1A	3661	1/1	0.81	0.17	45,45,45,45	0
55	MG	2a	1622	1/1	0.81	0.20	63,63,63,63	0
55	MG	2a	1633	1/1	0.81	0.27	51,51,51,51	0
55	MG	1a	3171	1/1	0.81	0.10	59,59,59,59	0
55	MG	2a	1723	1/1	0.82	0.24	65,65,65,65	0
55	MG	2A	3195	1/1	0.82	0.11	42,42,42,42	0
55	MG	1B	203	1/1	0.82	0.11	51,51,51,51	0
55	MG	2A	3272	1/1	0.82	0.23	56,56,56,56	0
55	MG	2a	1741	1/1	0.82	0.12	59,59,59,59	0
55	MG	1a	3179	1/1	0.82	0.15	47,47,47,47	0
55	MG	2A	3058	1/1	0.82	0.24	47,47,47,47	0
55	MG	23	102	1/1	0.82	0.15	52,52,52,52	0
55	MG	1A	3969	1/1	0.82	0.11	45,45,45,45	0
55	MG	1a	3027	1/1	0.82	0.15	45,45,45,45	0
55	MG	2A	3600	1/1	0.82	0.21	37,37,37,37	0
55	MG	2a	1798	1/1	0.82	0.15	53,53,53,53	0
55	MG	2a	1801	1/1	0.82	0.18	47,47,47,47	0
55	MG	2a	1802	1/1	0.82	0.17	58,58,58,58	0
55	MG	1A	4005	1/1	0.82	0.28	47,47,47,47	0
55	MG	1B	226	1/1	0.82	0.08	53,53,53,53	0
55	MG	2A	3663	1/1	0.82	0.13	43,43,43,43	0
55	MG	2A	3835	1/1	0.83	0.20	42,42,42,42	0
55	MG	2A	3197	1/1	0.83	0.16	34,34,34,34	0
55	MG	2A	3428	1/1	0.83	0.11	58,58,58,58	0
55	MG	2A	3724	1/1	0.83	0.12	41,41,41,41	0
55	MG	1A	3094	1/1	0.83	0.18	33,33,33,33	0
55	MG	1a	3047	1/1	0.83	0.28	55,55,55,55	0
55	MG	1A	4012	1/1	0.83	0.33	47,47,47,47	0
55	MG	2a	1790	1/1	0.83	0.19	62,62,62,62	0
55	MG	2A	3312	1/1	0.83	0.13	52,52,52,52	0
55	MG	2a	1702	1/1	0.83	0.31	55,55,55,55	0
55	MG	1A	3853	1/1	0.83	0.11	39,39,39,39	0
55	MG	1A	3508	1/1	0.83	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3072	1/1	0.83	0.24	60,60,60,60	0
55	MG	2A	3818	1/1	0.83	0.15	30,30,30,30	0
55	MG	2A	3714	1/1	0.83	0.10	56,56,56,56	0
55	MG	2B	203	1/1	0.84	0.10	52,52,52,52	0
55	MG	1A	3228	1/1	0.84	0.11	30,30,30,30	0
55	MG	2A	3568	1/1	0.84	0.15	50,50,50,50	0
55	MG	1A	3268	1/1	0.84	0.09	42,42,42,42	0
55	MG	2a	1604	1/1	0.84	0.16	47,47,47,47	0
55	MG	2a	1608	1/1	0.84	0.14	53,53,53,53	0
55	MG	2A	3178	1/1	0.84	0.34	42,42,42,42	0
55	MG	2A	3193	1/1	0.84	0.09	52,52,52,52	0
55	MG	1A	3199	1/1	0.84	0.11	43,43,43,43	0
55	MG	1a	3173	1/1	0.84	0.14	51,51,51,51	0
55	MG	2a	1648	1/1	0.84	0.13	58,58,58,58	0
55	MG	2a	1660	1/1	0.84	0.14	46,46,46,46	0
55	MG	2a	1691	1/1	0.84	0.30	53,53,53,53	0
55	MG	1A	3217	1/1	0.84	0.10	48,48,48,48	0
55	MG	1A	3887	1/1	0.84	0.14	55,55,55,55	0
55	MG	2A	3286	1/1	0.84	0.14	33,33,33,33	0
55	MG	1A	4033	1/1	0.84	0.10	42,42,42,42	0
55	MG	1a	3032	1/1	0.84	0.17	57,57,57,57	0
55	MG	2A	3319	1/1	0.84	0.12	38,38,38,38	0
55	MG	2A	3328	1/1	0.84	0.17	64,64,64,64	0
55	MG	1A	3750	1/1	0.84	0.15	58,58,58,58	0
55	MG	2A	3377	1/1	0.84	0.12	49,49,49,49	0
55	MG	1A	3015	1/1	0.84	0.18	36,36,36,36	0
55	MG	1A	3762	1/1	0.84	0.12	30,30,30,30	0
55	MG	1x	104	1/1	0.84	0.10	46,46,46,46	0
55	MG	2A	3425	1/1	0.84	0.19	42,42,42,42	0
55	MG	2A	3774	1/1	0.84	0.08	58,58,58,58	0
55	MG	2A	3021	1/1	0.84	0.26	55,55,55,55	0
55	MG	2A	3048	1/1	0.84	0.14	57,57,57,57	0
55	MG	1a	3061	1/1	0.84	0.14	61,61,61,61	0
55	MG	1A	3570	1/1	0.84	0.12	43,43,43,43	0
55	MG	1A	3684	1/1	0.84	0.10	52,52,52,52	0
55	MG	1B	233	1/1	0.84	0.10	42,42,42,42	0
55	MG	2A	3841	1/1	0.84	0.10	53,53,53,53	0
55	MG	1A	3814	1/1	0.85	0.09	25,25,25,25	0
55	MG	2A	3571	1/1	0.85	0.10	29,29,29,29	0
55	MG	2B	213	1/1	0.85	0.21	50,50,50,50	0
55	MG	2A	3576	1/1	0.85	0.14	48,48,48,48	0
55	MG	2B	219	1/1	0.85	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3236	1/1	0.85	0.12	38,38,38,38	0
55	MG	2a	1603	1/1	0.85	0.10	43,43,43,43	0
55	MG	2A	3251	1/1	0.85	0.17	21,21,21,21	0
55	MG	2A	3262	1/1	0.85	0.34	50,50,50,50	0
55	MG	1A	3889	1/1	0.85	0.10	45,45,45,45	0
55	MG	1a	3104	1/1	0.85	0.15	48,48,48,48	0
55	MG	1x	112	1/1	0.85	0.11	51,51,51,51	0
55	MG	2A	3673	1/1	0.85	0.08	56,56,56,56	0
55	MG	2A	3005	1/1	0.85	0.10	45,45,45,45	0
55	MG	2A	3008	1/1	0.85	0.08	24,24,24,24	0
55	MG	1a	3114	1/1	0.85	0.11	51,51,51,51	0
55	MG	2A	3350	1/1	0.85	0.08	38,38,38,38	0
55	MG	2A	3711	1/1	0.85	0.11	47,47,47,47	0
55	MG	2A	3027	1/1	0.85	0.18	46,46,46,46	0
55	MG	1a	3142	1/1	0.85	0.13	44,44,44,44	0
55	MG	1a	3016	1/1	0.85	0.12	46,46,46,46	0
55	MG	2A	3388	1/1	0.85	0.18	34,34,34,34	0
55	MG	1a	3155	1/1	0.85	0.17	49,49,49,49	0
55	MG	2A	3401	1/1	0.85	0.24	38,38,38,38	0
55	MG	2A	3763	1/1	0.85	0.12	60,60,60,60	0
55	MG	2A	3408	1/1	0.85	0.06	34,34,34,34	0
55	MG	1A	3306	1/1	0.85	0.06	38,38,38,38	0
55	MG	2A	3095	1/1	0.85	0.16	37,37,37,37	0
55	MG	1A	3524	1/1	0.85	0.07	35,35,35,35	0
55	MG	2A	3802	1/1	0.85	0.09	17,17,17,17	0
55	MG	1B	231	1/1	0.85	0.08	39,39,39,39	0
55	MG	1A	3342	1/1	0.85	0.17	46,46,46,46	0
55	MG	1A	4024	1/1	0.85	0.13	35,35,35,35	0
55	MG	1a	3058	1/1	0.85	0.09	48,48,48,48	0
55	MG	1A	3542	1/1	0.85	0.18	51,51,51,51	0
55	MG	1A	3406	1/1	0.85	0.11	31,31,31,31	0
55	MG	2q	202	1/1	0.85	0.16	55,55,55,55	0
55	MG	2A	3850	1/1	0.85	0.14	54,54,54,54	0
55	MG	2T	203	1/1	0.86	0.09	51,51,51,51	0
55	MG	1A	3712	1/1	0.86	0.14	36,36,36,36	0
55	MG	2A	3347	1/1	0.86	0.06	48,48,48,48	0
55	MG	2A	3087	1/1	0.86	0.08	31,31,31,31	0
55	MG	2A	3090	1/1	0.86	0.19	40,40,40,40	0
55	MG	1A	3111	1/1	0.86	0.10	40,40,40,40	0
55	MG	1A	3354	1/1	0.86	0.10	37,37,37,37	0
55	MG	1A	3849	1/1	0.86	0.21	22,22,22,22	0
55	MG	2a	1636	1/1	0.86	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3079	1/1	0.86	0.17	41,41,41,41	0
55	MG	1a	3184	1/1	0.86	0.34	55,55,55,55	0
55	MG	2a	1651	1/1	0.86	0.12	58,58,58,58	0
55	MG	2a	1656	1/1	0.86	0.14	44,44,44,44	0
55	MG	2A	3150	1/1	0.86	0.21	45,45,45,45	0
55	MG	2a	1665	1/1	0.86	0.16	57,57,57,57	0
55	MG	2a	1687	1/1	0.86	0.12	44,44,44,44	0
55	MG	1a	3080	1/1	0.86	0.20	63,63,63,63	0
55	MG	2A	3187	1/1	0.86	0.22	62,62,62,62	0
55	MG	2a	1707	1/1	0.86	0.11	43,43,43,43	0
55	MG	2a	1712	1/1	0.86	0.14	41,41,41,41	0
55	MG	2a	1714	1/1	0.86	0.24	50,50,50,50	0
55	MG	2A	3759	1/1	0.86	0.16	43,43,43,43	0
55	MG	1a	3088	1/1	0.86	0.26	51,51,51,51	0
55	MG	1A	3543	1/1	0.86	0.15	30,30,30,30	0
55	MG	2a	1724	1/1	0.86	0.23	49,49,49,49	0
55	MG	2A	3504	1/1	0.86	0.07	37,37,37,37	0
55	MG	1A	3295	1/1	0.86	0.07	26,26,26,26	0
55	MG	2A	3777	1/1	0.86	0.14	46,46,46,46	0
55	MG	2a	1740	1/1	0.86	0.11	75,75,75,75	0
55	MG	1a	3108	1/1	0.86	0.17	63,63,63,63	0
55	MG	2A	3531	1/1	0.86	0.17	43,43,43,43	0
55	MG	2A	3234	1/1	0.86	0.13	53,53,53,53	0
55	MG	1x	107	1/1	0.86	0.18	48,48,48,48	0
55	MG	2a	1761	1/1	0.86	0.10	49,49,49,49	0
55	MG	2A	3248	1/1	0.86	0.09	33,33,33,33	0
55	MG	1A	3225	1/1	0.86	0.28	54,54,54,54	0
55	MG	1a	3041	1/1	0.86	0.16	45,45,45,45	0
55	MG	2A	3836	1/1	0.86	0.24	39,39,39,39	0
55	MG	1A	3687	1/1	0.86	0.11	59,59,59,59	0
55	MG	1A	3154	1/1	0.86	0.07	17,17,17,17	0
55	MG	2A	3292	1/1	0.86	0.19	48,48,48,48	0
55	MG	2a	1806	1/1	0.86	0.13	55,55,55,55	0
55	MG	1a	3166	1/1	0.86	0.14	84,84,84,84	0
55	MG	2a	1811	1/1	0.86	0.30	42,42,42,42	0
55	MG	2A	3301	1/1	0.86	0.14	44,44,44,44	0
55	MG	2d	302	1/1	0.86	0.12	47,47,47,47	0
55	MG	1a	3169	1/1	0.86	0.12	55,55,55,55	0
57	ZN	14	102	1/1	0.86	0.17	159,159,159,159	0
55	MG	1A	3898	1/1	0.86	0.17	54,54,54,54	0
55	MG	1B	216	1/1	0.87	0.13	67,67,67,67	0
55	MG	2I	101	1/1	0.87	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3035	1/1	0.87	0.18	30,30,30,30	0
55	MG	2A	3045	1/1	0.87	0.10	45,45,45,45	0
55	MG	1A	3200	1/1	0.87	0.12	37,37,37,37	0
55	MG	2A	3051	1/1	0.87	0.08	42,42,42,42	0
55	MG	1A	3083	1/1	0.87	0.13	42,42,42,42	0
55	MG	2A	3646	1/1	0.87	0.11	54,54,54,54	0
55	MG	2A	3660	1/1	0.87	0.12	38,38,38,38	0
55	MG	2a	1634	1/1	0.87	0.17	51,51,51,51	0
55	MG	2a	1635	1/1	0.87	0.13	31,31,31,31	0
55	MG	1A	3145	1/1	0.87	0.14	45,45,45,45	0
55	MG	2A	3670	1/1	0.87	0.12	43,43,43,43	0
55	MG	2A	3068	1/1	0.87	0.25	32,32,32,32	0
55	MG	2A	3316	1/1	0.87	0.06	36,36,36,36	0
55	MG	2a	1652	1/1	0.87	0.20	40,40,40,40	0
55	MG	1A	3618	1/1	0.87	0.07	46,46,46,46	0
55	MG	2A	3088	1/1	0.87	0.14	45,45,45,45	0
55	MG	2A	3333	1/1	0.87	0.13	34,34,34,34	0
55	MG	1A	3362	1/1	0.87	0.12	44,44,44,44	0
55	MG	2A	3349	1/1	0.87	0.15	49,49,49,49	0
55	MG	1A	3025	1/1	0.87	0.26	51,51,51,51	0
55	MG	2A	3718	1/1	0.87	0.10	62,62,62,62	0
55	MG	1A	3815	1/1	0.87	0.18	31,31,31,31	0
55	MG	1A	3553	1/1	0.87	0.09	27,27,27,27	0
55	MG	1E	312	1/1	0.87	0.39	54,54,54,54	0
55	MG	1A	4020	1/1	0.87	0.13	35,35,35,35	0
55	MG	1A	4021	1/1	0.87	0.14	42,42,42,42	0
55	MG	2A	3760	1/1	0.87	0.11	50,50,50,50	0
55	MG	2A	3171	1/1	0.87	0.23	35,35,35,35	0
55	MG	1A	3912	1/1	0.87	0.14	39,39,39,39	0
55	MG	2A	3422	1/1	0.87	0.21	52,52,52,52	0
55	MG	2A	3772	1/1	0.87	0.21	31,31,31,31	0
55	MG	13	102	1/1	0.87	0.30	59,59,59,59	0
55	MG	1A	3747	1/1	0.87	0.11	38,38,38,38	0
55	MG	1a	3140	1/1	0.87	0.15	42,42,42,42	0
55	MG	2a	1754	1/1	0.87	0.25	45,45,45,45	0
55	MG	2A	3794	1/1	0.87	0.11	37,37,37,37	0
55	MG	2A	3457	1/1	0.87	0.09	54,54,54,54	0
55	MG	1a	3017	1/1	0.87	0.17	48,48,48,48	0
55	MG	2A	3482	1/1	0.87	0.13	35,35,35,35	0
55	MG	1A	3935	1/1	0.87	0.07	56,56,56,56	0
55	MG	2A	3207	1/1	0.87	0.17	48,48,48,48	0
55	MG	2a	1796	1/1	0.87	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3225	1/1	0.87	0.11	42,42,42,42	0
55	MG	2A	3011	1/1	0.87	0.14	41,41,41,41	0
55	MG	2A	3015	1/1	0.87	0.09	55,55,55,55	0
55	MG	2A	3242	1/1	0.87	0.10	62,62,62,62	0
55	MG	2A	3546	1/1	0.87	0.13	54,54,54,54	0
55	MG	2A	3558	1/1	0.87	0.10	28,28,28,28	0
55	MG	2A	3244	1/1	0.87	0.07	35,35,35,35	0
55	MG	1B	215	1/1	0.87	0.11	56,56,56,56	0
55	MG	2g	201	1/1	0.87	0.09	65,65,65,65	0
55	MG	2B	216	1/1	0.87	0.10	57,57,57,57	0
55	MG	2A	3249	1/1	0.87	0.07	25,25,25,25	0
55	MG	2Q	202	1/1	0.87	0.12	38,38,38,38	0
57	ZN	25	105	1/1	0.87	0.12	164,164,164,164	0
55	MG	2A	3613	1/1	0.88	0.27	28,28,28,28	0
55	MG	25	104	1/1	0.88	0.13	34,34,34,34	0
55	MG	27	102	1/1	0.88	0.11	36,36,36,36	0
55	MG	1a	3055	1/1	0.88	0.07	46,46,46,46	0
55	MG	1A	3915	1/1	0.88	0.11	53,53,53,53	0
55	MG	2A	3630	1/1	0.88	0.16	32,32,32,32	0
55	MG	1A	3820	1/1	0.88	0.22	14,14,14,14	0
55	MG	1B	230	1/1	0.88	0.14	44,44,44,44	0
55	MG	2a	1626	1/1	0.88	0.11	46,46,46,46	0
55	MG	2A	3122	1/1	0.88	0.11	49,49,49,49	0
55	MG	1a	3202	1/1	0.88	0.11	47,47,47,47	0
55	MG	1b	301	1/1	0.88	0.13	54,54,54,54	0
55	MG	2A	3336	1/1	0.88	0.19	59,59,59,59	0
55	MG	2A	3346	1/1	0.88	0.10	47,47,47,47	0
55	MG	2A	3145	1/1	0.88	0.07	51,51,51,51	0
55	MG	2A	3149	1/1	0.88	0.06	43,43,43,43	0
55	MG	1n	102	1/1	0.88	0.12	55,55,55,55	0
55	MG	2A	3356	1/1	0.88	0.12	36,36,36,36	0
55	MG	2A	3160	1/1	0.88	0.17	58,58,58,58	0
55	MG	2A	3169	1/1	0.88	0.10	40,40,40,40	0
55	MG	1A	3172	1/1	0.88	0.08	22,22,22,22	0
55	MG	2A	3173	1/1	0.88	0.16	31,31,31,31	0
55	MG	2A	3727	1/1	0.88	0.07	40,40,40,40	0
55	MG	2a	1704	1/1	0.88	0.15	47,47,47,47	0
55	MG	1A	3835	1/1	0.88	0.17	24,24,24,24	0
55	MG	1A	3841	1/1	0.88	0.14	41,41,41,41	0
55	MG	2A	3191	1/1	0.88	0.13	50,50,50,50	0
55	MG	1A	3401	1/1	0.88	0.09	37,37,37,37	0
55	MG	1A	3226	1/1	0.88	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
55	MG	1A	3315	1/1	0.88	0.07	21,21,21,21	0
55	MG	1A	3323	1/1	0.88	0.12	30,30,30,30	0
55	MG	2A	3447	1/1	0.88	0.20	39,39,39,39	0
55	MG	1A	3868	1/1	0.88	0.12	29,29,29,29	0
55	MG	2A	3465	1/1	0.88	0.21	50,50,50,50	0
55	MG	2A	3778	1/1	0.88	0.14	50,50,50,50	0
55	MG	2A	3214	1/1	0.88	0.12	33,33,33,33	0
55	MG	2a	1742	1/1	0.88	0.29	44,44,44,44	0
55	MG	2A	3217	1/1	0.88	0.25	50,50,50,50	0
55	MG	1A	3869	1/1	0.88	0.10	61,61,61,61	0
55	MG	13	103	1/1	0.88	0.14	53,53,53,53	0
55	MG	1A	3528	1/1	0.88	0.19	59,59,59,59	0
55	MG	1A	3760	1/1	0.88	0.14	22,22,22,22	0
55	MG	1a	3165	1/1	0.88	0.14	48,48,48,48	0
55	MG	2a	1769	1/1	0.88	0.18	64,64,64,64	0
55	MG	2A	3832	1/1	0.88	0.20	36,36,36,36	0
55	MG	1A	3287	1/1	0.88	0.14	48,48,48,48	0
55	MG	1A	3532	1/1	0.88	0.13	40,40,40,40	0
55	MG	2A	3549	1/1	0.88	0.11	61,61,61,61	0
55	MG	2A	3847	1/1	0.88	0.14	47,47,47,47	0
55	MG	2A	3849	1/1	0.88	0.17	50,50,50,50	0
55	MG	1A	3905	1/1	0.88	0.10	63,63,63,63	0
55	MG	1A	3290	1/1	0.88	0.12	39,39,39,39	0
55	MG	2A	3267	1/1	0.88	0.12	54,54,54,54	0
55	MG	1A	3293	1/1	0.88	0.10	41,41,41,41	0
55	MG	2A	3275	1/1	0.88	0.14	45,45,45,45	0
55	MG	2d	301	1/1	0.88	0.19	38,38,38,38	0
55	MG	2A	3277	1/1	0.88	0.10	42,42,42,42	0
55	MG	2A	3587	1/1	0.88	0.12	60,60,60,60	0
55	MG	2i	201	1/1	0.88	0.09	70,70,70,70	0
55	MG	2n	101	1/1	0.88	0.16	56,56,56,56	0
55	MG	2F	304	1/1	0.88	0.13	54,54,54,54	0
55	MG	2t	201	1/1	0.88	0.18	36,36,36,36	0
55	MG	1A	3358	1/1	0.88	0.20	35,35,35,35	0
55	MG	1a	3053	1/1	0.88	0.09	38,38,38,38	0
55	MG	2A	3610	1/1	0.88	0.19	41,41,41,41	0
55	MG	2A	3569	1/1	0.89	0.12	35,35,35,35	0
55	MG	1A	3308	1/1	0.89	0.08	45,45,45,45	0
55	MG	1A	3370	1/1	0.89	0.19	35,35,35,35	0
55	MG	2Z	302	1/1	0.89	0.13	26,26,26,26	0
55	MG	1a	3082	1/1	0.89	0.18	28,28,28,28	0
55	MG	1A	3383	1/1	0.89	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3263	1/1	0.89	0.05	33,33,33,33	0
55	MG	1a	3089	1/1	0.89	0.17	49,49,49,49	0
55	MG	1A	3067	1/1	0.89	0.11	21,21,21,21	0
55	MG	2A	3273	1/1	0.89	0.10	24,24,24,24	0
55	MG	1A	3840	1/1	0.89	0.11	28,28,28,28	0
55	MG	1A	3956	1/1	0.89	0.16	39,39,39,39	0
55	MG	2a	1621	1/1	0.89	0.10	40,40,40,40	0
55	MG	2A	3622	1/1	0.89	0.11	37,37,37,37	0
55	MG	2A	3279	1/1	0.89	0.11	33,33,33,33	0
55	MG	2A	3280	1/1	0.89	0.22	39,39,39,39	0
55	MG	1F	313	1/1	0.89	0.13	49,49,49,49	0
55	MG	1a	3117	1/1	0.89	0.16	46,46,46,46	0
55	MG	1a	3122	1/1	0.89	0.15	42,42,42,42	0
55	MG	1G	202	1/1	0.89	0.11	40,40,40,40	0
55	MG	1A	3166	1/1	0.89	0.09	36,36,36,36	0
55	MG	2A	3680	1/1	0.89	0.08	46,46,46,46	0
55	MG	1a	3144	1/1	0.89	0.09	56,56,56,56	0
55	MG	2a	1654	1/1	0.89	0.14	35,35,35,35	0
55	MG	1a	3148	1/1	0.89	0.21	40,40,40,40	0
55	MG	2A	3686	1/1	0.89	0.16	31,31,31,31	0
55	MG	2a	1662	1/1	0.89	0.16	52,52,52,52	0
55	MG	2A	3688	1/1	0.89	0.08	53,53,53,53	0
55	MG	2a	1670	1/1	0.89	0.16	49,49,49,49	0
55	MG	2a	1673	1/1	0.89	0.06	50,50,50,50	0
55	MG	2A	3697	1/1	0.89	0.10	30,30,30,30	0
55	MG	2A	3700	1/1	0.89	0.21	31,31,31,31	0
55	MG	2a	1699	1/1	0.89	0.10	36,36,36,36	0
55	MG	1A	3583	1/1	0.89	0.09	43,43,43,43	0
55	MG	2A	3708	1/1	0.89	0.13	20,20,20,20	0
55	MG	2a	1705	1/1	0.89	0.07	54,54,54,54	0
55	MG	2A	3709	1/1	0.89	0.09	42,42,42,42	0
55	MG	1Q	203	1/1	0.89	0.09	45,45,45,45	0
55	MG	2A	3111	1/1	0.89	0.10	56,56,56,56	0
55	MG	1a	3162	1/1	0.89	0.11	47,47,47,47	0
55	MG	1A	3746	1/1	0.89	0.15	51,51,51,51	0
55	MG	2A	3135	1/1	0.89	0.16	49,49,49,49	0
55	MG	1R	207	1/1	0.89	0.18	55,55,55,55	0
55	MG	1T	202	1/1	0.89	0.10	46,46,46,46	0
55	MG	1V	204	1/1	0.89	0.05	51,51,51,51	0
55	MG	2a	1736	1/1	0.89	0.17	54,54,54,54	0
55	MG	2A	3363	1/1	0.89	0.08	49,49,49,49	0
55	MG	1A	3411	1/1	0.89	0.16	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3992	1/1	0.89	0.08	40,40,40,40	0
55	MG	2A	3158	1/1	0.89	0.10	38,38,38,38	0
55	MG	1a	3003	1/1	0.89	0.08	54,54,54,54	0
55	MG	1A	3996	1/1	0.89	0.14	51,51,51,51	0
55	MG	2A	3770	1/1	0.89	0.10	45,45,45,45	0
55	MG	1a	3180	1/1	0.89	0.08	55,55,55,55	0
55	MG	2a	1756	1/1	0.89	0.13	33,33,33,33	0
55	MG	2a	1757	1/1	0.89	0.18	44,44,44,44	0
55	MG	2a	1759	1/1	0.89	0.15	50,50,50,50	0
55	MG	2A	3411	1/1	0.89	0.16	43,43,43,43	0
55	MG	2A	3172	1/1	0.89	0.10	43,43,43,43	0
55	MG	1A	3436	1/1	0.89	0.17	53,53,53,53	0
55	MG	1A	3865	1/1	0.89	0.11	49,49,49,49	0
55	MG	2a	1776	1/1	0.89	0.16	55,55,55,55	0
55	MG	2a	1787	1/1	0.89	0.12	49,49,49,49	0
55	MG	1A	3605	1/1	0.89	0.13	53,53,53,53	0
55	MG	1A	3751	1/1	0.89	0.13	44,44,44,44	0
55	MG	1a	3198	1/1	0.89	0.10	56,56,56,56	0
55	MG	1A	3881	1/1	0.89	0.10	44,44,44,44	0
55	MG	1a	3206	1/1	0.89	0.09	60,60,60,60	0
55	MG	1A	3455	1/1	0.89	0.12	35,35,35,35	0
55	MG	2A	3205	1/1	0.89	0.09	54,54,54,54	0
55	MG	1A	3035	1/1	0.89	0.12	18,18,18,18	0
55	MG	2A	3528	1/1	0.89	0.11	24,24,24,24	0
55	MG	1A	3250	1/1	0.89	0.11	46,46,46,46	0
55	MG	1A	3895	1/1	0.89	0.09	48,48,48,48	0
55	MG	1x	103	1/1	0.89	0.27	50,50,50,50	0
55	MG	2A	3232	1/1	0.89	0.13	43,43,43,43	0
55	MG	2A	3545	1/1	0.89	0.08	57,57,57,57	0
55	MG	2j	201	1/1	0.89	0.08	64,64,64,64	0
55	MG	2B	210	1/1	0.89	0.09	45,45,45,45	0
55	MG	1A	3770	1/1	0.89	0.10	32,32,32,32	0
55	MG	2A	3235	1/1	0.89	0.11	34,34,34,34	0
55	MG	1A	3301	1/1	0.89	0.19	29,29,29,29	0
55	MG	1A	3805	1/1	0.89	0.16	41,41,41,41	0
55	MG	1A	3104	1/1	0.89	0.36	32,32,32,32	0
58	V7A	2a	1817	35/35	0.89	0.16	61,80,87,88	0
55	MG	1A	3809	1/1	0.90	0.17	32,32,32,32	0
55	MG	2B	211	1/1	0.90	0.15	35,35,35,35	0
55	MG	1B	205	1/1	0.90	0.14	44,44,44,44	0
55	MG	1a	3209	1/1	0.90	0.13	38,38,38,38	0
55	MG	2A	3202	1/1	0.90	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3204	1/1	0.90	0.06	18,18,18,18	0
55	MG	1A	3350	1/1	0.90	0.08	28,28,28,28	0
55	MG	2B	220	1/1	0.90	0.11	50,50,50,50	0
55	MG	1e	201	1/1	0.90	0.19	54,54,54,54	0
55	MG	2P	203	1/1	0.90	0.07	46,46,46,46	0
55	MG	1f	202	1/1	0.90	0.18	38,38,38,38	0
55	MG	1A	3591	1/1	0.90	0.08	29,29,29,29	0
55	MG	2W	201	1/1	0.90	0.17	45,45,45,45	0
55	MG	2Z	301	1/1	0.90	0.14	68,68,68,68	0
55	MG	1n	103	1/1	0.90	0.19	37,37,37,37	0
55	MG	1a	3050	1/1	0.90	0.08	25,25,25,25	0
55	MG	1B	217	1/1	0.90	0.20	32,32,32,32	0
55	MG	1A	3908	1/1	0.90	0.12	29,29,29,29	0
55	MG	1B	219	1/1	0.90	0.07	40,40,40,40	0
55	MG	1A	3392	1/1	0.90	0.16	31,31,31,31	0
55	MG	1B	224	1/1	0.90	0.10	40,40,40,40	0
55	MG	1A	3822	1/1	0.90	0.15	26,26,26,26	0
55	MG	2a	1609	1/1	0.90	0.22	39,39,39,39	0
55	MG	2a	1610	1/1	0.90	0.19	55,55,55,55	0
55	MG	2a	1614	1/1	0.90	0.30	53,53,53,53	0
55	MG	1A	3914	1/1	0.90	0.11	62,62,62,62	0
55	MG	1a	3073	1/1	0.90	0.14	50,50,50,50	0
55	MG	2A	3254	1/1	0.90	0.08	41,41,41,41	0
55	MG	2a	1624	1/1	0.90	0.24	38,38,38,38	0
55	MG	1A	3736	1/1	0.90	0.11	33,33,33,33	0
55	MG	1A	3296	1/1	0.90	0.19	48,48,48,48	0
55	MG	2A	3614	1/1	0.90	0.18	13,13,13,13	0
55	MG	2A	3023	1/1	0.90	0.24	41,41,41,41	0
55	MG	1A	3744	1/1	0.90	0.22	21,21,21,21	0
55	MG	2a	1637	1/1	0.90	0.24	39,39,39,39	0
55	MG	1a	3085	1/1	0.90	0.17	38,38,38,38	0
55	MG	2a	1643	1/1	0.90	0.16	49,49,49,49	0
55	MG	1A	3612	1/1	0.90	0.09	14,14,14,14	0
55	MG	2A	3634	1/1	0.90	0.16	40,40,40,40	0
55	MG	2A	3639	1/1	0.90	0.17	44,44,44,44	0
55	MG	2A	3276	1/1	0.90	0.09	59,59,59,59	0
55	MG	2A	3649	1/1	0.90	0.20	47,47,47,47	0
55	MG	1A	3615	1/1	0.90	0.16	15,15,15,15	0
55	MG	1a	3090	1/1	0.90	0.12	46,46,46,46	0
55	MG	2A	3669	1/1	0.90	0.09	37,37,37,37	0
55	MG	1A	3165	1/1	0.90	0.20	40,40,40,40	0
55	MG	2A	3282	1/1	0.90	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1F	301	1/1	0.90	0.20	29,29,29,29	0
55	MG	1F	309	1/1	0.90	0.16	45,45,45,45	0
55	MG	2A	3294	1/1	0.90	0.14	33,33,33,33	0
55	MG	2A	3079	1/1	0.90	0.26	50,50,50,50	0
55	MG	1A	3629	1/1	0.90	0.13	16,16,16,16	0
55	MG	2A	3687	1/1	0.90	0.19	49,49,49,49	0
55	MG	1A	3089	1/1	0.90	0.12	39,39,39,39	0
55	MG	2a	1709	1/1	0.90	0.12	44,44,44,44	0
55	MG	2A	3313	1/1	0.90	0.23	52,52,52,52	0
55	MG	1N	205	1/1	0.90	0.13	22,22,22,22	0
55	MG	2A	3701	1/1	0.90	0.17	48,48,48,48	0
55	MG	2a	1719	1/1	0.90	0.22	43,43,43,43	0
55	MG	1A	3364	1/1	0.90	0.09	43,43,43,43	0
55	MG	2A	3094	1/1	0.90	0.20	49,49,49,49	0
55	MG	1O	205	1/1	0.90	0.09	31,31,31,31	0
55	MG	1P	203	1/1	0.90	0.14	44,44,44,44	0
55	MG	2A	3340	1/1	0.90	0.14	43,43,43,43	0
55	MG	2a	1732	1/1	0.90	0.20	39,39,39,39	0
55	MG	2A	3345	1/1	0.90	0.10	41,41,41,41	0
55	MG	1P	204	1/1	0.90	0.23	19,19,19,19	0
55	MG	1A	3972	1/1	0.90	0.26	37,37,37,37	0
55	MG	2A	3133	1/1	0.90	0.19	33,33,33,33	0
55	MG	1P	206	1/1	0.90	0.19	34,34,34,34	0
55	MG	1A	3167	1/1	0.90	0.18	30,30,30,30	0
55	MG	2A	3736	1/1	0.90	0.08	54,54,54,54	0
55	MG	2A	3740	1/1	0.90	0.09	42,42,42,42	0
55	MG	1A	3995	1/1	0.90	0.12	48,48,48,48	0
55	MG	2A	3758	1/1	0.90	0.23	59,59,59,59	0
55	MG	1A	3663	1/1	0.90	0.10	44,44,44,44	0
55	MG	1A	4003	1/1	0.90	0.13	42,42,42,42	0
55	MG	1A	3875	1/1	0.90	0.07	39,39,39,39	0
55	MG	2A	3151	1/1	0.90	0.07	56,56,56,56	0
55	MG	12	101	1/1	0.90	0.08	34,34,34,34	0
55	MG	1A	3474	1/1	0.90	0.05	23,23,23,23	0
55	MG	1A	4016	1/1	0.90	0.07	54,54,54,54	0
55	MG	2a	1778	1/1	0.90	0.07	61,61,61,61	0
55	MG	2a	1783	1/1	0.90	0.19	56,56,56,56	0
55	MG	2A	3773	1/1	0.90	0.08	36,36,36,36	0
55	MG	13	104	1/1	0.90	0.12	38,38,38,38	0
55	MG	2A	3412	1/1	0.90	0.21	45,45,45,45	0
55	MG	2A	3420	1/1	0.90	0.20	38,38,38,38	0
55	MG	18	103	1/1	0.90	0.30	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3776	1/1	0.90	0.06	32,32,32,32	0
55	MG	1A	3787	1/1	0.90	0.09	58,58,58,58	0
55	MG	2A	3183	1/1	0.90	0.16	39,39,39,39	0
55	MG	2A	3442	1/1	0.90	0.09	33,33,33,33	0
55	MG	2A	3185	1/1	0.90	0.07	54,54,54,54	0
55	MG	2A	3819	1/1	0.90	0.12	21,21,21,21	0
55	MG	2A	3452	1/1	0.90	0.18	37,37,37,37	0
55	MG	2A	3456	1/1	0.90	0.18	38,38,38,38	0
55	MG	2A	3834	1/1	0.90	0.15	43,43,43,43	0
55	MG	2A	3186	1/1	0.90	0.19	43,43,43,43	0
55	MG	1A	3492	1/1	0.90	0.10	47,47,47,47	0
55	MG	2A	3837	1/1	0.90	0.24	23,23,23,23	0
55	MG	2A	3838	1/1	0.90	0.14	49,49,49,49	0
55	MG	1a	3021	1/1	0.90	0.15	34,34,34,34	0
55	MG	1A	3499	1/1	0.90	0.11	39,39,39,39	0
55	MG	2A	3483	1/1	0.90	0.16	29,29,29,29	0
55	MG	2A	3497	1/1	0.90	0.12	51,51,51,51	0
58	V7A	1a	3213	35/35	0.90	0.14	47,61,72,74	0
55	MG	2A	3502	1/1	0.90	0.19	56,56,56,56	0
55	MG	2A	3826	1/1	0.91	0.08	35,35,35,35	0
55	MG	1A	3616	1/1	0.91	0.17	12,12,12,12	0
55	MG	2A	3126	1/1	0.91	0.17	46,46,46,46	0
55	MG	1A	3910	1/1	0.91	0.07	35,35,35,35	0
55	MG	1a	3096	1/1	0.91	0.10	42,42,42,42	0
55	MG	1a	3101	1/1	0.91	0.15	45,45,45,45	0
55	MG	1D	303	1/1	0.91	0.07	31,31,31,31	0
55	MG	2A	3839	1/1	0.91	0.08	30,30,30,30	0
55	MG	2A	3840	1/1	0.91	0.09	51,51,51,51	0
55	MG	1A	3501	1/1	0.91	0.26	36,36,36,36	0
55	MG	2A	3843	1/1	0.91	0.23	39,39,39,39	0
55	MG	2A	3440	1/1	0.91	0.08	40,40,40,40	0
55	MG	1A	3623	1/1	0.91	0.13	15,15,15,15	0
55	MG	1a	3110	1/1	0.91	0.10	40,40,40,40	0
55	MG	2B	201	1/1	0.91	0.11	40,40,40,40	0
55	MG	1E	311	1/1	0.91	0.07	48,48,48,48	0
55	MG	2B	204	1/1	0.91	0.20	47,47,47,47	0
55	MG	2A	3453	1/1	0.91	0.14	31,31,31,31	0
55	MG	2A	3155	1/1	0.91	0.09	54,54,54,54	0
55	MG	1A	3322	1/1	0.91	0.04	20,20,20,20	0
55	MG	1a	3120	1/1	0.91	0.14	42,42,42,42	0
55	MG	1a	3121	1/1	0.91	0.28	54,54,54,54	0
55	MG	1A	3634	1/1	0.91	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3923	1/1	0.91	0.12	36,36,36,36	0
55	MG	1A	3803	1/1	0.91	0.25	29,29,29,29	0
55	MG	2E	301	1/1	0.91	0.07	31,31,31,31	0
55	MG	2E	305	1/1	0.91	0.08	27,27,27,27	0
55	MG	2A	3499	1/1	0.91	0.21	45,45,45,45	0
55	MG	1A	3514	1/1	0.91	0.29	33,33,33,33	0
55	MG	1N	202	1/1	0.91	0.09	41,41,41,41	0
55	MG	1A	3948	1/1	0.91	0.14	43,43,43,43	0
55	MG	2V	201	1/1	0.91	0.14	53,53,53,53	0
55	MG	2A	3526	1/1	0.91	0.13	27,27,27,27	0
55	MG	2X	101	1/1	0.91	0.07	34,34,34,34	0
55	MG	1A	3371	1/1	0.91	0.21	45,45,45,45	0
55	MG	1A	3812	1/1	0.91	0.10	39,39,39,39	0
55	MG	1a	3164	1/1	0.91	0.10	52,52,52,52	0
55	MG	2A	3539	1/1	0.91	0.10	41,41,41,41	0
55	MG	2A	3540	1/1	0.91	0.14	32,32,32,32	0
55	MG	1A	3059	1/1	0.91	0.06	35,35,35,35	0
55	MG	28	103	1/1	0.91	0.10	53,53,53,53	0
55	MG	1A	3961	1/1	0.91	0.15	37,37,37,37	0
55	MG	1A	3330	1/1	0.91	0.10	33,33,33,33	0
55	MG	1A	3184	1/1	0.91	0.14	43,43,43,43	0
55	MG	1A	3683	1/1	0.91	0.09	39,39,39,39	0
55	MG	1A	3971	1/1	0.91	0.13	20,20,20,20	0
55	MG	1A	3160	1/1	0.91	0.24	45,45,45,45	0
55	MG	2a	1615	1/1	0.91	0.22	37,37,37,37	0
55	MG	1A	3983	1/1	0.91	0.18	25,25,25,25	0
55	MG	1V	203	1/1	0.91	0.09	22,22,22,22	0
55	MG	1A	3826	1/1	0.91	0.09	29,29,29,29	0
55	MG	2A	3575	1/1	0.91	0.11	26,26,26,26	0
55	MG	2A	3218	1/1	0.91	0.11	43,43,43,43	0
55	MG	2a	1628	1/1	0.91	0.16	41,41,41,41	0
55	MG	2a	1631	1/1	0.91	0.19	42,42,42,42	0
55	MG	2A	3222	1/1	0.91	0.10	47,47,47,47	0
55	MG	1W	204	1/1	0.91	0.10	43,43,43,43	0
55	MG	1W	205	1/1	0.91	0.17	34,34,34,34	0
55	MG	2A	3595	1/1	0.91	0.07	45,45,45,45	0
55	MG	2A	3598	1/1	0.91	0.15	32,32,32,32	0
55	MG	1W	208	1/1	0.91	0.12	27,27,27,27	0
55	MG	1Y	201	1/1	0.91	0.13	33,33,33,33	0
55	MG	2A	3611	1/1	0.91	0.16	43,43,43,43	0
55	MG	10	101	1/1	0.91	0.05	33,33,33,33	0
55	MG	2A	3240	1/1	0.91	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1I	103	1/1	0.91	0.09	47,47,47,47	0
55	MG	2A	3243	1/1	0.91	0.07	51,51,51,51	0
55	MG	1A	3685	1/1	0.91	0.10	26,26,26,26	0
55	MG	2A	3628	1/1	0.91	0.21	31,31,31,31	0
55	MG	1a	3210	1/1	0.91	0.09	34,34,34,34	0
55	MG	2a	1666	1/1	0.91	0.20	44,44,44,44	0
55	MG	1A	3297	1/1	0.91	0.11	40,40,40,40	0
55	MG	1A	3416	1/1	0.91	0.18	44,44,44,44	0
55	MG	2a	1680	1/1	0.91	0.16	40,40,40,40	0
55	MG	2a	1686	1/1	0.91	0.14	37,37,37,37	0
55	MG	2A	3252	1/1	0.91	0.07	36,36,36,36	0
55	MG	2A	3647	1/1	0.91	0.11	41,41,41,41	0
55	MG	1A	3693	1/1	0.91	0.13	46,46,46,46	0
55	MG	2A	3651	1/1	0.91	0.16	48,48,48,48	0
55	MG	2a	1703	1/1	0.91	0.15	38,38,38,38	0
55	MG	1A	3706	1/1	0.91	0.13	39,39,39,39	0
55	MG	1A	3707	1/1	0.91	0.10	24,24,24,24	0
55	MG	2A	3264	1/1	0.91	0.09	52,52,52,52	0
55	MG	1a	3012	1/1	0.91	0.10	43,43,43,43	0
55	MG	1a	3013	1/1	0.91	0.07	56,56,56,56	0
55	MG	1a	3015	1/1	0.91	0.12	31,31,31,31	0
55	MG	2A	3678	1/1	0.91	0.14	43,43,43,43	0
55	MG	1A	3567	1/1	0.91	0.07	27,27,27,27	0
55	MG	1A	3863	1/1	0.91	0.07	49,49,49,49	0
55	MG	1A	3718	1/1	0.91	0.10	46,46,46,46	0
55	MG	1A	4029	1/1	0.91	0.18	36,36,36,36	0
55	MG	1A	3418	1/1	0.91	0.07	36,36,36,36	0
55	MG	1A	4034	1/1	0.91	0.11	54,54,54,54	0
55	MG	2A	3283	1/1	0.91	0.05	31,31,31,31	0
55	MG	2a	1733	1/1	0.91	0.13	44,44,44,44	0
55	MG	1a	3042	1/1	0.91	0.28	53,53,53,53	0
55	MG	2A	3290	1/1	0.91	0.07	30,30,30,30	0
55	MG	2A	3705	1/1	0.91	0.10	55,55,55,55	0
55	MG	2A	3016	1/1	0.91	0.08	33,33,33,33	0
55	MG	1A	4036	1/1	0.91	0.10	48,48,48,48	0
55	MG	1A	3127	1/1	0.91	0.09	18,18,18,18	0
55	MG	1a	3049	1/1	0.91	0.11	63,63,63,63	0
55	MG	2A	3307	1/1	0.91	0.09	38,38,38,38	0
55	MG	2A	3716	1/1	0.91	0.12	45,45,45,45	0
55	MG	2A	3308	1/1	0.91	0.09	44,44,44,44	0
55	MG	1A	3448	1/1	0.91	0.17	37,37,37,37	0
55	MG	1B	208	1/1	0.91	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3314	1/1	0.91	0.07	39,39,39,39	0
55	MG	2A	3046	1/1	0.91	0.11	56,56,56,56	0
55	MG	1B	211	1/1	0.91	0.10	39,39,39,39	0
55	MG	2A	3734	1/1	0.91	0.07	39,39,39,39	0
55	MG	2a	1775	1/1	0.91	0.07	68,68,68,68	0
55	MG	1A	3876	1/1	0.91	0.10	42,42,42,42	0
55	MG	1A	3453	1/1	0.91	0.24	24,24,24,24	0
55	MG	2a	1780	1/1	0.91	0.18	62,62,62,62	0
55	MG	1A	3600	1/1	0.91	0.11	33,33,33,33	0
55	MG	2A	3337	1/1	0.91	0.15	35,35,35,35	0
55	MG	2A	3061	1/1	0.91	0.13	50,50,50,50	0
55	MG	2a	1793	1/1	0.91	0.15	57,57,57,57	0
55	MG	1a	3065	1/1	0.91	0.07	51,51,51,51	0
55	MG	2A	3762	1/1	0.91	0.14	67,67,67,67	0
55	MG	1A	3355	1/1	0.91	0.11	37,37,37,37	0
55	MG	2A	3086	1/1	0.91	0.06	48,48,48,48	0
55	MG	1a	3068	1/1	0.91	0.05	30,30,30,30	0
55	MG	1A	3602	1/1	0.91	0.07	28,28,28,28	0
55	MG	1A	3080	1/1	0.91	0.12	41,41,41,41	0
55	MG	1A	3896	1/1	0.91	0.06	28,28,28,28	0
55	MG	1B	225	1/1	0.91	0.14	49,49,49,49	0
55	MG	2a	1815	1/1	0.91	0.08	53,53,53,53	0
55	MG	2A	3373	1/1	0.91	0.06	31,31,31,31	0
55	MG	1A	3610	1/1	0.91	0.10	24,24,24,24	0
55	MG	2A	3105	1/1	0.91	0.10	45,45,45,45	0
55	MG	2A	3793	1/1	0.91	0.14	13,13,13,13	0
55	MG	2A	3381	1/1	0.91	0.14	68,68,68,68	0
55	MG	2A	3110	1/1	0.91	0.05	17,17,17,17	0
55	MG	1A	3048	1/1	0.91	0.08	33,33,33,33	0
55	MG	2A	3814	1/1	0.91	0.09	44,44,44,44	0
55	MG	2x	104	1/1	0.91	0.25	50,50,50,50	0
55	MG	2A	3398	1/1	0.91	0.09	38,38,38,38	0
55	MG	2A	3113	1/1	0.91	0.14	50,50,50,50	0
55	MG	2A	3405	1/1	0.91	0.16	41,41,41,41	0
55	MG	2A	3821	1/1	0.91	0.13	33,33,33,33	0
55	MG	1A	3168	1/1	0.91	0.20	31,31,31,31	0
55	MG	1a	3062	1/1	0.92	0.20	51,51,51,51	0
55	MG	2A	3364	1/1	0.92	0.20	33,33,33,33	0
55	MG	2A	3367	1/1	0.92	0.11	27,27,27,27	0
55	MG	1A	3513	1/1	0.92	0.07	53,53,53,53	0
55	MG	2A	3376	1/1	0.92	0.11	33,33,33,33	0
55	MG	1A	3360	1/1	0.92	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3379	1/1	0.92	0.07	43,43,43,43	0
55	MG	1A	3518	1/1	0.92	0.08	45,45,45,45	0
55	MG	1A	3062	1/1	0.92	0.06	36,36,36,36	0
55	MG	1A	3695	1/1	0.92	0.10	10,10,10,10	0
55	MG	1a	3076	1/1	0.92	0.12	59,59,59,59	0
55	MG	1a	3078	1/1	0.92	0.19	19,19,19,19	0
55	MG	1A	3084	1/1	0.92	0.06	32,32,32,32	0
55	MG	1A	3185	1/1	0.92	0.06	23,23,23,23	0
55	MG	2A	3112	1/1	0.92	0.08	42,42,42,42	0
55	MG	1A	3147	1/1	0.92	0.10	41,41,41,41	0
55	MG	1A	3714	1/1	0.92	0.12	11,11,11,11	0
55	MG	2A	3413	1/1	0.92	0.18	30,30,30,30	0
55	MG	2A	3118	1/1	0.92	0.14	51,51,51,51	0
55	MG	1B	234	1/1	0.92	0.14	48,48,48,48	0
55	MG	1A	3377	1/1	0.92	0.14	38,38,38,38	0
55	MG	2A	3851	1/1	0.92	0.13	47,47,47,47	0
55	MG	1D	309	1/1	0.92	0.14	21,21,21,21	0
55	MG	2A	3134	1/1	0.92	0.11	40,40,40,40	0
55	MG	2A	3431	1/1	0.92	0.12	37,37,37,37	0
55	MG	1a	3091	1/1	0.92	0.09	53,53,53,53	0
55	MG	2A	3137	1/1	0.92	0.10	39,39,39,39	0
55	MG	1A	3381	1/1	0.92	0.10	22,22,22,22	0
55	MG	1a	3100	1/1	0.92	0.09	31,31,31,31	0
55	MG	1E	303	1/1	0.92	0.09	22,22,22,22	0
55	MG	2A	3147	1/1	0.92	0.26	51,51,51,51	0
55	MG	1E	306	1/1	0.92	0.07	33,33,33,33	0
55	MG	2A	3460	1/1	0.92	0.23	32,32,32,32	0
55	MG	1A	3735	1/1	0.92	0.17	37,37,37,37	0
55	MG	1A	3909	1/1	0.92	0.09	80,80,80,80	0
55	MG	2A	3470	1/1	0.92	0.23	21,21,21,21	0
55	MG	2A	3472	1/1	0.92	0.26	15,15,15,15	0
55	MG	2A	3480	1/1	0.92	0.06	38,38,38,38	0
55	MG	1A	3307	1/1	0.92	0.16	39,39,39,39	0
55	MG	2U	201	1/1	0.92	0.23	48,48,48,48	0
55	MG	2A	3157	1/1	0.92	0.07	20,20,20,20	0
55	MG	2A	3487	1/1	0.92	0.12	44,44,44,44	0
55	MG	1E	313	1/1	0.92	0.07	43,43,43,43	0
55	MG	1A	3556	1/1	0.92	0.11	26,26,26,26	0
55	MG	2A	3161	1/1	0.92	0.10	51,51,51,51	0
55	MG	2A	3167	1/1	0.92	0.11	51,51,51,51	0
55	MG	2I	104	1/1	0.92	0.15	27,27,27,27	0
55	MG	2I	106	1/1	0.92	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3232	1/1	0.92	0.04	26,26,26,26	0
55	MG	2A	3519	1/1	0.92	0.07	60,60,60,60	0
55	MG	1A	3311	1/1	0.92	0.11	41,41,41,41	0
55	MG	2A	3527	1/1	0.92	0.08	40,40,40,40	0
55	MG	1A	3580	1/1	0.92	0.11	42,42,42,42	0
55	MG	1a	3133	1/1	0.92	0.17	47,47,47,47	0
55	MG	1A	3922	1/1	0.92	0.06	68,68,68,68	0
55	MG	2A	3534	1/1	0.92	0.15	21,21,21,21	0
55	MG	2A	3180	1/1	0.92	0.12	38,38,38,38	0
55	MG	2a	1612	1/1	0.92	0.11	39,39,39,39	0
55	MG	2A	3181	1/1	0.92	0.05	10,10,10,10	0
55	MG	1A	3193	1/1	0.92	0.16	15,15,15,15	0
55	MG	2A	3542	1/1	0.92	0.12	29,29,29,29	0
55	MG	1a	3143	1/1	0.92	0.09	34,34,34,34	0
55	MG	1A	3931	1/1	0.92	0.09	20,20,20,20	0
55	MG	1A	3407	1/1	0.92	0.08	37,37,37,37	0
55	MG	2A	3188	1/1	0.92	0.04	30,30,30,30	0
55	MG	1A	3589	1/1	0.92	0.10	25,25,25,25	0
55	MG	1a	3150	1/1	0.92	0.10	41,41,41,41	0
55	MG	2a	1632	1/1	0.92	0.19	51,51,51,51	0
55	MG	1A	3409	1/1	0.92	0.06	50,50,50,50	0
55	MG	1a	3157	1/1	0.92	0.15	34,34,34,34	0
55	MG	1A	3594	1/1	0.92	0.10	25,25,25,25	0
55	MG	1a	3163	1/1	0.92	0.12	42,42,42,42	0
55	MG	2A	3203	1/1	0.92	0.05	44,44,44,44	0
55	MG	1A	3595	1/1	0.92	0.10	24,24,24,24	0
55	MG	1A	3763	1/1	0.92	0.08	37,37,37,37	0
55	MG	2a	1646	1/1	0.92	0.12	58,58,58,58	0
55	MG	1A	3767	1/1	0.92	0.19	40,40,40,40	0
55	MG	1a	3168	1/1	0.92	0.13	50,50,50,50	0
55	MG	1A	3318	1/1	0.92	0.12	27,27,27,27	0
55	MG	2a	1653	1/1	0.92	0.10	42,42,42,42	0
55	MG	1A	3771	1/1	0.92	0.08	44,44,44,44	0
55	MG	1A	3319	1/1	0.92	0.14	16,16,16,16	0
55	MG	2A	3223	1/1	0.92	0.15	51,51,51,51	0
55	MG	1A	3266	1/1	0.92	0.25	52,52,52,52	0
55	MG	2A	3226	1/1	0.92	0.22	32,32,32,32	0
55	MG	2A	3229	1/1	0.92	0.05	22,22,22,22	0
55	MG	2a	1667	1/1	0.92	0.12	40,40,40,40	0
55	MG	1A	3435	1/1	0.92	0.07	54,54,54,54	0
55	MG	1A	3974	1/1	0.92	0.08	30,30,30,30	0
55	MG	2a	1678	1/1	0.92	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3976	1/1	0.92	0.15	26,26,26,26	0
55	MG	2a	1681	1/1	0.92	0.12	54,54,54,54	0
55	MG	2a	1685	1/1	0.92	0.12	51,51,51,51	0
55	MG	1A	3058	1/1	0.92	0.11	39,39,39,39	0
55	MG	1Y	202	1/1	0.92	0.07	44,44,44,44	0
55	MG	1a	3186	1/1	0.92	0.10	31,31,31,31	0
55	MG	2a	1698	1/1	0.92	0.15	40,40,40,40	0
55	MG	1A	3270	1/1	0.92	0.09	41,41,41,41	0
55	MG	1a	3193	1/1	0.92	0.14	62,62,62,62	0
55	MG	1A	3286	1/1	0.92	0.09	41,41,41,41	0
55	MG	1A	3121	1/1	0.92	0.11	27,27,27,27	0
55	MG	2A	3654	1/1	0.92	0.10	41,41,41,41	0
55	MG	1a	3199	1/1	0.92	0.07	55,55,55,55	0
55	MG	1A	3457	1/1	0.92	0.15	38,38,38,38	0
55	MG	2A	3666	1/1	0.92	0.12	26,26,26,26	0
55	MG	1A	4004	1/1	0.92	0.08	31,31,31,31	0
55	MG	2A	3261	1/1	0.92	0.16	43,43,43,43	0
55	MG	2A	3671	1/1	0.92	0.06	35,35,35,35	0
55	MG	1a	3207	1/1	0.92	0.14	50,50,50,50	0
55	MG	1A	3458	1/1	0.92	0.08	25,25,25,25	0
55	MG	14	101	1/1	0.92	0.11	40,40,40,40	0
55	MG	2A	3265	1/1	0.92	0.14	37,37,37,37	0
55	MG	2a	1726	1/1	0.92	0.28	26,26,26,26	0
55	MG	2a	1728	1/1	0.92	0.15	41,41,41,41	0
55	MG	1a	3212	1/1	0.92	0.15	66,66,66,66	0
55	MG	18	102	1/1	0.92	0.16	26,26,26,26	0
55	MG	1A	3628	1/1	0.92	0.09	22,22,22,22	0
55	MG	19	101	1/1	0.92	0.10	58,58,58,58	0
55	MG	1A	3471	1/1	0.92	0.08	47,47,47,47	0
55	MG	2A	3696	1/1	0.92	0.07	50,50,50,50	0
55	MG	1a	3004	1/1	0.92	0.08	57,57,57,57	0
55	MG	2A	3278	1/1	0.92	0.13	36,36,36,36	0
55	MG	1a	3005	1/1	0.92	0.31	51,51,51,51	0
55	MG	1v	103	1/1	0.92	0.31	55,55,55,55	0
55	MG	2a	1749	1/1	0.92	0.14	53,53,53,53	0
55	MG	2a	1751	1/1	0.92	0.10	34,34,34,34	0
55	MG	1A	3212	1/1	0.92	0.06	10,10,10,10	0
55	MG	1A	3643	1/1	0.92	0.07	35,35,35,35	0
55	MG	1A	3831	1/1	0.92	0.07	26,26,26,26	0
55	MG	2A	3289	1/1	0.92	0.15	49,49,49,49	0
55	MG	1A	3479	1/1	0.92	0.09	48,48,48,48	0
55	MG	1A	4031	1/1	0.92	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3018	1/1	0.92	0.25	42,42,42,42	0
55	MG	1a	3020	1/1	0.92	0.16	34,34,34,34	0
55	MG	2a	1771	1/1	0.92	0.08	39,39,39,39	0
55	MG	2A	3719	1/1	0.92	0.17	47,47,47,47	0
55	MG	2A	3721	1/1	0.92	0.12	40,40,40,40	0
55	MG	1A	3652	1/1	0.92	0.10	29,29,29,29	0
55	MG	1A	3655	1/1	0.92	0.12	41,41,41,41	0
55	MG	1A	3658	1/1	0.92	0.13	32,32,32,32	0
55	MG	1a	3037	1/1	0.92	0.13	39,39,39,39	0
55	MG	2A	3731	1/1	0.92	0.14	46,46,46,46	0
55	MG	1A	4038	1/1	0.92	0.08	35,35,35,35	0
55	MG	1A	4041	1/1	0.92	0.10	29,29,29,29	0
55	MG	2A	3737	1/1	0.92	0.16	51,51,51,51	0
55	MG	2A	3032	1/1	0.92	0.15	28,28,28,28	0
55	MG	2a	1797	1/1	0.92	0.15	47,47,47,47	0
55	MG	2A	3318	1/1	0.92	0.14	44,44,44,44	0
55	MG	1A	3292	1/1	0.92	0.06	25,25,25,25	0
55	MG	2A	3037	1/1	0.92	0.18	17,17,17,17	0
55	MG	2A	3332	1/1	0.92	0.05	33,33,33,33	0
55	MG	2a	1809	1/1	0.92	0.10	26,26,26,26	0
55	MG	1B	204	1/1	0.92	0.09	25,25,25,25	0
55	MG	1A	3493	1/1	0.92	0.12	37,37,37,37	0
55	MG	2a	1812	1/1	0.92	0.14	54,54,54,54	0
55	MG	1A	3215	1/1	0.92	0.10	44,44,44,44	0
55	MG	2A	3766	1/1	0.92	0.09	37,37,37,37	0
55	MG	2A	3050	1/1	0.92	0.13	31,31,31,31	0
55	MG	1A	3666	1/1	0.92	0.06	23,23,23,23	0
55	MG	2f	202	1/1	0.92	0.14	52,52,52,52	0
55	MG	1A	3169	1/1	0.92	0.09	38,38,38,38	0
55	MG	2A	3055	1/1	0.92	0.09	48,48,48,48	0
55	MG	1a	3054	1/1	0.92	0.10	46,46,46,46	0
55	MG	2k	201	1/1	0.92	0.09	54,54,54,54	0
55	MG	1A	3866	1/1	0.92	0.08	62,62,62,62	0
55	MG	2A	3351	1/1	0.92	0.12	38,38,38,38	0
55	MG	2A	3780	1/1	0.92	0.12	51,51,51,51	0
55	MG	2A	3781	1/1	0.92	0.15	43,43,43,43	0
55	MG	2x	107	1/1	0.92	0.19	47,47,47,47	0
56	K	2A	3433	1/1	0.92	0.07	43,43,43,43	0
55	MG	2A	3785	1/1	0.92	0.15	43,43,43,43	0
55	MG	2A	3355	1/1	0.92	0.17	30,30,30,30	0
57	ZN	24	501	1/1	0.92	0.14	147,147,147,147	0
55	MG	1A	3359	1/1	0.92	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3358	1/1	0.92	0.05	17,17,17,17	0
55	MG	1A	3512	1/1	0.92	0.07	23,23,23,23	0
55	MG	2A	3764	1/1	0.93	0.08	37,37,37,37	0
55	MG	2A	3341	1/1	0.93	0.13	43,43,43,43	0
55	MG	1A	3141	1/1	0.93	0.10	37,37,37,37	0
55	MG	1a	3059	1/1	0.93	0.06	41,41,41,41	0
55	MG	1a	3060	1/1	0.93	0.12	44,44,44,44	0
55	MG	1A	3521	1/1	0.93	0.13	25,25,25,25	0
55	MG	1A	3070	1/1	0.93	0.06	41,41,41,41	0
55	MG	2A	3074	1/1	0.93	0.10	44,44,44,44	0
55	MG	2A	3077	1/1	0.93	0.11	23,23,23,23	0
55	MG	1a	3064	1/1	0.93	0.17	59,59,59,59	0
55	MG	1A	3171	1/1	0.93	0.08	34,34,34,34	0
55	MG	2A	3359	1/1	0.93	0.19	33,33,33,33	0
55	MG	1A	3298	1/1	0.93	0.05	38,38,38,38	0
55	MG	1A	3873	1/1	0.93	0.07	50,50,50,50	0
55	MG	1A	3090	1/1	0.93	0.13	42,42,42,42	0
55	MG	1A	3538	1/1	0.93	0.16	29,29,29,29	0
55	MG	2A	3795	1/1	0.93	0.11	30,30,30,30	0
55	MG	2A	3371	1/1	0.93	0.10	27,27,27,27	0
55	MG	2A	3372	1/1	0.93	0.13	42,42,42,42	0
55	MG	2A	3806	1/1	0.93	0.15	36,36,36,36	0
55	MG	1A	3878	1/1	0.93	0.08	20,20,20,20	0
55	MG	1B	228	1/1	0.93	0.09	33,33,33,33	0
55	MG	2A	3097	1/1	0.93	0.24	40,40,40,40	0
55	MG	1A	3879	1/1	0.93	0.12	41,41,41,41	0
55	MG	2A	3106	1/1	0.93	0.13	23,23,23,23	0
55	MG	1A	3704	1/1	0.93	0.07	41,41,41,41	0
55	MG	2A	3382	1/1	0.93	0.16	22,22,22,22	0
55	MG	2A	3827	1/1	0.93	0.10	45,45,45,45	0
55	MG	1A	3180	1/1	0.93	0.12	56,56,56,56	0
55	MG	2A	3389	1/1	0.93	0.14	28,28,28,28	0
55	MG	2A	3391	1/1	0.93	0.19	30,30,30,30	0
55	MG	2A	3392	1/1	0.93	0.15	25,25,25,25	0
55	MG	1B	232	1/1	0.93	0.08	59,59,59,59	0
55	MG	1A	3182	1/1	0.93	0.11	42,42,42,42	0
55	MG	1A	3077	1/1	0.93	0.05	24,24,24,24	0
55	MG	2A	3117	1/1	0.93	0.09	33,33,33,33	0
55	MG	1A	3893	1/1	0.93	0.08	35,35,35,35	0
55	MG	2A	3409	1/1	0.93	0.14	28,28,28,28	0
55	MG	2A	3120	1/1	0.93	0.19	30,30,30,30	0
55	MG	1A	3240	1/1	0.93	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3093	1/1	0.93	0.13	53,53,53,53	0
55	MG	2A	3416	1/1	0.93	0.10	33,33,33,33	0
55	MG	2A	3130	1/1	0.93	0.07	28,28,28,28	0
55	MG	2A	3131	1/1	0.93	0.11	49,49,49,49	0
55	MG	1A	3558	1/1	0.93	0.13	21,21,21,21	0
55	MG	2B	205	1/1	0.93	0.14	34,34,34,34	0
55	MG	1A	3242	1/1	0.93	0.10	28,28,28,28	0
55	MG	1A	3729	1/1	0.93	0.08	29,29,29,29	0
55	MG	1A	3733	1/1	0.93	0.11	17,17,17,17	0
55	MG	2A	3435	1/1	0.93	0.13	24,24,24,24	0
55	MG	2A	3439	1/1	0.93	0.07	15,15,15,15	0
55	MG	1a	3103	1/1	0.93	0.12	44,44,44,44	0
55	MG	2A	3441	1/1	0.93	0.06	31,31,31,31	0
55	MG	1A	3568	1/1	0.93	0.06	31,31,31,31	0
55	MG	2A	3444	1/1	0.93	0.23	36,36,36,36	0
55	MG	1a	3105	1/1	0.93	0.15	35,35,35,35	0
55	MG	2A	3449	1/1	0.93	0.15	32,32,32,32	0
55	MG	1A	3249	1/1	0.93	0.37	49,49,49,49	0
55	MG	2Q	201	1/1	0.93	0.09	53,53,53,53	0
55	MG	1A	3737	1/1	0.93	0.09	33,33,33,33	0
55	MG	2A	3455	1/1	0.93	0.24	32,32,32,32	0
55	MG	1a	3113	1/1	0.93	0.13	41,41,41,41	0
55	MG	1A	3001	1/1	0.93	0.07	26,26,26,26	0
55	MG	1F	304	1/1	0.93	0.22	30,30,30,30	0
55	MG	2A	3461	1/1	0.93	0.28	51,51,51,51	0
55	MG	2A	3156	1/1	0.93	0.25	32,32,32,32	0
55	MG	1F	308	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3320	1/1	0.93	0.10	28,28,28,28	0
55	MG	1A	3426	1/1	0.93	0.10	15,15,15,15	0
55	MG	2A	3473	1/1	0.93	0.27	19,19,19,19	0
55	MG	2A	3479	1/1	0.93	0.17	23,23,23,23	0
55	MG	1A	3262	1/1	0.93	0.21	27,27,27,27	0
55	MG	26	101	1/1	0.93	0.20	40,40,40,40	0
55	MG	2A	3166	1/1	0.93	0.05	38,38,38,38	0
55	MG	28	101	1/1	0.93	0.06	31,31,31,31	0
55	MG	1a	3137	1/1	0.93	0.07	34,34,34,34	0
55	MG	2A	3486	1/1	0.93	0.14	29,29,29,29	0
55	MG	1G	204	1/1	0.93	0.08	51,51,51,51	0
55	MG	2a	1607	1/1	0.93	0.07	31,31,31,31	0
55	MG	2A	3489	1/1	0.93	0.15	17,17,17,17	0
55	MG	2A	3493	1/1	0.93	0.07	42,42,42,42	0
55	MG	1H	201	1/1	0.93	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	1611	1/1	0.93	0.16	47,47,47,47	0
55	MG	1A	3590	1/1	0.93	0.06	21,21,21,21	0
55	MG	1A	3189	1/1	0.93	0.08	22,22,22,22	0
55	MG	2A	3503	1/1	0.93	0.15	26,26,26,26	0
55	MG	1A	3437	1/1	0.93	0.07	29,29,29,29	0
55	MG	2A	3509	1/1	0.93	0.11	26,26,26,26	0
55	MG	2A	3511	1/1	0.93	0.18	27,27,27,27	0
55	MG	1A	3933	1/1	0.93	0.06	51,51,51,51	0
55	MG	2A	3516	1/1	0.93	0.14	36,36,36,36	0
55	MG	1A	3023	1/1	0.93	0.05	24,24,24,24	0
55	MG	2a	1630	1/1	0.93	0.14	48,48,48,48	0
55	MG	2A	3520	1/1	0.93	0.08	48,48,48,48	0
55	MG	2A	3522	1/1	0.93	0.15	34,34,34,34	0
55	MG	1a	3153	1/1	0.93	0.06	26,26,26,26	0
55	MG	1a	3154	1/1	0.93	0.07	41,41,41,41	0
55	MG	1A	3451	1/1	0.93	0.18	47,47,47,47	0
55	MG	1a	3156	1/1	0.93	0.13	39,39,39,39	0
55	MG	1A	3331	1/1	0.93	0.05	21,21,21,21	0
55	MG	2a	1638	1/1	0.93	0.10	42,42,42,42	0
55	MG	2a	1640	1/1	0.93	0.06	42,42,42,42	0
55	MG	1A	3191	1/1	0.93	0.07	44,44,44,44	0
55	MG	1A	3764	1/1	0.93	0.09	41,41,41,41	0
55	MG	2A	3194	1/1	0.93	0.10	26,26,26,26	0
55	MG	1A	3274	1/1	0.93	0.09	40,40,40,40	0
55	MG	1A	3281	1/1	0.93	0.05	12,12,12,12	0
55	MG	1A	3459	1/1	0.93	0.14	28,28,28,28	0
55	MG	2A	3201	1/1	0.93	0.25	51,51,51,51	0
55	MG	1A	3464	1/1	0.93	0.12	29,29,29,29	0
55	MG	1A	3968	1/1	0.93	0.07	42,42,42,42	0
55	MG	2a	1659	1/1	0.93	0.18	45,45,45,45	0
55	MG	2A	3552	1/1	0.93	0.20	15,15,15,15	0
55	MG	2A	3554	1/1	0.93	0.14	28,28,28,28	0
55	MG	1A	3777	1/1	0.93	0.07	51,51,51,51	0
55	MG	2A	3559	1/1	0.93	0.11	24,24,24,24	0
55	MG	1A	3778	1/1	0.93	0.14	55,55,55,55	0
55	MG	2a	1669	1/1	0.93	0.09	40,40,40,40	0
55	MG	1A	3467	1/1	0.93	0.19	28,28,28,28	0
55	MG	2A	3209	1/1	0.93	0.07	24,24,24,24	0
55	MG	1a	3174	1/1	0.93	0.13	49,49,49,49	0
55	MG	1a	3175	1/1	0.93	0.08	74,74,74,74	0
55	MG	1A	3790	1/1	0.93	0.06	28,28,28,28	0
55	MG	1A	3351	1/1	0.93	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3578	1/1	0.93	0.11	22,22,22,22	0
55	MG	1A	3794	1/1	0.93	0.06	35,35,35,35	0
55	MG	2A	3589	1/1	0.93	0.08	42,42,42,42	0
55	MG	2a	1695	1/1	0.93	0.14	43,43,43,43	0
55	MG	2A	3590	1/1	0.93	0.26	27,27,27,27	0
55	MG	2A	3591	1/1	0.93	0.09	41,41,41,41	0
55	MG	2A	3593	1/1	0.93	0.25	50,50,50,50	0
55	MG	10	106	1/1	0.93	0.11	35,35,35,35	0
55	MG	1a	3183	1/1	0.93	0.10	44,44,44,44	0
55	MG	1A	3283	1/1	0.93	0.12	12,12,12,12	0
55	MG	1A	3993	1/1	0.93	0.26	10,10,10,10	0
55	MG	2A	3607	1/1	0.93	0.14	44,44,44,44	0
55	MG	2a	1710	1/1	0.93	0.07	57,57,57,57	0
55	MG	1A	3284	1/1	0.93	0.06	14,14,14,14	0
55	MG	1a	3192	1/1	0.93	0.08	33,33,33,33	0
55	MG	1A	3488	1/1	0.93	0.06	30,30,30,30	0
55	MG	2A	3239	1/1	0.93	0.09	34,34,34,34	0
55	MG	1A	3998	1/1	0.93	0.07	44,44,44,44	0
55	MG	2A	3618	1/1	0.93	0.16	22,22,22,22	0
55	MG	2A	3241	1/1	0.93	0.09	32,32,32,32	0
55	MG	1A	3999	1/1	0.93	0.13	32,32,32,32	0
55	MG	16	103	1/1	0.93	0.10	42,42,42,42	0
55	MG	1A	4001	1/1	0.93	0.12	41,41,41,41	0
55	MG	2A	3631	1/1	0.93	0.19	19,19,19,19	0
55	MG	2A	3246	1/1	0.93	0.09	48,48,48,48	0
55	MG	1a	3203	1/1	0.93	0.07	39,39,39,39	0
55	MG	1A	3356	1/1	0.93	0.05	29,29,29,29	0
55	MG	2a	1737	1/1	0.93	0.20	28,28,28,28	0
55	MG	1A	3639	1/1	0.93	0.09	15,15,15,15	0
55	MG	1A	3641	1/1	0.93	0.24	17,17,17,17	0
55	MG	1A	4006	1/1	0.93	0.11	42,42,42,42	0
55	MG	1A	3357	1/1	0.93	0.27	39,39,39,39	0
55	MG	2A	3658	1/1	0.93	0.10	52,52,52,52	0
55	MG	1a	3009	1/1	0.93	0.08	28,28,28,28	0
55	MG	1a	3010	1/1	0.93	0.16	55,55,55,55	0
55	MG	1A	4014	1/1	0.93	0.09	51,51,51,51	0
55	MG	2a	1752	1/1	0.93	0.29	37,37,37,37	0
55	MG	1A	3644	1/1	0.93	0.16	28,28,28,28	0
55	MG	1A	4018	1/1	0.93	0.07	40,40,40,40	0
55	MG	1A	3824	1/1	0.93	0.07	14,14,14,14	0
55	MG	1A	3496	1/1	0.93	0.15	26,26,26,26	0
55	MG	1A	3498	1/1	0.93	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3830	1/1	0.93	0.07	30,30,30,30	0
55	MG	1A	3162	1/1	0.93	0.08	36,36,36,36	0
55	MG	2a	1764	1/1	0.93	0.10	41,41,41,41	0
55	MG	1x	105	1/1	0.93	0.26	54,54,54,54	0
55	MG	1a	3025	1/1	0.93	0.17	30,30,30,30	0
55	MG	1x	110	1/1	0.93	0.14	29,29,29,29	0
55	MG	1A	3066	1/1	0.93	0.11	23,23,23,23	0
55	MG	1x	113	1/1	0.93	0.21	50,50,50,50	0
55	MG	2A	3284	1/1	0.93	0.10	33,33,33,33	0
55	MG	1a	3029	1/1	0.93	0.14	30,30,30,30	0
55	MG	2A	3287	1/1	0.93	0.27	46,46,46,46	0
55	MG	1A	3837	1/1	0.93	0.12	51,51,51,51	0
55	MG	1a	3033	1/1	0.93	0.22	40,40,40,40	0
55	MG	2A	3291	1/1	0.93	0.05	39,39,39,39	0
55	MG	1A	3839	1/1	0.93	0.06	36,36,36,36	0
55	MG	1a	3038	1/1	0.93	0.08	54,54,54,54	0
55	MG	2A	3295	1/1	0.93	0.09	31,31,31,31	0
55	MG	1A	4037	1/1	0.93	0.09	33,33,33,33	0
55	MG	2A	3715	1/1	0.93	0.08	46,46,46,46	0
55	MG	2A	3022	1/1	0.93	0.10	27,27,27,27	0
55	MG	2A	3302	1/1	0.93	0.06	40,40,40,40	0
55	MG	2A	3303	1/1	0.93	0.11	44,44,44,44	0
55	MG	2A	3304	1/1	0.93	0.07	39,39,39,39	0
55	MG	1A	3027	1/1	0.93	0.24	28,28,28,28	0
55	MG	2A	3026	1/1	0.93	0.08	27,27,27,27	0
55	MG	2A	3310	1/1	0.93	0.06	28,28,28,28	0
55	MG	2A	3726	1/1	0.93	0.11	52,52,52,52	0
55	MG	1a	3044	1/1	0.93	0.11	56,56,56,56	0
55	MG	2A	3028	1/1	0.93	0.09	35,35,35,35	0
55	MG	2f	201	1/1	0.93	0.05	44,44,44,44	0
55	MG	2A	3730	1/1	0.93	0.14	54,54,54,54	0
55	MG	1A	3206	1/1	0.93	0.11	28,28,28,28	0
55	MG	1B	202	1/1	0.93	0.11	48,48,48,48	0
55	MG	1A	3134	1/1	0.93	0.33	34,34,34,34	0
55	MG	2A	3039	1/1	0.93	0.10	32,32,32,32	0
55	MG	2A	3738	1/1	0.93	0.07	27,27,27,27	0
55	MG	2A	3323	1/1	0.93	0.07	38,38,38,38	0
55	MG	2A	3744	1/1	0.93	0.07	51,51,51,51	0
55	MG	2x	102	1/1	0.93	0.10	41,41,41,41	0
55	MG	2x	103	1/1	0.93	0.13	29,29,29,29	0
55	MG	2A	3745	1/1	0.93	0.20	17,17,17,17	0
55	MG	2x	105	1/1	0.93	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3747	1/1	0.93	0.12	49,49,49,49	0
55	MG	1A	3365	1/1	0.93	0.06	41,41,41,41	0
55	MG	1A	3851	1/1	0.93	0.08	43,43,43,43	0
55	MG	1A	3668	1/1	0.93	0.22	10,10,10,10	0
55	MG	1A	3516	1/1	0.93	0.18	31,31,31,31	0
55	MG	2A	3761	1/1	0.93	0.15	55,55,55,55	0
55	MG	1B	212	1/1	0.93	0.07	25,25,25,25	0
55	MG	2A	3053	1/1	0.93	0.11	34,34,34,34	0
55	MG	1a	3134	1/1	0.94	0.10	28,28,28,28	0
55	MG	2A	3792	1/1	0.94	0.14	30,30,30,30	0
55	MG	1Q	202	1/1	0.94	0.06	30,30,30,30	0
55	MG	1A	3216	1/1	0.94	0.07	30,30,30,30	0
55	MG	2A	3427	1/1	0.94	0.18	45,45,45,45	0
55	MG	2A	3797	1/1	0.94	0.11	21,21,21,21	0
55	MG	2A	3798	1/1	0.94	0.19	23,23,23,23	0
55	MG	1A	3635	1/1	0.94	0.08	22,22,22,22	0
55	MG	1A	3146	1/1	0.94	0.12	49,49,49,49	0
55	MG	2A	3432	1/1	0.94	0.12	45,45,45,45	0
55	MG	2A	3807	1/1	0.94	0.20	21,21,21,21	0
55	MG	1S	201	1/1	0.94	0.17	47,47,47,47	0
55	MG	2A	3815	1/1	0.94	0.11	44,44,44,44	0
55	MG	2A	3437	1/1	0.94	0.08	37,37,37,37	0
55	MG	1a	3145	1/1	0.94	0.09	23,23,23,23	0
55	MG	1A	3640	1/1	0.94	0.11	47,47,47,47	0
55	MG	2A	3820	1/1	0.94	0.11	33,33,33,33	0
55	MG	1V	202	1/1	0.94	0.18	35,35,35,35	0
55	MG	1A	3497	1/1	0.94	0.12	37,37,37,37	0
55	MG	2A	3443	1/1	0.94	0.20	46,46,46,46	0
55	MG	1a	3152	1/1	0.94	0.08	40,40,40,40	0
55	MG	2A	3831	1/1	0.94	0.09	35,35,35,35	0
55	MG	2A	3446	1/1	0.94	0.12	59,59,59,59	0
55	MG	2A	3833	1/1	0.94	0.22	47,47,47,47	0
55	MG	1A	3979	1/1	0.94	0.10	36,36,36,36	0
55	MG	1A	3980	1/1	0.94	0.07	24,24,24,24	0
55	MG	2A	3168	1/1	0.94	0.18	47,47,47,47	0
55	MG	1A	3982	1/1	0.94	0.07	36,36,36,36	0
55	MG	1A	3811	1/1	0.94	0.11	39,39,39,39	0
55	MG	1A	3988	1/1	0.94	0.09	36,36,36,36	0
55	MG	1A	3223	1/1	0.94	0.08	31,31,31,31	0
55	MG	2A	3459	1/1	0.94	0.16	29,29,29,29	0
55	MG	2A	3174	1/1	0.94	0.07	33,33,33,33	0
55	MG	2A	3846	1/1	0.94	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3173	1/1	0.94	0.06	28,28,28,28	0
55	MG	2A	3464	1/1	0.94	0.12	20,20,20,20	0
55	MG	10	104	1/1	0.94	0.16	46,46,46,46	0
55	MG	10	105	1/1	0.94	0.15	29,29,29,29	0
55	MG	1A	3008	1/1	0.94	0.11	21,21,21,21	0
55	MG	2A	3184	1/1	0.94	0.14	29,29,29,29	0
55	MG	1a	3167	1/1	0.94	0.13	31,31,31,31	0
55	MG	1A	3506	1/1	0.94	0.09	23,23,23,23	0
55	MG	2B	206	1/1	0.94	0.11	40,40,40,40	0
55	MG	1A	3055	1/1	0.94	0.16	29,29,29,29	0
55	MG	1A	3657	1/1	0.94	0.08	19,19,19,19	0
55	MG	1A	4000	1/1	0.94	0.07	32,32,32,32	0
55	MG	1A	3155	1/1	0.94	0.05	23,23,23,23	0
55	MG	2B	214	1/1	0.94	0.17	49,49,49,49	0
55	MG	1A	3378	1/1	0.94	0.04	29,29,29,29	0
55	MG	16	101	1/1	0.94	0.07	28,28,28,28	0
55	MG	1A	3380	1/1	0.94	0.20	24,24,24,24	0
55	MG	2A	3496	1/1	0.94	0.08	27,27,27,27	0
55	MG	2D	302	1/1	0.94	0.11	28,28,28,28	0
55	MG	17	103	1/1	0.94	0.10	41,41,41,41	0
55	MG	2E	304	1/1	0.94	0.08	30,30,30,30	0
55	MG	1A	3157	1/1	0.94	0.09	29,29,29,29	0
55	MG	1A	3300	1/1	0.94	0.06	27,27,27,27	0
55	MG	2G	201	1/1	0.94	0.05	42,42,42,42	0
55	MG	2P	201	1/1	0.94	0.07	40,40,40,40	0
55	MG	1a	3182	1/1	0.94	0.09	39,39,39,39	0
55	MG	18	104	1/1	0.94	0.05	33,33,33,33	0
55	MG	2A	3506	1/1	0.94	0.12	33,33,33,33	0
55	MG	18	105	1/1	0.94	0.13	35,35,35,35	0
55	MG	1A	3836	1/1	0.94	0.06	45,45,45,45	0
55	MG	19	102	1/1	0.94	0.08	31,31,31,31	0
55	MG	2A	3515	1/1	0.94	0.16	24,24,24,24	0
55	MG	1a	3002	1/1	0.94	0.14	30,30,30,30	0
55	MG	1A	3389	1/1	0.94	0.10	21,21,21,21	0
55	MG	1A	3523	1/1	0.94	0.07	42,42,42,42	0
55	MG	2A	3521	1/1	0.94	0.12	33,33,33,33	0
55	MG	2A	3220	1/1	0.94	0.11	38,38,38,38	0
55	MG	1A	3233	1/1	0.94	0.21	24,24,24,24	0
55	MG	23	101	1/1	0.94	0.13	21,21,21,21	0
55	MG	1a	3007	1/1	0.94	0.08	27,27,27,27	0
55	MG	25	101	1/1	0.94	0.10	38,38,38,38	0
55	MG	25	102	1/1	0.94	0.05	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3526	1/1	0.94	0.11	31,31,31,31	0
55	MG	1A	3304	1/1	0.94	0.06	35,35,35,35	0
55	MG	2A	3228	1/1	0.94	0.19	45,45,45,45	0
55	MG	1A	3402	1/1	0.94	0.07	35,35,35,35	0
55	MG	2A	3536	1/1	0.94	0.18	15,15,15,15	0
55	MG	1A	3236	1/1	0.94	0.23	28,28,28,28	0
55	MG	2A	3233	1/1	0.94	0.06	50,50,50,50	0
55	MG	2a	1606	1/1	0.94	0.21	30,30,30,30	0
55	MG	1a	3014	1/1	0.94	0.08	33,33,33,33	0
55	MG	1A	3692	1/1	0.94	0.07	44,44,44,44	0
55	MG	1A	3856	1/1	0.94	0.14	39,39,39,39	0
55	MG	1A	3535	1/1	0.94	0.10	22,22,22,22	0
55	MG	1A	3110	1/1	0.94	0.13	43,43,43,43	0
55	MG	2A	3547	1/1	0.94	0.10	29,29,29,29	0
55	MG	2a	1613	1/1	0.94	0.20	45,45,45,45	0
55	MG	1f	201	1/1	0.94	0.10	33,33,33,33	0
55	MG	1A	3540	1/1	0.94	0.08	14,14,14,14	0
55	MG	2A	3553	1/1	0.94	0.11	45,45,45,45	0
55	MG	1l	201	1/1	0.94	0.19	24,24,24,24	0
55	MG	2A	3555	1/1	0.94	0.11	32,32,32,32	0
55	MG	1n	101	1/1	0.94	0.06	34,34,34,34	0
55	MG	2a	1625	1/1	0.94	0.11	43,43,43,43	0
55	MG	2A	3245	1/1	0.94	0.06	24,24,24,24	0
55	MG	1A	3017	1/1	0.94	0.09	10,10,10,10	0
55	MG	2A	3247	1/1	0.94	0.08	25,25,25,25	0
55	MG	1a	3023	1/1	0.94	0.15	44,44,44,44	0
55	MG	1t	201	1/1	0.94	0.23	42,42,42,42	0
55	MG	2A	3572	1/1	0.94	0.10	50,50,50,50	0
55	MG	1a	3024	1/1	0.94	0.10	30,30,30,30	0
55	MG	1A	3246	1/1	0.94	0.05	37,37,37,37	0
55	MG	1A	3313	1/1	0.94	0.09	21,21,21,21	0
55	MG	2A	3255	1/1	0.94	0.09	51,51,51,51	0
55	MG	2A	3258	1/1	0.94	0.06	23,23,23,23	0
55	MG	1a	3028	1/1	0.94	0.24	52,52,52,52	0
55	MG	1A	3417	1/1	0.94	0.07	30,30,30,30	0
55	MG	1a	3030	1/1	0.94	0.10	50,50,50,50	0
55	MG	2a	1645	1/1	0.94	0.06	46,46,46,46	0
55	MG	1x	106	1/1	0.94	0.16	39,39,39,39	0
55	MG	2a	1647	1/1	0.94	0.17	60,60,60,60	0
55	MG	1A	3716	1/1	0.94	0.07	20,20,20,20	0
55	MG	2a	1649	1/1	0.94	0.14	62,62,62,62	0
55	MG	2a	1650	1/1	0.94	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1x	109	1/1	0.94	0.05	53,53,53,53	0
55	MG	2A	3596	1/1	0.94	0.08	26,26,26,26	0
55	MG	1A	3113	1/1	0.94	0.07	36,36,36,36	0
55	MG	1x	111	1/1	0.94	0.10	32,32,32,32	0
55	MG	2A	3601	1/1	0.94	0.16	44,44,44,44	0
55	MG	2a	1657	1/1	0.94	0.10	45,45,45,45	0
55	MG	2A	3604	1/1	0.94	0.13	34,34,34,34	0
55	MG	1a	3034	1/1	0.94	0.11	49,49,49,49	0
55	MG	2a	1661	1/1	0.94	0.08	46,46,46,46	0
55	MG	2A	3608	1/1	0.94	0.10	31,31,31,31	0
55	MG	1A	3719	1/1	0.94	0.12	19,19,19,19	0
55	MG	1A	3425	1/1	0.94	0.13	33,33,33,33	0
55	MG	2A	3007	1/1	0.94	0.14	38,38,38,38	0
55	MG	1A	3019	1/1	0.94	0.06	30,30,30,30	0
55	MG	2A	3010	1/1	0.94	0.11	42,42,42,42	0
55	MG	1A	3251	1/1	0.94	0.15	26,26,26,26	0
55	MG	1a	3043	1/1	0.94	0.16	35,35,35,35	0
55	MG	2a	1679	1/1	0.94	0.19	45,45,45,45	0
55	MG	1A	3885	1/1	0.94	0.10	46,46,46,46	0
55	MG	2A	3285	1/1	0.94	0.07	21,21,21,21	0
55	MG	1A	3252	1/1	0.94	0.06	35,35,35,35	0
55	MG	1A	3582	1/1	0.94	0.09	45,45,45,45	0
55	MG	2A	3288	1/1	0.94	0.07	30,30,30,30	0
55	MG	2A	3638	1/1	0.94	0.14	26,26,26,26	0
55	MG	1A	3257	1/1	0.94	0.14	25,25,25,25	0
55	MG	2A	3643	1/1	0.94	0.10	43,43,43,43	0
55	MG	1A	3585	1/1	0.94	0.10	22,22,22,22	0
55	MG	1B	223	1/1	0.94	0.07	28,28,28,28	0
55	MG	1a	3052	1/1	0.94	0.20	53,53,53,53	0
55	MG	1A	3438	1/1	0.94	0.06	33,33,33,33	0
55	MG	2A	3653	1/1	0.94	0.11	41,41,41,41	0
55	MG	1A	3260	1/1	0.94	0.12	35,35,35,35	0
55	MG	2A	3656	1/1	0.94	0.07	35,35,35,35	0
55	MG	1A	3903	1/1	0.94	0.18	37,37,37,37	0
55	MG	2A	3038	1/1	0.94	0.23	51,51,51,51	0
55	MG	1A	3261	1/1	0.94	0.19	23,23,23,23	0
55	MG	2a	1716	1/1	0.94	0.27	47,47,47,47	0
55	MG	2A	3664	1/1	0.94	0.08	34,34,34,34	0
55	MG	2A	3041	1/1	0.94	0.12	29,29,29,29	0
55	MG	1A	3748	1/1	0.94	0.09	27,27,27,27	0
55	MG	1A	3198	1/1	0.94	0.08	29,29,29,29	0
55	MG	1A	3263	1/1	0.94	0.10	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3672	1/1	0.94	0.19	39,39,39,39	0
55	MG	2A	3309	1/1	0.94	0.09	48,48,48,48	0
55	MG	1A	3013	1/1	0.94	0.09	20,20,20,20	0
55	MG	1a	3063	1/1	0.94	0.17	42,42,42,42	0
55	MG	1A	3758	1/1	0.94	0.30	49,49,49,49	0
55	MG	1A	3759	1/1	0.94	0.05	20,20,20,20	0
55	MG	1B	235	1/1	0.94	0.07	38,38,38,38	0
55	MG	2A	3684	1/1	0.94	0.14	36,36,36,36	0
55	MG	1D	302	1/1	0.94	0.20	30,30,30,30	0
55	MG	2A	3059	1/1	0.94	0.16	32,32,32,32	0
55	MG	1a	3071	1/1	0.94	0.12	37,37,37,37	0
55	MG	2A	3327	1/1	0.94	0.22	43,43,43,43	0
55	MG	2A	3066	1/1	0.94	0.20	46,46,46,46	0
55	MG	2a	1745	1/1	0.94	0.09	53,53,53,53	0
55	MG	2A	3067	1/1	0.94	0.09	27,27,27,27	0
55	MG	1A	3599	1/1	0.94	0.10	27,27,27,27	0
55	MG	2A	3071	1/1	0.94	0.20	45,45,45,45	0
55	MG	1A	3348	1/1	0.94	0.07	28,28,28,28	0
55	MG	2a	1753	1/1	0.94	0.17	33,33,33,33	0
55	MG	2A	3075	1/1	0.94	0.16	30,30,30,30	0
55	MG	2A	3076	1/1	0.94	0.06	30,30,30,30	0
55	MG	2A	3343	1/1	0.94	0.04	25,25,25,25	0
55	MG	1A	3916	1/1	0.94	0.09	21,21,21,21	0
55	MG	2a	1758	1/1	0.94	0.06	46,46,46,46	0
55	MG	1A	3918	1/1	0.94	0.18	19,19,19,19	0
55	MG	2A	3081	1/1	0.94	0.09	54,54,54,54	0
55	MG	1A	3267	1/1	0.94	0.07	37,37,37,37	0
55	MG	1E	308	1/1	0.94	0.10	34,34,34,34	0
55	MG	1A	3133	1/1	0.94	0.04	27,27,27,27	0
55	MG	2A	3720	1/1	0.94	0.12	44,44,44,44	0
55	MG	2a	1773	1/1	0.94	0.11	48,48,48,48	0
55	MG	1A	3927	1/1	0.94	0.12	31,31,31,31	0
55	MG	1A	3928	1/1	0.94	0.09	33,33,33,33	0
55	MG	1A	3202	1/1	0.94	0.09	33,33,33,33	0
55	MG	1A	3932	1/1	0.94	0.05	15,15,15,15	0
55	MG	2A	3096	1/1	0.94	0.12	44,44,44,44	0
55	MG	2A	3362	1/1	0.94	0.05	42,42,42,42	0
55	MG	2a	1784	1/1	0.94	0.17	32,32,32,32	0
55	MG	2a	1785	1/1	0.94	0.08	37,37,37,37	0
55	MG	2A	3729	1/1	0.94	0.14	24,24,24,24	0
55	MG	2a	1789	1/1	0.94	0.18	44,44,44,44	0
55	MG	1A	3040	1/1	0.94	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3102	1/1	0.94	0.21	31,31,31,31	0
55	MG	2A	3732	1/1	0.94	0.07	28,28,28,28	0
55	MG	1A	3208	1/1	0.94	0.15	28,28,28,28	0
55	MG	1a	3094	1/1	0.94	0.10	41,41,41,41	0
55	MG	2A	3108	1/1	0.94	0.07	41,41,41,41	0
55	MG	1A	3937	1/1	0.94	0.10	29,29,29,29	0
55	MG	1A	3477	1/1	0.94	0.04	25,25,25,25	0
55	MG	2a	1805	1/1	0.94	0.09	50,50,50,50	0
55	MG	1A	3773	1/1	0.94	0.11	21,21,21,21	0
55	MG	2a	1808	1/1	0.94	0.07	56,56,56,56	0
55	MG	1A	3210	1/1	0.94	0.06	25,25,25,25	0
55	MG	2A	3746	1/1	0.94	0.19	31,31,31,31	0
55	MG	1A	3954	1/1	0.94	0.07	38,38,38,38	0
55	MG	2A	3748	1/1	0.94	0.05	44,44,44,44	0
55	MG	2A	3749	1/1	0.94	0.12	35,35,35,35	0
55	MG	2a	1814	1/1	0.94	0.06	46,46,46,46	0
55	MG	1H	202	1/1	0.94	0.07	22,22,22,22	0
55	MG	2A	3756	1/1	0.94	0.07	25,25,25,25	0
55	MG	2A	3757	1/1	0.94	0.14	34,34,34,34	0
55	MG	1A	3480	1/1	0.94	0.09	20,20,20,20	0
55	MG	1N	203	1/1	0.94	0.09	45,45,45,45	0
55	MG	1a	3109	1/1	0.94	0.12	40,40,40,40	0
55	MG	1A	3041	1/1	0.94	0.16	30,30,30,30	0
55	MG	2A	3127	1/1	0.94	0.16	32,32,32,32	0
55	MG	1O	201	1/1	0.94	0.06	40,40,40,40	0
55	MG	2l	201	1/1	0.94	0.10	47,47,47,47	0
55	MG	1A	3782	1/1	0.94	0.10	29,29,29,29	0
55	MG	2A	3132	1/1	0.94	0.12	38,38,38,38	0
55	MG	2r	101	1/1	0.94	0.15	40,40,40,40	0
55	MG	2A	3402	1/1	0.94	0.12	34,34,34,34	0
55	MG	2A	3768	1/1	0.94	0.11	35,35,35,35	0
55	MG	1A	3489	1/1	0.94	0.18	28,28,28,28	0
55	MG	2A	3406	1/1	0.94	0.05	30,30,30,30	0
55	MG	1a	3118	1/1	0.94	0.20	42,42,42,42	0
55	MG	2x	106	1/1	0.94	0.24	60,60,60,60	0
55	MG	1A	3964	1/1	0.94	0.11	40,40,40,40	0
55	MG	1A	3789	1/1	0.94	0.16	24,24,24,24	0
55	MG	1A	3966	1/1	0.94	0.07	28,28,28,28	0
55	MG	1A	3069	1/1	0.94	0.18	29,29,29,29	0
55	MG	2A	3779	1/1	0.94	0.14	34,34,34,34	0
55	MG	2A	3143	1/1	0.94	0.09	44,44,44,44	0
55	MG	2A	3418	1/1	0.94	0.30	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3144	1/1	0.94	0.14	44,44,44,44	0
55	MG	2A	3786	1/1	0.95	0.12	37,37,37,37	0
55	MG	2A	3128	1/1	0.95	0.18	36,36,36,36	0
55	MG	1a	3107	1/1	0.95	0.17	36,36,36,36	0
55	MG	1A	3517	1/1	0.95	0.16	34,34,34,34	0
55	MG	1A	3701	1/1	0.95	0.09	42,42,42,42	0
55	MG	2A	3419	1/1	0.95	0.13	31,31,31,31	0
55	MG	1A	3702	1/1	0.95	0.15	21,21,21,21	0
55	MG	1a	3112	1/1	0.95	0.15	54,54,54,54	0
55	MG	2A	3801	1/1	0.95	0.10	44,44,44,44	0
55	MG	1A	3207	1/1	0.95	0.15	22,22,22,22	0
55	MG	1A	3316	1/1	0.95	0.06	14,14,14,14	0
55	MG	2A	3138	1/1	0.95	0.09	31,31,31,31	0
55	MG	1a	3115	1/1	0.95	0.17	38,38,38,38	0
55	MG	2A	3808	1/1	0.95	0.10	22,22,22,22	0
55	MG	2A	3429	1/1	0.95	0.10	32,32,32,32	0
55	MG	1A	3522	1/1	0.95	0.07	33,33,33,33	0
55	MG	1A	3403	1/1	0.95	0.06	30,30,30,30	0
55	MG	1A	3405	1/1	0.95	0.08	32,32,32,32	0
55	MG	1A	3715	1/1	0.95	0.09	21,21,21,21	0
55	MG	2A	3146	1/1	0.95	0.20	40,40,40,40	0
55	MG	1I	201	1/1	0.95	0.06	52,52,52,52	0
55	MG	2A	3823	1/1	0.95	0.09	26,26,26,26	0
55	MG	2A	3148	1/1	0.95	0.20	31,31,31,31	0
55	MG	2A	3825	1/1	0.95	0.15	31,31,31,31	0
55	MG	1a	3123	1/1	0.95	0.09	27,27,27,27	0
55	MG	1A	3128	1/1	0.95	0.05	23,23,23,23	0
55	MG	2A	3829	1/1	0.95	0.09	33,33,33,33	0
55	MG	1A	3082	1/1	0.95	0.08	36,36,36,36	0
55	MG	2A	3152	1/1	0.95	0.17	50,50,50,50	0
55	MG	1A	3529	1/1	0.95	0.12	38,38,38,38	0
55	MG	1A	3720	1/1	0.95	0.05	56,56,56,56	0
55	MG	1A	3924	1/1	0.95	0.11	47,47,47,47	0
55	MG	1A	3926	1/1	0.95	0.07	34,34,34,34	0
55	MG	1A	3264	1/1	0.95	0.18	42,42,42,42	0
55	MG	1A	3007	1/1	0.95	0.06	27,27,27,27	0
55	MG	2A	3162	1/1	0.95	0.05	37,37,37,37	0
55	MG	2A	3163	1/1	0.95	0.06	33,33,33,33	0
55	MG	2A	3164	1/1	0.95	0.15	36,36,36,36	0
55	MG	2A	3842	1/1	0.95	0.17	42,42,42,42	0
55	MG	1A	3930	1/1	0.95	0.10	17,17,17,17	0
55	MG	2A	3462	1/1	0.95	0.19	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3463	1/1	0.95	0.23	16,16,16,16	0
55	MG	2A	3848	1/1	0.95	0.08	31,31,31,31	0
55	MG	1A	3730	1/1	0.95	0.15	37,37,37,37	0
55	MG	1Q	201	1/1	0.95	0.21	26,26,26,26	0
55	MG	1A	3732	1/1	0.95	0.11	18,18,18,18	0
55	MG	2A	3469	1/1	0.95	0.16	21,21,21,21	0
55	MG	2A	3170	1/1	0.95	0.15	47,47,47,47	0
55	MG	1A	3214	1/1	0.95	0.06	23,23,23,23	0
55	MG	1A	3934	1/1	0.95	0.07	49,49,49,49	0
55	MG	2A	3475	1/1	0.95	0.20	17,17,17,17	0
55	MG	2A	3477	1/1	0.95	0.18	16,16,16,16	0
55	MG	1R	204	1/1	0.95	0.06	41,41,41,41	0
55	MG	1A	3324	1/1	0.95	0.08	31,31,31,31	0
55	MG	2A	3175	1/1	0.95	0.07	37,37,37,37	0
55	MG	1A	3136	1/1	0.95	0.10	30,30,30,30	0
55	MG	2A	3484	1/1	0.95	0.11	29,29,29,29	0
55	MG	1a	3158	1/1	0.95	0.13	19,19,19,19	0
55	MG	2B	217	1/1	0.95	0.12	53,53,53,53	0
55	MG	2B	218	1/1	0.95	0.17	37,37,37,37	0
55	MG	1a	3159	1/1	0.95	0.06	34,34,34,34	0
55	MG	1S	203	1/1	0.95	0.09	44,44,44,44	0
55	MG	2D	301	1/1	0.95	0.23	42,42,42,42	0
55	MG	2A	3490	1/1	0.95	0.07	23,23,23,23	0
55	MG	2D	308	1/1	0.95	0.20	22,22,22,22	0
55	MG	1A	3938	1/1	0.95	0.16	18,18,18,18	0
55	MG	1U	202	1/1	0.95	0.12	28,28,28,28	0
55	MG	1A	3941	1/1	0.95	0.07	15,15,15,15	0
55	MG	2F	301	1/1	0.95	0.06	28,28,28,28	0
55	MG	2F	303	1/1	0.95	0.10	30,30,30,30	0
55	MG	1A	3419	1/1	0.95	0.08	49,49,49,49	0
55	MG	2F	306	1/1	0.95	0.12	54,54,54,54	0
55	MG	1A	3138	1/1	0.95	0.39	29,29,29,29	0
55	MG	2A	3189	1/1	0.95	0.13	32,32,32,32	0
55	MG	1A	3951	1/1	0.95	0.12	33,33,33,33	0
55	MG	2P	204	1/1	0.95	0.09	44,44,44,44	0
55	MG	1A	3332	1/1	0.95	0.06	47,47,47,47	0
55	MG	2A	3507	1/1	0.95	0.17	10,10,10,10	0
55	MG	2T	201	1/1	0.95	0.08	36,36,36,36	0
55	MG	1A	3953	1/1	0.95	0.07	46,46,46,46	0
55	MG	1W	209	1/1	0.95	0.10	29,29,29,29	0
55	MG	2A	3513	1/1	0.95	0.04	56,56,56,56	0
55	MG	1X	101	1/1	0.95	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3199	1/1	0.95	0.21	38,38,38,38	0
55	MG	2Y	201	1/1	0.95	0.10	27,27,27,27	0
55	MG	1X	102	1/1	0.95	0.17	34,34,34,34	0
55	MG	1A	3555	1/1	0.95	0.07	34,34,34,34	0
55	MG	1a	3176	1/1	0.95	0.06	71,71,71,71	0
55	MG	1A	3433	1/1	0.95	0.11	28,28,28,28	0
55	MG	2I	105	1/1	0.95	0.12	49,49,49,49	0
55	MG	1A	3333	1/1	0.95	0.16	30,30,30,30	0
55	MG	2A	3525	1/1	0.95	0.17	29,29,29,29	0
55	MG	1A	3559	1/1	0.95	0.14	42,42,42,42	0
55	MG	2A	3206	1/1	0.95	0.12	42,42,42,42	0
55	MG	1A	3561	1/1	0.95	0.09	52,52,52,52	0
55	MG	2A	3529	1/1	0.95	0.13	28,28,28,28	0
55	MG	1A	3563	1/1	0.95	0.17	19,19,19,19	0
55	MG	1I	102	1/1	0.95	0.06	28,28,28,28	0
55	MG	2A	3215	1/1	0.95	0.07	24,24,24,24	0
55	MG	2A	3535	1/1	0.95	0.20	24,24,24,24	0
55	MG	1A	3752	1/1	0.95	0.19	24,24,24,24	0
55	MG	1A	3755	1/1	0.95	0.09	26,26,26,26	0
55	MG	2a	1605	1/1	0.95	0.15	42,42,42,42	0
55	MG	1a	3187	1/1	0.95	0.08	76,76,76,76	0
55	MG	1A	3967	1/1	0.95	0.09	38,38,38,38	0
55	MG	1A	3139	1/1	0.95	0.05	35,35,35,35	0
55	MG	1A	3336	1/1	0.95	0.11	32,32,32,32	0
55	MG	1a	3195	1/1	0.95	0.12	25,25,25,25	0
55	MG	1A	3339	1/1	0.95	0.17	33,33,33,33	0
55	MG	15	103	1/1	0.95	0.06	23,23,23,23	0
55	MG	2A	3548	1/1	0.95	0.17	22,22,22,22	0
55	MG	2A	3230	1/1	0.95	0.05	42,42,42,42	0
55	MG	2A	3550	1/1	0.95	0.07	10,10,10,10	0
55	MG	2a	1616	1/1	0.95	0.26	52,52,52,52	0
55	MG	2A	3551	1/1	0.95	0.13	32,32,32,32	0
55	MG	2A	3231	1/1	0.95	0.08	55,55,55,55	0
55	MG	1A	3439	1/1	0.95	0.08	26,26,26,26	0
55	MG	2a	1623	1/1	0.95	0.17	48,48,48,48	0
55	MG	1A	3443	1/1	0.95	0.09	39,39,39,39	0
55	MG	1A	3280	1/1	0.95	0.10	19,19,19,19	0
55	MG	17	104	1/1	0.95	0.10	28,28,28,28	0
55	MG	17	106	1/1	0.95	0.06	17,17,17,17	0
55	MG	2a	1629	1/1	0.95	0.12	30,30,30,30	0
55	MG	2A	3562	1/1	0.95	0.17	29,29,29,29	0
55	MG	1A	3449	1/1	0.95	0.16	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3343	1/1	0.95	0.12	25,25,25,25	0
55	MG	1A	3588	1/1	0.95	0.07	35,35,35,35	0
55	MG	1A	3452	1/1	0.95	0.12	21,21,21,21	0
55	MG	1d	301	1/1	0.95	0.16	21,21,21,21	0
55	MG	1A	3985	1/1	0.95	0.09	37,37,37,37	0
55	MG	1A	3987	1/1	0.95	0.06	34,34,34,34	0
55	MG	1A	3772	1/1	0.95	0.14	47,47,47,47	0
55	MG	1A	3991	1/1	0.95	0.14	34,34,34,34	0
55	MG	2A	3580	1/1	0.95	0.16	40,40,40,40	0
55	MG	2a	1642	1/1	0.95	0.09	43,43,43,43	0
55	MG	2A	3585	1/1	0.95	0.08	43,43,43,43	0
55	MG	1A	3179	1/1	0.95	0.08	44,44,44,44	0
55	MG	2A	3588	1/1	0.95	0.10	42,42,42,42	0
55	MG	1A	3775	1/1	0.95	0.06	40,40,40,40	0
55	MG	1a	3006	1/1	0.95	0.06	56,56,56,56	0
55	MG	1A	3030	1/1	0.95	0.09	21,21,21,21	0
55	MG	1A	3593	1/1	0.95	0.07	22,22,22,22	0
55	MG	1A	3181	1/1	0.95	0.14	27,27,27,27	0
55	MG	1A	3780	1/1	0.95	0.07	41,41,41,41	0
55	MG	1A	3285	1/1	0.95	0.13	42,42,42,42	0
55	MG	2A	3597	1/1	0.95	0.13	26,26,26,26	0
55	MG	2a	1655	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3786	1/1	0.95	0.10	37,37,37,37	0
55	MG	2A	3599	1/1	0.95	0.13	40,40,40,40	0
55	MG	1A	3033	1/1	0.95	0.10	35,35,35,35	0
55	MG	1A	3460	1/1	0.95	0.08	41,41,41,41	0
55	MG	2A	3603	1/1	0.95	0.09	45,45,45,45	0
55	MG	1A	3461	1/1	0.95	0.15	38,38,38,38	0
55	MG	2a	1663	1/1	0.95	0.12	31,31,31,31	0
55	MG	1A	3463	1/1	0.95	0.05	45,45,45,45	0
55	MG	2A	3268	1/1	0.95	0.06	32,32,32,32	0
55	MG	1a	3019	1/1	0.95	0.07	50,50,50,50	0
55	MG	1A	4009	1/1	0.95	0.10	41,41,41,41	0
55	MG	1A	3603	1/1	0.95	0.07	36,36,36,36	0
55	MG	1A	3227	1/1	0.95	0.09	37,37,37,37	0
55	MG	2a	1674	1/1	0.95	0.10	67,67,67,67	0
55	MG	2a	1676	1/1	0.95	0.10	40,40,40,40	0
55	MG	2A	3615	1/1	0.95	0.08	25,25,25,25	0
55	MG	2A	3002	1/1	0.95	0.07	26,26,26,26	0
55	MG	2A	3004	1/1	0.95	0.10	24,24,24,24	0
55	MG	1A	3466	1/1	0.95	0.22	38,38,38,38	0
55	MG	2a	1684	1/1	0.95	0.08	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3620	1/1	0.95	0.05	21,21,21,21	0
55	MG	1A	3611	1/1	0.95	0.09	59,59,59,59	0
55	MG	2A	3625	1/1	0.95	0.10	24,24,24,24	0
55	MG	2a	1689	1/1	0.95	0.23	42,42,42,42	0
55	MG	2a	1690	1/1	0.95	0.22	39,39,39,39	0
55	MG	2A	3281	1/1	0.95	0.12	40,40,40,40	0
55	MG	2a	1692	1/1	0.95	0.10	46,46,46,46	0
55	MG	2a	1693	1/1	0.95	0.05	57,57,57,57	0
55	MG	2A	3629	1/1	0.95	0.12	39,39,39,39	0
55	MG	1a	3026	1/1	0.95	0.12	27,27,27,27	0
55	MG	2A	3009	1/1	0.95	0.09	27,27,27,27	0
55	MG	2a	1701	1/1	0.95	0.10	48,48,48,48	0
55	MG	1A	3034	1/1	0.95	0.09	22,22,22,22	0
55	MG	1A	3469	1/1	0.95	0.14	25,25,25,25	0
55	MG	2A	3013	1/1	0.95	0.06	36,36,36,36	0
55	MG	1A	3003	1/1	0.95	0.12	28,28,28,28	0
55	MG	1A	3472	1/1	0.95	0.07	30,30,30,30	0
55	MG	2a	1708	1/1	0.95	0.06	69,69,69,69	0
55	MG	2A	3017	1/1	0.95	0.16	24,24,24,24	0
55	MG	1a	3031	1/1	0.95	0.17	29,29,29,29	0
55	MG	2a	1711	1/1	0.95	0.13	49,49,49,49	0
55	MG	1A	4030	1/1	0.95	0.10	20,20,20,20	0
55	MG	1A	3473	1/1	0.95	0.12	27,27,27,27	0
55	MG	2A	3024	1/1	0.95	0.09	25,25,25,25	0
55	MG	2A	3655	1/1	0.95	0.11	26,26,26,26	0
55	MG	2a	1718	1/1	0.95	0.11	38,38,38,38	0
55	MG	1A	3626	1/1	0.95	0.16	14,14,14,14	0
55	MG	1a	3035	1/1	0.95	0.06	52,52,52,52	0
55	MG	2a	1722	1/1	0.95	0.09	26,26,26,26	0
55	MG	1A	3021	1/1	0.95	0.06	21,21,21,21	0
55	MG	2A	3661	1/1	0.95	0.08	41,41,41,41	0
55	MG	2A	3031	1/1	0.95	0.19	46,46,46,46	0
55	MG	1A	3105	1/1	0.95	0.09	19,19,19,19	0
55	MG	2a	1727	1/1	0.95	0.21	44,44,44,44	0
55	MG	1A	3632	1/1	0.95	0.05	27,27,27,27	0
55	MG	2a	1729	1/1	0.95	0.14	48,48,48,48	0
55	MG	1A	3633	1/1	0.95	0.07	26,26,26,26	0
55	MG	1A	4040	1/1	0.95	0.16	33,33,33,33	0
55	MG	1A	3478	1/1	0.95	0.16	27,27,27,27	0
55	MG	2a	1735	1/1	0.95	0.13	33,33,33,33	0
55	MG	1a	3045	1/1	0.95	0.11	30,30,30,30	0
55	MG	1B	201	1/1	0.95	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3832	1/1	0.95	0.09	17,17,17,17	0
55	MG	1A	3156	1/1	0.95	0.10	24,24,24,24	0
55	MG	2A	3315	1/1	0.95	0.08	14,14,14,14	0
55	MG	1A	3192	1/1	0.95	0.11	39,39,39,39	0
55	MG	2a	1743	1/1	0.95	0.06	38,38,38,38	0
55	MG	2A	3682	1/1	0.95	0.13	61,61,61,61	0
55	MG	1A	3485	1/1	0.95	0.06	39,39,39,39	0
55	MG	1A	3486	1/1	0.95	0.09	38,38,38,38	0
55	MG	2a	1747	1/1	0.95	0.11	29,29,29,29	0
55	MG	2a	1748	1/1	0.95	0.08	61,61,61,61	0
55	MG	2A	3321	1/1	0.95	0.07	37,37,37,37	0
55	MG	2A	3322	1/1	0.95	0.04	33,33,33,33	0
55	MG	1B	209	1/1	0.95	0.12	27,27,27,27	0
55	MG	2A	3689	1/1	0.95	0.08	51,51,51,51	0
55	MG	2A	3690	1/1	0.95	0.08	43,43,43,43	0
55	MG	2A	3694	1/1	0.95	0.05	21,21,21,21	0
55	MG	2A	3324	1/1	0.95	0.07	26,26,26,26	0
55	MG	2A	3326	1/1	0.95	0.04	34,34,34,34	0
55	MG	1A	3642	1/1	0.95	0.13	21,21,21,21	0
55	MG	1A	3245	1/1	0.95	0.15	48,48,48,48	0
55	MG	2a	1760	1/1	0.95	0.15	38,38,38,38	0
55	MG	2A	3330	1/1	0.95	0.09	26,26,26,26	0
55	MG	2A	3331	1/1	0.95	0.08	45,45,45,45	0
55	MG	1A	3011	1/1	0.95	0.14	16,16,16,16	0
55	MG	1A	3846	1/1	0.95	0.09	18,18,18,18	0
55	MG	2a	1770	1/1	0.95	0.08	40,40,40,40	0
55	MG	2A	3710	1/1	0.95	0.09	27,27,27,27	0
55	MG	2A	3064	1/1	0.95	0.06	33,33,33,33	0
55	MG	1A	3072	1/1	0.95	0.13	27,27,27,27	0
55	MG	2A	3338	1/1	0.95	0.12	32,32,32,32	0
55	MG	1A	3373	1/1	0.95	0.05	28,28,28,28	0
55	MG	1A	3852	1/1	0.95	0.07	62,62,62,62	0
55	MG	2A	3342	1/1	0.95	0.04	21,21,21,21	0
55	MG	1B	220	1/1	0.95	0.13	25,25,25,25	0
55	MG	1A	3653	1/1	0.95	0.14	21,21,21,21	0
55	MG	1B	222	1/1	0.95	0.12	22,22,22,22	0
55	MG	1A	3376	1/1	0.95	0.13	24,24,24,24	0
55	MG	2A	3348	1/1	0.95	0.09	32,32,32,32	0
55	MG	1A	3005	1/1	0.95	0.06	20,20,20,20	0
55	MG	2a	1792	1/1	0.95	0.07	72,72,72,72	0
55	MG	1A	3006	1/1	0.95	0.08	25,25,25,25	0
55	MG	2A	3080	1/1	0.95	0.08	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3353	1/1	0.95	0.18	36,36,36,36	0
55	MG	1A	3379	1/1	0.95	0.09	27,27,27,27	0
55	MG	2A	3082	1/1	0.95	0.29	44,44,44,44	0
55	MG	2A	3085	1/1	0.95	0.06	27,27,27,27	0
55	MG	1A	3124	1/1	0.95	0.07	27,27,27,27	0
55	MG	2a	1803	1/1	0.95	0.04	29,29,29,29	0
55	MG	2a	1804	1/1	0.95	0.10	31,31,31,31	0
55	MG	1a	3074	1/1	0.95	0.11	42,42,42,42	0
55	MG	1a	3075	1/1	0.95	0.11	43,43,43,43	0
55	MG	2A	3089	1/1	0.95	0.06	32,32,32,32	0
55	MG	1A	3502	1/1	0.95	0.05	24,24,24,24	0
55	MG	2A	3365	1/1	0.95	0.16	34,34,34,34	0
55	MG	1A	3664	1/1	0.95	0.07	20,20,20,20	0
55	MG	2A	3370	1/1	0.95	0.07	25,25,25,25	0
55	MG	2A	3093	1/1	0.95	0.06	22,22,22,22	0
55	MG	1A	3665	1/1	0.95	0.05	10,10,10,10	0
55	MG	1A	3505	1/1	0.95	0.06	27,27,27,27	0
55	MG	2A	3375	1/1	0.95	0.09	35,35,35,35	0
55	MG	2A	3755	1/1	0.95	0.09	42,42,42,42	0
55	MG	1a	3081	1/1	0.95	0.07	41,41,41,41	0
55	MG	1A	3254	1/1	0.95	0.12	27,27,27,27	0
55	MG	2A	3098	1/1	0.95	0.14	42,42,42,42	0
55	MG	1A	3669	1/1	0.95	0.05	26,26,26,26	0
55	MG	1A	3670	1/1	0.95	0.06	57,57,57,57	0
55	MG	2j	202	1/1	0.95	0.09	49,49,49,49	0
55	MG	1A	3672	1/1	0.95	0.06	32,32,32,32	0
55	MG	2A	3383	1/1	0.95	0.10	37,37,37,37	0
55	MG	1A	3678	1/1	0.95	0.09	16,16,16,16	0
55	MG	2q	201	1/1	0.95	0.16	30,30,30,30	0
55	MG	1D	306	1/1	0.95	0.06	35,35,35,35	0
55	MG	1A	3507	1/1	0.95	0.19	37,37,37,37	0
55	MG	1A	3310	1/1	0.95	0.12	36,36,36,36	0
55	MG	2A	3395	1/1	0.95	0.07	38,38,38,38	0
55	MG	1a	3095	1/1	0.95	0.08	28,28,28,28	0
55	MG	1A	3509	1/1	0.95	0.16	24,24,24,24	0
55	MG	1A	3892	1/1	0.95	0.06	25,25,25,25	0
55	MG	1A	3511	1/1	0.95	0.07	21,21,21,21	0
55	MG	2A	3403	1/1	0.95	0.21	35,35,35,35	0
55	MG	2A	3775	1/1	0.95	0.14	30,30,30,30	0
55	MG	2A	3119	1/1	0.95	0.08	29,29,29,29	0
55	MG	1A	3386	1/1	0.95	0.19	10,10,10,10	0
55	MG	1A	3204	1/1	0.95	0.21	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3390	1/1	0.95	0.12	30,30,30,30	0
55	MG	2A	3410	1/1	0.95	0.06	43,43,43,43	0
55	MG	1A	3056	1/1	0.95	0.11	42,42,42,42	0
55	MG	1A	3045	1/1	0.96	0.16	15,15,15,15	0
55	MG	1E	302	1/1	0.96	0.13	32,32,32,32	0
55	MG	2A	3139	1/1	0.96	0.14	22,22,22,22	0
55	MG	2A	3140	1/1	0.96	0.05	37,37,37,37	0
55	MG	1A	3681	1/1	0.96	0.12	22,22,22,22	0
55	MG	2A	3438	1/1	0.96	0.18	30,30,30,30	0
55	MG	2A	3809	1/1	0.96	0.06	40,40,40,40	0
55	MG	2A	3810	1/1	0.96	0.10	29,29,29,29	0
55	MG	1A	3682	1/1	0.96	0.08	56,56,56,56	0
55	MG	1A	3412	1/1	0.96	0.05	27,27,27,27	0
55	MG	1A	3183	1/1	0.96	0.10	29,29,29,29	0
55	MG	1E	310	1/1	0.96	0.09	20,20,20,20	0
55	MG	1A	3317	1/1	0.96	0.06	24,24,24,24	0
55	MG	1A	3888	1/1	0.96	0.07	58,58,58,58	0
55	MG	1A	3686	1/1	0.96	0.13	39,39,39,39	0
55	MG	1E	314	1/1	0.96	0.07	36,36,36,36	0
55	MG	2A	3448	1/1	0.96	0.12	32,32,32,32	0
55	MG	1a	3116	1/1	0.96	0.27	32,32,32,32	0
55	MG	2A	3450	1/1	0.96	0.08	19,19,19,19	0
55	MG	2A	3451	1/1	0.96	0.17	19,19,19,19	0
55	MG	2A	3828	1/1	0.96	0.08	24,24,24,24	0
55	MG	1A	3890	1/1	0.96	0.06	43,43,43,43	0
55	MG	1F	302	1/1	0.96	0.09	16,16,16,16	0
55	MG	2A	3153	1/1	0.96	0.15	50,50,50,50	0
55	MG	1A	3047	1/1	0.96	0.14	21,21,21,21	0
55	MG	1F	306	1/1	0.96	0.05	11,11,11,11	0
55	MG	1F	307	1/1	0.96	0.09	30,30,30,30	0
55	MG	1A	3688	1/1	0.96	0.08	33,33,33,33	0
55	MG	2A	3159	1/1	0.96	0.08	31,31,31,31	0
55	MG	1a	3126	1/1	0.96	0.12	30,30,30,30	0
55	MG	1a	3129	1/1	0.96	0.13	32,32,32,32	0
55	MG	1a	3132	1/1	0.96	0.15	31,31,31,31	0
55	MG	1A	3248	1/1	0.96	0.13	16,16,16,16	0
55	MG	1F	312	1/1	0.96	0.04	19,19,19,19	0
55	MG	2A	3468	1/1	0.96	0.24	19,19,19,19	0
55	MG	2A	3844	1/1	0.96	0.13	40,40,40,40	0
55	MG	2A	3845	1/1	0.96	0.12	38,38,38,38	0
55	MG	1A	3420	1/1	0.96	0.09	29,29,29,29	0
55	MG	1G	201	1/1	0.96	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3471	1/1	0.96	0.06	43,43,43,43	0
55	MG	1a	3141	1/1	0.96	0.08	45,45,45,45	0
55	MG	1A	3897	1/1	0.96	0.06	42,42,42,42	0
55	MG	2A	3474	1/1	0.96	0.12	10,10,10,10	0
55	MG	1G	203	1/1	0.96	0.07	40,40,40,40	0
55	MG	1A	3421	1/1	0.96	0.17	33,33,33,33	0
55	MG	2A	3478	1/1	0.96	0.14	15,15,15,15	0
55	MG	1A	3902	1/1	0.96	0.05	25,25,25,25	0
55	MG	1A	3694	1/1	0.96	0.07	35,35,35,35	0
55	MG	2B	207	1/1	0.96	0.33	60,60,60,60	0
55	MG	1A	3536	1/1	0.96	0.17	16,16,16,16	0
55	MG	1A	3423	1/1	0.96	0.06	34,34,34,34	0
55	MG	2A	3176	1/1	0.96	0.06	19,19,19,19	0
55	MG	2A	3177	1/1	0.96	0.07	33,33,33,33	0
55	MG	1A	3539	1/1	0.96	0.15	20,20,20,20	0
55	MG	2A	3488	1/1	0.96	0.17	16,16,16,16	0
55	MG	2A	3179	1/1	0.96	0.10	30,30,30,30	0
55	MG	1A	3703	1/1	0.96	0.17	25,25,25,25	0
55	MG	1A	3143	1/1	0.96	0.07	28,28,28,28	0
55	MG	2A	3494	1/1	0.96	0.10	50,50,50,50	0
55	MG	2A	3495	1/1	0.96	0.04	17,17,17,17	0
55	MG	1A	3541	1/1	0.96	0.14	32,32,32,32	0
55	MG	1A	3144	1/1	0.96	0.11	38,38,38,38	0
55	MG	2D	305	1/1	0.96	0.19	41,41,41,41	0
55	MG	1A	3091	1/1	0.96	0.07	32,32,32,32	0
55	MG	2A	3500	1/1	0.96	0.17	33,33,33,33	0
55	MG	2E	303	1/1	0.96	0.05	28,28,28,28	0
55	MG	1A	3544	1/1	0.96	0.13	40,40,40,40	0
55	MG	1A	3545	1/1	0.96	0.14	22,22,22,22	0
55	MG	1A	3546	1/1	0.96	0.17	35,35,35,35	0
55	MG	1A	3919	1/1	0.96	0.11	33,33,33,33	0
55	MG	1A	3921	1/1	0.96	0.10	54,54,54,54	0
55	MG	1A	3547	1/1	0.96	0.13	24,24,24,24	0
55	MG	1A	3548	1/1	0.96	0.13	23,23,23,23	0
55	MG	1R	203	1/1	0.96	0.19	30,30,30,30	0
55	MG	1A	3434	1/1	0.96	0.07	43,43,43,43	0
55	MG	2A	3198	1/1	0.96	0.17	26,26,26,26	0
55	MG	1R	206	1/1	0.96	0.05	24,24,24,24	0
55	MG	2A	3517	1/1	0.96	0.12	44,44,44,44	0
55	MG	2Q	204	1/1	0.96	0.05	33,33,33,33	0
55	MG	1a	3170	1/1	0.96	0.11	36,36,36,36	0
55	MG	1A	3029	1/1	0.96	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2T	204	1/1	0.96	0.13	39,39,39,39	0
55	MG	1A	3726	1/1	0.96	0.07	18,18,18,18	0
55	MG	1A	3727	1/1	0.96	0.10	39,39,39,39	0
55	MG	2A	3523	1/1	0.96	0.06	27,27,27,27	0
55	MG	2A	3524	1/1	0.96	0.15	23,23,23,23	0
55	MG	1A	3329	1/1	0.96	0.11	25,25,25,25	0
55	MG	1U	201	1/1	0.96	0.07	24,24,24,24	0
55	MG	1A	3253	1/1	0.96	0.12	21,21,21,21	0
55	MG	1U	206	1/1	0.96	0.08	19,19,19,19	0
55	MG	1a	3178	1/1	0.96	0.08	36,36,36,36	0
55	MG	2A	3210	1/1	0.96	0.09	15,15,15,15	0
55	MG	2A	3212	1/1	0.96	0.11	26,26,26,26	0
55	MG	2A	3532	1/1	0.96	0.06	24,24,24,24	0
55	MG	1U	208	1/1	0.96	0.17	36,36,36,36	0
55	MG	23	103	1/1	0.96	0.20	17,17,17,17	0
55	MG	1V	201	1/1	0.96	0.07	27,27,27,27	0
55	MG	1A	3097	1/1	0.96	0.10	30,30,30,30	0
55	MG	1A	3255	1/1	0.96	0.18	32,32,32,32	0
55	MG	1A	3734	1/1	0.96	0.11	12,12,12,12	0
55	MG	27	101	1/1	0.96	0.13	31,31,31,31	0
55	MG	1W	203	1/1	0.96	0.05	13,13,13,13	0
55	MG	1A	3440	1/1	0.96	0.09	19,19,19,19	0
55	MG	1A	3564	1/1	0.96	0.14	15,15,15,15	0
55	MG	1a	3188	1/1	0.96	0.10	41,41,41,41	0
55	MG	2A	3227	1/1	0.96	0.22	29,29,29,29	0
55	MG	1a	3189	1/1	0.96	0.06	44,44,44,44	0
55	MG	1A	3565	1/1	0.96	0.14	16,16,16,16	0
55	MG	1A	3150	1/1	0.96	0.10	27,27,27,27	0
55	MG	1A	3741	1/1	0.96	0.07	16,16,16,16	0
55	MG	1A	3944	1/1	0.96	0.09	20,20,20,20	0
55	MG	1A	3259	1/1	0.96	0.10	10,10,10,10	0
55	MG	1A	3195	1/1	0.96	0.15	31,31,31,31	0
55	MG	1Z	302	1/1	0.96	0.03	32,32,32,32	0
55	MG	1a	3200	1/1	0.96	0.08	53,53,53,53	0
55	MG	1A	3571	1/1	0.96	0.08	25,25,25,25	0
55	MG	1A	3572	1/1	0.96	0.10	36,36,36,36	0
55	MG	2A	3561	1/1	0.96	0.10	27,27,27,27	0
55	MG	1A	3578	1/1	0.96	0.11	26,26,26,26	0
55	MG	2a	1618	1/1	0.96	0.10	40,40,40,40	0
55	MG	2a	1619	1/1	0.96	0.05	27,27,27,27	0
55	MG	2a	1620	1/1	0.96	0.07	63,63,63,63	0
55	MG	1A	3196	1/1	0.96	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	10	107	1/1	0.96	0.05	24,24,24,24	0
55	MG	1A	3581	1/1	0.96	0.06	15,15,15,15	0
55	MG	1a	3211	1/1	0.96	0.08	36,36,36,36	0
55	MG	1A	3959	1/1	0.96	0.16	56,56,56,56	0
55	MG	1A	3340	1/1	0.96	0.06	39,39,39,39	0
55	MG	12	102	1/1	0.96	0.19	32,32,32,32	0
55	MG	1A	3152	1/1	0.96	0.10	29,29,29,29	0
55	MG	2A	3250	1/1	0.96	0.05	44,44,44,44	0
55	MG	2A	3579	1/1	0.96	0.07	25,25,25,25	0
55	MG	1A	3963	1/1	0.96	0.07	42,42,42,42	0
55	MG	2A	3584	1/1	0.96	0.04	40,40,40,40	0
55	MG	1A	3757	1/1	0.96	0.09	23,23,23,23	0
55	MG	1A	3101	1/1	0.96	0.12	34,34,34,34	0
55	MG	1A	3586	1/1	0.96	0.07	31,31,31,31	0
55	MG	1A	3456	1/1	0.96	0.17	24,24,24,24	0
55	MG	1A	3345	1/1	0.96	0.15	21,21,21,21	0
55	MG	2a	1639	1/1	0.96	0.05	34,34,34,34	0
55	MG	17	101	1/1	0.96	0.08	19,19,19,19	0
55	MG	1A	3103	1/1	0.96	0.15	32,32,32,32	0
55	MG	1A	3349	1/1	0.96	0.09	26,26,26,26	0
55	MG	1v	105	1/1	0.96	0.15	35,35,35,35	0
55	MG	2a	1644	1/1	0.96	0.04	31,31,31,31	0
55	MG	2A	3266	1/1	0.96	0.05	32,32,32,32	0
55	MG	1A	3051	1/1	0.96	0.04	16,16,16,16	0
55	MG	17	107	1/1	0.96	0.11	32,32,32,32	0
55	MG	2A	3270	1/1	0.96	0.19	25,25,25,25	0
55	MG	1A	3973	1/1	0.96	0.07	38,38,38,38	0
55	MG	1A	3765	1/1	0.96	0.20	26,26,26,26	0
55	MG	2A	3602	1/1	0.96	0.08	36,36,36,36	0
55	MG	2A	3274	1/1	0.96	0.09	46,46,46,46	0
55	MG	1A	3052	1/1	0.96	0.09	19,19,19,19	0
55	MG	2A	3605	1/1	0.96	0.18	33,33,33,33	0
55	MG	1A	3768	1/1	0.96	0.14	24,24,24,24	0
55	MG	1x	108	1/1	0.96	0.12	28,28,28,28	0
55	MG	1A	3769	1/1	0.96	0.07	48,48,48,48	0
55	MG	2a	1658	1/1	0.96	0.10	20,20,20,20	0
55	MG	1A	3981	1/1	0.96	0.15	47,47,47,47	0
55	MG	2A	3612	1/1	0.96	0.15	26,26,26,26	0
55	MG	1A	3352	1/1	0.96	0.06	16,16,16,16	0
55	MG	1A	3353	1/1	0.96	0.18	34,34,34,34	0
55	MG	1A	3984	1/1	0.96	0.07	43,43,43,43	0
55	MG	2a	1664	1/1	0.96	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3106	1/1	0.96	0.09	33,33,33,33	0
55	MG	1A	3986	1/1	0.96	0.12	23,23,23,23	0
55	MG	1A	3269	1/1	0.96	0.10	25,25,25,25	0
55	MG	2a	1668	1/1	0.96	0.12	28,28,28,28	0
55	MG	1A	3159	1/1	0.96	0.04	28,28,28,28	0
55	MG	2A	3621	1/1	0.96	0.08	21,21,21,21	0
55	MG	2a	1671	1/1	0.96	0.05	42,42,42,42	0
55	MG	1A	3989	1/1	0.96	0.06	35,35,35,35	0
55	MG	1a	3011	1/1	0.96	0.06	70,70,70,70	0
55	MG	2a	1675	1/1	0.96	0.14	44,44,44,44	0
55	MG	1A	3271	1/1	0.96	0.05	32,32,32,32	0
55	MG	1A	3073	1/1	0.96	0.06	22,22,22,22	0
55	MG	2A	3012	1/1	0.96	0.06	40,40,40,40	0
55	MG	1A	3277	1/1	0.96	0.06	25,25,25,25	0
55	MG	2A	3632	1/1	0.96	0.08	37,37,37,37	0
55	MG	2a	1682	1/1	0.96	0.12	26,26,26,26	0
55	MG	2a	1683	1/1	0.96	0.08	36,36,36,36	0
55	MG	1A	3607	1/1	0.96	0.06	15,15,15,15	0
55	MG	2A	3637	1/1	0.96	0.17	31,31,31,31	0
55	MG	1A	3209	1/1	0.96	0.10	24,24,24,24	0
55	MG	2A	3296	1/1	0.96	0.07	35,35,35,35	0
55	MG	2a	1688	1/1	0.96	0.08	33,33,33,33	0
55	MG	2A	3641	1/1	0.96	0.13	41,41,41,41	0
55	MG	1A	3476	1/1	0.96	0.14	38,38,38,38	0
55	MG	2A	3020	1/1	0.96	0.07	26,26,26,26	0
55	MG	1A	3161	1/1	0.96	0.08	29,29,29,29	0
55	MG	1A	3363	1/1	0.96	0.09	33,33,33,33	0
55	MG	2a	1694	1/1	0.96	0.04	46,46,46,46	0
55	MG	2A	3650	1/1	0.96	0.09	41,41,41,41	0
55	MG	2a	1697	1/1	0.96	0.07	23,23,23,23	0
55	MG	1A	3282	1/1	0.96	0.08	24,24,24,24	0
55	MG	2A	3305	1/1	0.96	0.07	29,29,29,29	0
55	MG	2a	1700	1/1	0.96	0.16	43,43,43,43	0
55	MG	2A	3306	1/1	0.96	0.07	19,19,19,19	0
55	MG	1A	3791	1/1	0.96	0.09	46,46,46,46	0
55	MG	1A	3024	1/1	0.96	0.12	38,38,38,38	0
55	MG	2A	3657	1/1	0.96	0.07	50,50,50,50	0
55	MG	1A	3622	1/1	0.96	0.11	39,39,39,39	0
55	MG	2A	3659	1/1	0.96	0.06	41,41,41,41	0
55	MG	1A	3798	1/1	0.96	0.08	17,17,17,17	0
55	MG	1A	4007	1/1	0.96	0.15	50,50,50,50	0
55	MG	2A	3662	1/1	0.96	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3481	1/1	0.96	0.20	31,31,31,31	0
55	MG	1A	4010	1/1	0.96	0.06	54,54,54,54	0
55	MG	2A	3665	1/1	0.96	0.17	37,37,37,37	0
55	MG	2A	3036	1/1	0.96	0.04	23,23,23,23	0
55	MG	1A	4011	1/1	0.96	0.14	54,54,54,54	0
55	MG	2A	3317	1/1	0.96	0.14	49,49,49,49	0
55	MG	1A	3804	1/1	0.96	0.17	35,35,35,35	0
55	MG	1A	4013	1/1	0.96	0.06	28,28,28,28	0
55	MG	2A	3040	1/1	0.96	0.08	28,28,28,28	0
55	MG	2A	3675	1/1	0.96	0.11	42,42,42,42	0
55	MG	1A	3624	1/1	0.96	0.13	43,43,43,43	0
55	MG	2A	3677	1/1	0.96	0.10	37,37,37,37	0
55	MG	2A	3042	1/1	0.96	0.06	42,42,42,42	0
55	MG	2A	3679	1/1	0.96	0.07	40,40,40,40	0
55	MG	2A	3043	1/1	0.96	0.13	20,20,20,20	0
55	MG	1A	3806	1/1	0.96	0.05	30,30,30,30	0
55	MG	1A	3808	1/1	0.96	0.14	22,22,22,22	0
55	MG	2a	1731	1/1	0.96	0.11	33,33,33,33	0
55	MG	1A	3483	1/1	0.96	0.29	40,40,40,40	0
55	MG	2A	3329	1/1	0.96	0.07	23,23,23,23	0
55	MG	2a	1734	1/1	0.96	0.08	40,40,40,40	0
55	MG	2A	3685	1/1	0.96	0.13	10,10,10,10	0
55	MG	1a	3036	1/1	0.96	0.06	34,34,34,34	0
55	MG	1A	3810	1/1	0.96	0.07	23,23,23,23	0
55	MG	2A	3052	1/1	0.96	0.07	34,34,34,34	0
55	MG	1A	3366	1/1	0.96	0.08	43,43,43,43	0
55	MG	1a	3039	1/1	0.96	0.14	20,20,20,20	0
55	MG	2A	3692	1/1	0.96	0.10	48,48,48,48	0
55	MG	2A	3693	1/1	0.96	0.19	20,20,20,20	0
55	MG	1A	3368	1/1	0.96	0.14	29,29,29,29	0
55	MG	2A	3057	1/1	0.96	0.11	38,38,38,38	0
55	MG	1A	3487	1/1	0.96	0.08	25,25,25,25	0
55	MG	2A	3698	1/1	0.96	0.06	34,34,34,34	0
55	MG	1A	3163	1/1	0.96	0.14	19,19,19,19	0
55	MG	2A	3060	1/1	0.96	0.28	41,41,41,41	0
55	MG	2A	3703	1/1	0.96	0.08	30,30,30,30	0
55	MG	1A	3816	1/1	0.96	0.13	15,15,15,15	0
55	MG	2A	3706	1/1	0.96	0.15	31,31,31,31	0
55	MG	2A	3344	1/1	0.96	0.06	37,37,37,37	0
55	MG	2A	3063	1/1	0.96	0.10	26,26,26,26	0
55	MG	1A	3818	1/1	0.96	0.17	28,28,28,28	0
55	MG	1A	3164	1/1	0.96	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3821	1/1	0.96	0.08	10,10,10,10	0
55	MG	2A	3712	1/1	0.96	0.15	22,22,22,22	0
55	MG	1A	3491	1/1	0.96	0.05	37,37,37,37	0
55	MG	2A	3070	1/1	0.96	0.10	34,34,34,34	0
55	MG	1A	4039	1/1	0.96	0.21	31,31,31,31	0
55	MG	1A	3636	1/1	0.96	0.05	29,29,29,29	0
55	MG	2a	1766	1/1	0.96	0.07	39,39,39,39	0
55	MG	2a	1767	1/1	0.96	0.06	52,52,52,52	0
55	MG	1A	3078	1/1	0.96	0.22	23,23,23,23	0
55	MG	1A	3036	1/1	0.96	0.13	30,30,30,30	0
55	MG	1A	3827	1/1	0.96	0.11	22,22,22,22	0
55	MG	2a	1772	1/1	0.96	0.09	28,28,28,28	0
55	MG	1A	3829	1/1	0.96	0.07	28,28,28,28	0
55	MG	2A	3360	1/1	0.96	0.04	38,38,38,38	0
55	MG	1a	3056	1/1	0.96	0.05	37,37,37,37	0
55	MG	2A	3725	1/1	0.96	0.13	25,25,25,25	0
55	MG	1a	3057	1/1	0.96	0.06	31,31,31,31	0
55	MG	1A	3220	1/1	0.96	0.14	34,34,34,34	0
55	MG	2a	1781	1/1	0.96	0.05	53,53,53,53	0
55	MG	2a	1782	1/1	0.96	0.06	40,40,40,40	0
55	MG	1A	3039	1/1	0.96	0.16	38,38,38,38	0
55	MG	1A	3126	1/1	0.96	0.05	48,48,48,48	0
55	MG	1A	3294	1/1	0.96	0.04	10,10,10,10	0
55	MG	2a	1786	1/1	0.96	0.07	39,39,39,39	0
55	MG	1A	3645	1/1	0.96	0.13	30,30,30,30	0
55	MG	1A	3649	1/1	0.96	0.09	31,31,31,31	0
55	MG	2A	3733	1/1	0.96	0.14	15,15,15,15	0
55	MG	1B	213	1/1	0.96	0.04	48,48,48,48	0
55	MG	1B	214	1/1	0.96	0.14	30,30,30,30	0
55	MG	2a	1794	1/1	0.96	0.07	51,51,51,51	0
55	MG	2A	3374	1/1	0.96	0.10	35,35,35,35	0
55	MG	1A	3031	1/1	0.96	0.10	26,26,26,26	0
55	MG	1a	3067	1/1	0.96	0.13	34,34,34,34	0
55	MG	2A	3742	1/1	0.96	0.09	50,50,50,50	0
55	MG	1A	3004	1/1	0.96	0.12	25,25,25,25	0
55	MG	1a	3069	1/1	0.96	0.12	23,23,23,23	0
55	MG	1A	3129	1/1	0.96	0.47	24,24,24,24	0
55	MG	1A	3063	1/1	0.96	0.08	21,21,21,21	0
55	MG	2A	3101	1/1	0.96	0.19	30,30,30,30	0
55	MG	1A	3843	1/1	0.96	0.18	35,35,35,35	0
55	MG	2a	1807	1/1	0.96	0.14	45,45,45,45	0
55	MG	2A	3384	1/1	0.96	0.16	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3385	1/1	0.96	0.15	21,21,21,21	0
55	MG	2A	3387	1/1	0.96	0.17	25,25,25,25	0
55	MG	1A	3229	1/1	0.96	0.09	29,29,29,29	0
55	MG	1A	3847	1/1	0.96	0.04	21,21,21,21	0
55	MG	2A	3390	1/1	0.96	0.10	37,37,37,37	0
55	MG	1A	3230	1/1	0.96	0.05	23,23,23,23	0
55	MG	2A	3109	1/1	0.96	0.08	41,41,41,41	0
55	MG	2a	1816	1/1	0.96	0.11	35,35,35,35	0
55	MG	2A	3393	1/1	0.96	0.09	31,31,31,31	0
55	MG	2A	3394	1/1	0.96	0.13	27,27,27,27	0
55	MG	2e	201	1/1	0.96	0.11	43,43,43,43	0
55	MG	2e	202	1/1	0.96	0.41	47,47,47,47	0
55	MG	1a	3077	1/1	0.96	0.10	46,46,46,46	0
55	MG	1A	3659	1/1	0.96	0.11	31,31,31,31	0
55	MG	1A	3400	1/1	0.96	0.07	27,27,27,27	0
55	MG	1A	3510	1/1	0.96	0.11	21,21,21,21	0
55	MG	1A	3855	1/1	0.96	0.07	36,36,36,36	0
55	MG	1A	3175	1/1	0.96	0.07	26,26,26,26	0
55	MG	1a	3083	1/1	0.96	0.09	40,40,40,40	0
55	MG	1A	3085	1/1	0.96	0.04	14,14,14,14	0
55	MG	2A	3407	1/1	0.96	0.39	50,50,50,50	0
55	MG	1A	3235	1/1	0.96	0.08	20,20,20,20	0
55	MG	2A	3776	1/1	0.96	0.07	57,57,57,57	0
55	MG	1A	3086	1/1	0.96	0.07	37,37,37,37	0
55	MG	2A	3124	1/1	0.96	0.12	29,29,29,29	0
55	MG	2x	101	1/1	0.96	0.09	35,35,35,35	0
55	MG	2A	3125	1/1	0.96	0.20	18,18,18,18	0
55	MG	1A	3237	1/1	0.96	0.06	25,25,25,25	0
55	MG	1A	3867	1/1	0.96	0.09	18,18,18,18	0
55	MG	2A	3783	1/1	0.96	0.13	19,19,19,19	0
55	MG	1A	3239	1/1	0.96	0.08	43,43,43,43	0
55	MG	2A	3129	1/1	0.96	0.15	27,27,27,27	0
56	K	1A	3470	1/1	0.96	0.07	51,51,51,51	0
55	MG	1A	3408	1/1	0.96	0.05	18,18,18,18	0
55	MG	1A	3872	1/1	0.96	0.08	52,52,52,52	0
55	MG	1A	3671	1/1	0.96	0.07	28,28,28,28	0
55	MG	1D	305	1/1	0.96	0.09	20,20,20,20	0
55	MG	1A	3088	1/1	0.96	0.15	28,28,28,28	0
55	MG	1A	3410	1/1	0.96	0.06	34,34,34,34	0
55	MG	2A	3136	1/1	0.96	0.06	39,39,39,39	0
55	MG	1a	3208	1/1	0.97	0.07	41,41,41,41	0
55	MG	1A	3098	1/1	0.97	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3413	1/1	0.97	0.11	21,21,21,21	0
55	MG	2A	3505	1/1	0.97	0.21	18,18,18,18	0
55	MG	1A	3994	1/1	0.97	0.12	10,10,10,10	0
55	MG	2A	3224	1/1	0.97	0.07	34,34,34,34	0
55	MG	2A	3508	1/1	0.97	0.23	15,15,15,15	0
55	MG	1A	3515	1/1	0.97	0.15	10,10,10,10	0
55	MG	2A	3510	1/1	0.97	0.29	32,32,32,32	0
55	MG	17	105	1/1	0.97	0.04	22,22,22,22	0
55	MG	2A	3512	1/1	0.97	0.09	27,27,27,27	0
55	MG	1A	3647	1/1	0.97	0.10	43,43,43,43	0
55	MG	2B	202	1/1	0.97	0.09	40,40,40,40	0
55	MG	1A	3997	1/1	0.97	0.05	37,37,37,37	0
55	MG	1A	3648	1/1	0.97	0.06	34,34,34,34	0
55	MG	1A	3415	1/1	0.97	0.15	26,26,26,26	0
55	MG	1A	3265	1/1	0.97	0.04	19,19,19,19	0
55	MG	1l	203	1/1	0.97	0.03	35,35,35,35	0
55	MG	2B	209	1/1	0.97	0.03	40,40,40,40	0
55	MG	1A	3651	1/1	0.97	0.09	15,15,15,15	0
55	MG	1A	3100	1/1	0.97	0.07	38,38,38,38	0
55	MG	1A	3519	1/1	0.97	0.12	26,26,26,26	0
55	MG	1a	3001	1/1	0.97	0.14	47,47,47,47	0
55	MG	2A	3237	1/1	0.97	0.09	40,40,40,40	0
55	MG	2A	3238	1/1	0.97	0.11	18,18,18,18	0
55	MG	1v	101	1/1	0.97	0.09	36,36,36,36	0
55	MG	1A	3654	1/1	0.97	0.06	43,43,43,43	0
55	MG	1A	3520	1/1	0.97	0.19	11,11,11,11	0
55	MG	1A	3218	1/1	0.97	0.09	22,22,22,22	0
55	MG	1x	101	1/1	0.97	0.22	38,38,38,38	0
55	MG	1A	3219	1/1	0.97	0.07	36,36,36,36	0
55	MG	1A	3142	1/1	0.97	0.06	25,25,25,25	0
55	MG	2D	304	1/1	0.97	0.10	22,22,22,22	0
55	MG	1A	3660	1/1	0.97	0.10	10,10,10,10	0
55	MG	2D	306	1/1	0.97	0.12	28,28,28,28	0
55	MG	1A	3221	1/1	0.97	0.27	30,30,30,30	0
55	MG	1A	3338	1/1	0.97	0.09	55,55,55,55	0
55	MG	2E	302	1/1	0.97	0.12	27,27,27,27	0
55	MG	2A	3537	1/1	0.97	0.09	22,22,22,22	0
55	MG	1A	3222	1/1	0.97	0.07	19,19,19,19	0
55	MG	1A	3272	1/1	0.97	0.07	23,23,23,23	0
55	MG	1A	4017	1/1	0.97	0.05	25,25,25,25	0
55	MG	1A	3427	1/1	0.97	0.04	22,22,22,22	0
55	MG	2A	3543	1/1	0.97	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3253	1/1	0.97	0.16	30,30,30,30	0
55	MG	1A	3531	1/1	0.97	0.20	30,30,30,30	0
55	MG	2O	201	1/1	0.97	0.06	31,31,31,31	0
55	MG	1A	3428	1/1	0.97	0.10	21,21,21,21	0
55	MG	2A	3256	1/1	0.97	0.04	55,55,55,55	0
55	MG	2A	3257	1/1	0.97	0.09	35,35,35,35	0
55	MG	1A	4023	1/1	0.97	0.05	40,40,40,40	0
55	MG	2A	3259	1/1	0.97	0.12	40,40,40,40	0
55	MG	2A	3001	1/1	0.97	0.24	29,29,29,29	0
55	MG	1A	3833	1/1	0.97	0.04	28,28,28,28	0
55	MG	2T	202	1/1	0.97	0.12	39,39,39,39	0
55	MG	1A	4025	1/1	0.97	0.06	45,45,45,45	0
55	MG	1A	3533	1/1	0.97	0.08	21,21,21,21	0
55	MG	1A	3534	1/1	0.97	0.09	37,37,37,37	0
55	MG	1a	3022	1/1	0.97	0.11	16,16,16,16	0
55	MG	1A	3431	1/1	0.97	0.04	14,14,14,14	0
55	MG	2A	3560	1/1	0.97	0.08	23,23,23,23	0
55	MG	1A	3341	1/1	0.97	0.07	43,43,43,43	0
55	MG	2A	3269	1/1	0.97	0.05	30,30,30,30	0
55	MG	2A	3565	1/1	0.97	0.15	22,22,22,22	0
55	MG	1A	3673	1/1	0.97	0.17	39,39,39,39	0
55	MG	2A	3567	1/1	0.97	0.07	33,33,33,33	0
55	MG	2A	3271	1/1	0.97	0.05	57,57,57,57	0
55	MG	1A	3675	1/1	0.97	0.04	43,43,43,43	0
55	MG	2A	3570	1/1	0.97	0.09	33,33,33,33	0
55	MG	1A	3676	1/1	0.97	0.06	25,25,25,25	0
55	MG	1A	3677	1/1	0.97	0.07	36,36,36,36	0
55	MG	2A	3574	1/1	0.97	0.09	31,31,31,31	0
55	MG	1A	3273	1/1	0.97	0.08	26,26,26,26	0
55	MG	1A	3176	1/1	0.97	0.16	21,21,21,21	0
55	MG	2A	3019	1/1	0.97	0.06	47,47,47,47	0
55	MG	1A	3344	1/1	0.97	0.09	19,19,19,19	0
55	MG	1A	3275	1/1	0.97	0.06	21,21,21,21	0
55	MG	1A	3347	1/1	0.97	0.05	34,34,34,34	0
55	MG	2A	3583	1/1	0.97	0.09	19,19,19,19	0
55	MG	1A	3276	1/1	0.97	0.07	40,40,40,40	0
55	MG	1A	3854	1/1	0.97	0.05	38,38,38,38	0
55	MG	2A	3586	1/1	0.97	0.11	31,31,31,31	0
55	MG	2A	3025	1/1	0.97	0.15	35,35,35,35	0
55	MG	1A	3044	1/1	0.97	0.07	22,22,22,22	0
55	MG	1B	206	1/1	0.97	0.04	45,45,45,45	0
55	MG	1B	207	1/1	0.97	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3029	1/1	0.97	0.12	21,21,21,21	0
55	MG	2A	3592	1/1	0.97	0.07	31,31,31,31	0
55	MG	1A	3279	1/1	0.97	0.04	16,16,16,16	0
55	MG	1a	3040	1/1	0.97	0.13	34,34,34,34	0
55	MG	2A	3033	1/1	0.97	0.13	22,22,22,22	0
55	MG	2A	3034	1/1	0.97	0.08	32,32,32,32	0
55	MG	1A	3857	1/1	0.97	0.08	23,23,23,23	0
55	MG	1A	3859	1/1	0.97	0.04	51,51,51,51	0
55	MG	1A	3860	1/1	0.97	0.06	45,45,45,45	0
55	MG	1A	3444	1/1	0.97	0.13	18,18,18,18	0
55	MG	2A	3297	1/1	0.97	0.05	17,17,17,17	0
55	MG	1A	3445	1/1	0.97	0.09	19,19,19,19	0
55	MG	2A	3300	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3864	1/1	0.97	0.06	31,31,31,31	0
55	MG	1A	3689	1/1	0.97	0.06	54,54,54,54	0
55	MG	1A	3690	1/1	0.97	0.09	27,27,27,27	0
55	MG	1A	3446	1/1	0.97	0.09	42,42,42,42	0
55	MG	2A	3609	1/1	0.97	0.11	27,27,27,27	0
55	MG	2A	3044	1/1	0.97	0.19	33,33,33,33	0
55	MG	1A	3550	1/1	0.97	0.07	24,24,24,24	0
55	MG	1A	3057	1/1	0.97	0.12	18,18,18,18	0
55	MG	1A	3037	1/1	0.97	0.05	15,15,15,15	0
55	MG	1A	3046	1/1	0.97	0.11	30,30,30,30	0
55	MG	1A	3696	1/1	0.97	0.14	25,25,25,25	0
55	MG	2A	3311	1/1	0.97	0.05	33,33,33,33	0
55	MG	2A	3617	1/1	0.97	0.09	23,23,23,23	0
55	MG	1A	3697	1/1	0.97	0.07	32,32,32,32	0
55	MG	1A	3877	1/1	0.97	0.07	37,37,37,37	0
55	MG	1A	3698	1/1	0.97	0.09	12,12,12,12	0
55	MG	1A	3699	1/1	0.97	0.07	22,22,22,22	0
55	MG	2A	3056	1/1	0.97	0.04	23,23,23,23	0
55	MG	2A	3623	1/1	0.97	0.12	14,14,14,14	0
55	MG	2A	3624	1/1	0.97	0.14	27,27,27,27	0
55	MG	1A	3880	1/1	0.97	0.07	55,55,55,55	0
55	MG	1A	3700	1/1	0.97	0.10	20,20,20,20	0
55	MG	1A	3882	1/1	0.97	0.04	24,24,24,24	0
55	MG	2A	3320	1/1	0.97	0.09	30,30,30,30	0
55	MG	1A	3883	1/1	0.97	0.06	55,55,55,55	0
55	MG	1A	3557	1/1	0.97	0.06	54,54,54,54	0
55	MG	1A	3038	1/1	0.97	0.06	21,21,21,21	0
55	MG	1A	3148	1/1	0.97	0.09	26,26,26,26	0
55	MG	2A	3065	1/1	0.97	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1D	301	1/1	0.97	0.16	22,22,22,22	0
55	MG	1A	3454	1/1	0.97	0.07	21,21,21,21	0
55	MG	1A	3705	1/1	0.97	0.15	36,36,36,36	0
55	MG	2A	3644	1/1	0.97	0.12	52,52,52,52	0
55	MG	2A	3069	1/1	0.97	0.14	28,28,28,28	0
55	MG	1a	3070	1/1	0.97	0.18	25,25,25,25	0
55	MG	2A	3648	1/1	0.97	0.06	32,32,32,32	0
55	MG	1D	304	1/1	0.97	0.24	30,30,30,30	0
55	MG	1A	3108	1/1	0.97	0.11	33,33,33,33	0
55	MG	2A	3334	1/1	0.97	0.16	30,30,30,30	0
55	MG	2A	3335	1/1	0.97	0.08	25,25,25,25	0
55	MG	1A	3151	1/1	0.97	0.09	25,25,25,25	0
55	MG	1D	307	1/1	0.97	0.18	10,10,10,10	0
55	MG	1A	3710	1/1	0.97	0.10	13,13,13,13	0
55	MG	2A	3339	1/1	0.97	0.06	34,34,34,34	0
55	MG	1A	3894	1/1	0.97	0.05	16,16,16,16	0
55	MG	1A	3014	1/1	0.97	0.15	30,30,30,30	0
55	MG	1A	3064	1/1	0.97	0.05	13,13,13,13	0
55	MG	1A	3291	1/1	0.97	0.07	18,18,18,18	0
55	MG	1A	3361	1/1	0.97	0.07	37,37,37,37	0
55	MG	1A	3900	1/1	0.97	0.07	22,22,22,22	0
55	MG	1A	3049	1/1	0.97	0.22	26,26,26,26	0
55	MG	1A	3117	1/1	0.97	0.08	24,24,24,24	0
55	MG	2a	1677	1/1	0.97	0.09	45,45,45,45	0
55	MG	1A	3904	1/1	0.97	0.05	32,32,32,32	0
55	MG	1a	3086	1/1	0.97	0.05	50,50,50,50	0
55	MG	1a	3087	1/1	0.97	0.09	36,36,36,36	0
55	MG	2A	3092	1/1	0.97	0.20	44,44,44,44	0
55	MG	2A	3352	1/1	0.97	0.05	31,31,31,31	0
55	MG	1A	3575	1/1	0.97	0.08	27,27,27,27	0
55	MG	2A	3354	1/1	0.97	0.05	31,31,31,31	0
55	MG	1A	3721	1/1	0.97	0.14	26,26,26,26	0
55	MG	1A	3577	1/1	0.97	0.11	15,15,15,15	0
55	MG	2A	3357	1/1	0.97	0.04	14,14,14,14	0
55	MG	1A	3238	1/1	0.97	0.06	27,27,27,27	0
55	MG	1a	3092	1/1	0.97	0.10	51,51,51,51	0
55	MG	1A	3194	1/1	0.97	0.05	32,32,32,32	0
55	MG	2A	3099	1/1	0.97	0.12	26,26,26,26	0
55	MG	1A	3911	1/1	0.97	0.13	47,47,47,47	0
55	MG	1A	3050	1/1	0.97	0.07	25,25,25,25	0
55	MG	2A	3103	1/1	0.97	0.13	34,34,34,34	0
55	MG	1A	3367	1/1	0.97	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	1696	1/1	0.97	0.04	53,53,53,53	0
55	MG	2A	3366	1/1	0.97	0.13	31,31,31,31	0
55	MG	1a	3098	1/1	0.97	0.03	26,26,26,26	0
55	MG	2A	3368	1/1	0.97	0.11	22,22,22,22	0
55	MG	1A	3122	1/1	0.97	0.05	22,22,22,22	0
55	MG	1A	3369	1/1	0.97	0.07	32,32,32,32	0
55	MG	1A	3243	1/1	0.97	0.17	26,26,26,26	0
55	MG	1A	3917	1/1	0.97	0.10	16,16,16,16	0
55	MG	2A	3695	1/1	0.97	0.09	44,44,44,44	0
55	MG	1A	3299	1/1	0.97	0.08	34,34,34,34	0
55	MG	2a	1706	1/1	0.97	0.11	30,30,30,30	0
55	MG	1A	3475	1/1	0.97	0.10	27,27,27,27	0
55	MG	2A	3114	1/1	0.97	0.07	30,30,30,30	0
55	MG	1A	3920	1/1	0.97	0.10	15,15,15,15	0
55	MG	2A	3378	1/1	0.97	0.17	44,44,44,44	0
55	MG	2A	3702	1/1	0.97	0.11	31,31,31,31	0
55	MG	1A	3372	1/1	0.97	0.06	22,22,22,22	0
55	MG	2a	1713	1/1	0.97	0.15	31,31,31,31	0
55	MG	2A	3704	1/1	0.97	0.10	26,26,26,26	0
55	MG	2a	1715	1/1	0.97	0.21	36,36,36,36	0
55	MG	1A	3123	1/1	0.97	0.14	10,10,10,10	0
55	MG	1A	3087	1/1	0.97	0.12	30,30,30,30	0
55	MG	1A	3742	1/1	0.97	0.05	22,22,22,22	0
55	MG	1A	3068	1/1	0.97	0.07	34,34,34,34	0
55	MG	2a	1720	1/1	0.97	0.15	23,23,23,23	0
55	MG	2A	3123	1/1	0.97	0.18	16,16,16,16	0
55	MG	1N	204	1/1	0.97	0.05	33,33,33,33	0
55	MG	2A	3386	1/1	0.97	0.16	31,31,31,31	0
55	MG	1A	3201	1/1	0.97	0.06	36,36,36,36	0
55	MG	2A	3713	1/1	0.97	0.06	39,39,39,39	0
55	MG	1A	3002	1/1	0.97	0.08	39,39,39,39	0
55	MG	1A	3596	1/1	0.97	0.04	34,34,34,34	0
55	MG	1O	204	1/1	0.97	0.12	38,38,38,38	0
55	MG	1a	3119	1/1	0.97	0.11	16,16,16,16	0
55	MG	1A	3598	1/1	0.97	0.08	35,35,35,35	0
55	MG	1P	201	1/1	0.97	0.05	15,15,15,15	0
55	MG	1A	3203	1/1	0.97	0.15	14,14,14,14	0
55	MG	1A	3484	1/1	0.97	0.07	24,24,24,24	0
55	MG	1a	3124	1/1	0.97	0.20	34,34,34,34	0
55	MG	2A	3723	1/1	0.97	0.06	36,36,36,36	0
55	MG	2A	3397	1/1	0.97	0.07	21,21,21,21	0
55	MG	1A	3016	1/1	0.97	0.08	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3399	1/1	0.97	0.06	32,32,32,32	0
55	MG	1a	3127	1/1	0.97	0.14	21,21,21,21	0
55	MG	1a	3128	1/1	0.97	0.07	30,30,30,30	0
55	MG	1A	3753	1/1	0.97	0.05	28,28,28,28	0
55	MG	1a	3131	1/1	0.97	0.11	42,42,42,42	0
55	MG	1A	3936	1/1	0.97	0.11	39,39,39,39	0
55	MG	1A	3382	1/1	0.97	0.12	26,26,26,26	0
55	MG	1A	3205	1/1	0.97	0.15	18,18,18,18	0
55	MG	1Q	204	1/1	0.97	0.04	35,35,35,35	0
55	MG	1a	3138	1/1	0.97	0.12	19,19,19,19	0
55	MG	1A	3939	1/1	0.97	0.06	14,14,14,14	0
55	MG	2a	1750	1/1	0.97	0.17	32,32,32,32	0
55	MG	1R	201	1/1	0.97	0.09	40,40,40,40	0
55	MG	1R	202	1/1	0.97	0.11	32,32,32,32	0
55	MG	2A	3741	1/1	0.97	0.08	25,25,25,25	0
55	MG	2A	3414	1/1	0.97	0.05	28,28,28,28	0
55	MG	2A	3743	1/1	0.97	0.06	35,35,35,35	0
55	MG	1A	3604	1/1	0.97	0.07	20,20,20,20	0
55	MG	1A	3312	1/1	0.97	0.08	40,40,40,40	0
55	MG	1A	3606	1/1	0.97	0.04	28,28,28,28	0
55	MG	1a	3147	1/1	0.97	0.04	44,44,44,44	0
55	MG	1A	3071	1/1	0.97	0.19	35,35,35,35	0
55	MG	1A	3608	1/1	0.97	0.14	19,19,19,19	0
55	MG	2A	3750	1/1	0.97	0.12	41,41,41,41	0
55	MG	2A	3424	1/1	0.97	0.04	40,40,40,40	0
55	MG	2A	3752	1/1	0.97	0.08	30,30,30,30	0
55	MG	2A	3753	1/1	0.97	0.07	31,31,31,31	0
55	MG	2a	1768	1/1	0.97	0.17	36,36,36,36	0
55	MG	2A	3154	1/1	0.97	0.07	32,32,32,32	0
55	MG	1S	202	1/1	0.97	0.13	33,33,33,33	0
55	MG	1A	3490	1/1	0.97	0.08	35,35,35,35	0
55	MG	1T	201	1/1	0.97	0.09	13,13,13,13	0
55	MG	2A	3430	1/1	0.97	0.13	29,29,29,29	0
55	MG	1A	3314	1/1	0.97	0.06	29,29,29,29	0
55	MG	1A	3131	1/1	0.97	0.06	21,21,21,21	0
55	MG	2A	3434	1/1	0.97	0.14	15,15,15,15	0
55	MG	1A	3955	1/1	0.97	0.11	39,39,39,39	0
55	MG	2a	1779	1/1	0.97	0.05	19,19,19,19	0
55	MG	2A	3436	1/1	0.97	0.14	33,33,33,33	0
55	MG	1U	203	1/1	0.97	0.07	32,32,32,32	0
55	MG	1A	3766	1/1	0.97	0.04	26,26,26,26	0
55	MG	1U	207	1/1	0.97	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	3160	1/1	0.97	0.11	39,39,39,39	0
55	MG	1a	3161	1/1	0.97	0.07	41,41,41,41	0
55	MG	1A	3393	1/1	0.97	0.30	21,21,21,21	0
55	MG	1A	3958	1/1	0.97	0.12	27,27,27,27	0
55	MG	2a	1788	1/1	0.97	0.04	54,54,54,54	0
55	MG	1A	3495	1/1	0.97	0.06	33,33,33,33	0
55	MG	1A	3617	1/1	0.97	0.11	27,27,27,27	0
55	MG	2a	1791	1/1	0.97	0.06	66,66,66,66	0
55	MG	1A	3394	1/1	0.97	0.05	31,31,31,31	0
55	MG	1W	201	1/1	0.97	0.18	35,35,35,35	0
55	MG	1W	202	1/1	0.97	0.05	20,20,20,20	0
55	MG	1A	3395	1/1	0.97	0.07	13,13,13,13	0
55	MG	1A	3397	1/1	0.97	0.07	16,16,16,16	0
55	MG	1A	3256	1/1	0.97	0.17	25,25,25,25	0
55	MG	1W	206	1/1	0.97	0.08	27,27,27,27	0
55	MG	2a	1799	1/1	0.97	0.11	49,49,49,49	0
55	MG	2a	1800	1/1	0.97	0.12	28,28,28,28	0
55	MG	2A	3784	1/1	0.97	0.09	43,43,43,43	0
55	MG	1A	3774	1/1	0.97	0.06	37,37,37,37	0
55	MG	1A	3053	1/1	0.97	0.07	31,31,31,31	0
55	MG	1A	3258	1/1	0.97	0.05	22,22,22,22	0
55	MG	2A	3788	1/1	0.97	0.08	40,40,40,40	0
55	MG	2A	3789	1/1	0.97	0.12	34,34,34,34	0
55	MG	2A	3790	1/1	0.97	0.06	42,42,42,42	0
55	MG	2A	3458	1/1	0.97	0.09	28,28,28,28	0
55	MG	1A	3503	1/1	0.97	0.06	40,40,40,40	0
55	MG	2A	3182	1/1	0.97	0.05	25,25,25,25	0
55	MG	1X	103	1/1	0.97	0.07	34,34,34,34	0
55	MG	2A	3796	1/1	0.97	0.14	22,22,22,22	0
55	MG	1A	3630	1/1	0.97	0.07	18,18,18,18	0
55	MG	1A	3779	1/1	0.97	0.08	27,27,27,27	0
55	MG	1Z	301	1/1	0.97	0.03	23,23,23,23	0
55	MG	1A	3504	1/1	0.97	0.04	25,25,25,25	0
55	MG	2A	3804	1/1	0.97	0.09	31,31,31,31	0
55	MG	1A	3781	1/1	0.97	0.09	41,41,41,41	0
55	MG	10	102	1/1	0.97	0.06	34,34,34,34	0
55	MG	1A	3095	1/1	0.97	0.14	29,29,29,29	0
55	MG	1a	3185	1/1	0.97	0.04	32,32,32,32	0
55	MG	1A	3096	1/1	0.97	0.05	23,23,23,23	0
55	MG	1A	3321	1/1	0.97	0.05	18,18,18,18	0
55	MG	2A	3813	1/1	0.97	0.11	34,34,34,34	0
55	MG	2A	3196	1/1	0.97	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3137	1/1	0.97	0.07	30,30,30,30	0
55	MG	1A	3637	1/1	0.97	0.17	16,16,16,16	0
55	MG	1A	3638	1/1	0.97	0.12	10,10,10,10	0
55	MG	1A	3792	1/1	0.97	0.05	37,37,37,37	0
55	MG	1A	3170	1/1	0.97	0.12	32,32,32,32	0
55	MG	1A	3043	1/1	0.97	0.07	25,25,25,25	0
55	MG	1a	3196	1/1	0.97	0.03	34,34,34,34	0
55	MG	1A	3795	1/1	0.97	0.06	27,27,27,27	0
55	MG	1A	3326	1/1	0.97	0.04	26,26,26,26	0
55	MG	13	105	1/1	0.97	0.07	26,26,26,26	0
55	MG	1A	3800	1/1	0.97	0.09	24,24,24,24	0
55	MG	2A	3208	1/1	0.97	0.12	37,37,37,37	0
55	MG	15	101	1/1	0.97	0.12	36,36,36,36	0
55	MG	1A	3990	1/1	0.97	0.05	25,25,25,25	0
55	MG	2A	3491	1/1	0.97	0.19	27,27,27,27	0
55	MG	2A	3492	1/1	0.97	0.03	10,10,10,10	0
55	MG	2A	3211	1/1	0.97	0.11	26,26,26,26	0
55	MG	1a	3204	1/1	0.97	0.16	22,22,22,22	0
55	MG	2A	3213	1/1	0.97	0.05	32,32,32,32	0
55	MG	1a	3205	1/1	0.97	0.07	41,41,41,41	0
55	MG	1A	3328	1/1	0.97	0.05	22,22,22,22	0
55	MG	2A	3216	1/1	0.97	0.04	28,28,28,28	0
55	MG	16	102	1/1	0.97	0.05	18,18,18,18	0
55	MG	1A	3213	1/1	0.98	0.08	35,35,35,35	0
55	MG	1A	3844	1/1	0.98	0.08	23,23,23,23	0
55	MG	2A	3116	1/1	0.98	0.05	38,38,38,38	0
55	MG	1A	3325	1/1	0.98	0.07	41,41,41,41	0
55	MG	1A	3429	1/1	0.98	0.09	23,23,23,23	0
55	MG	1A	3848	1/1	0.98	0.05	22,22,22,22	0
55	MG	1F	303	1/1	0.98	0.07	29,29,29,29	0
55	MG	1A	3738	1/1	0.98	0.04	42,42,42,42	0
55	MG	1a	3190	1/1	0.98	0.08	44,44,44,44	0
55	MG	1F	305	1/1	0.98	0.04	34,34,34,34	0
55	MG	2A	3498	1/1	0.98	0.07	32,32,32,32	0
55	MG	1A	3850	1/1	0.98	0.07	17,17,17,17	0
55	MG	1A	3430	1/1	0.98	0.19	32,32,32,32	0
55	MG	2A	3501	1/1	0.98	0.04	26,26,26,26	0
55	MG	1a	3194	1/1	0.98	0.04	27,27,27,27	0
55	MG	1A	3970	1/1	0.98	0.12	22,22,22,22	0
55	MG	1A	3560	1/1	0.98	0.07	19,19,19,19	0
55	MG	1F	310	1/1	0.98	0.14	25,25,25,25	0
55	MG	1F	311	1/1	0.98	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3102	1/1	0.98	0.05	17,17,17,17	0
55	MG	1A	3562	1/1	0.98	0.09	25,25,25,25	0
55	MG	1a	3201	1/1	0.98	0.03	33,33,33,33	0
55	MG	1A	3074	1/1	0.98	0.19	19,19,19,19	0
55	MG	1A	3975	1/1	0.98	0.03	23,23,23,23	0
55	MG	1A	3374	1/1	0.98	0.04	33,33,33,33	0
55	MG	1A	3977	1/1	0.98	0.03	23,23,23,23	0
55	MG	1A	3076	1/1	0.98	0.05	42,42,42,42	0
55	MG	1a	3046	1/1	0.98	0.06	33,33,33,33	0
55	MG	1A	3858	1/1	0.98	0.08	41,41,41,41	0
55	MG	1A	3566	1/1	0.98	0.05	18,18,18,18	0
55	MG	2A	3735	1/1	0.98	0.04	22,22,22,22	0
55	MG	1N	201	1/1	0.98	0.05	47,47,47,47	0
55	MG	1A	3130	1/1	0.98	0.14	18,18,18,18	0
55	MG	1A	3288	1/1	0.98	0.05	27,27,27,27	0
55	MG	2A	3739	1/1	0.98	0.10	43,43,43,43	0
55	MG	1A	3862	1/1	0.98	0.04	39,39,39,39	0
55	MG	1A	3569	1/1	0.98	0.08	28,28,28,28	0
55	MG	1A	3289	1/1	0.98	0.03	10,10,10,10	0
55	MG	1O	202	1/1	0.98	0.04	47,47,47,47	0
55	MG	1A	3754	1/1	0.98	0.07	33,33,33,33	0
55	MG	1A	3656	1/1	0.98	0.04	36,36,36,36	0
55	MG	1l	202	1/1	0.98	0.05	18,18,18,18	0
55	MG	1A	3756	1/1	0.98	0.04	23,23,23,23	0
55	MG	1A	3186	1/1	0.98	0.07	34,34,34,34	0
55	MG	1P	202	1/1	0.98	0.12	15,15,15,15	0
55	MG	1A	3187	1/1	0.98	0.16	33,33,33,33	0
55	MG	2A	3533	1/1	0.98	0.06	42,42,42,42	0
55	MG	1A	3870	1/1	0.98	0.05	14,14,14,14	0
55	MG	1A	3871	1/1	0.98	0.09	12,12,12,12	0
55	MG	2A	3754	1/1	0.98	0.06	43,43,43,43	0
55	MG	1A	3574	1/1	0.98	0.07	46,46,46,46	0
55	MG	1A	3441	1/1	0.98	0.11	38,38,38,38	0
55	MG	1v	104	1/1	0.98	0.07	35,35,35,35	0
55	MG	1A	3874	1/1	0.98	0.04	30,30,30,30	0
55	MG	1A	3576	1/1	0.98	0.09	10,10,10,10	0
55	MG	1A	3442	1/1	0.98	0.09	22,22,22,22	0
55	MG	2A	3165	1/1	0.98	0.09	33,33,33,33	0
55	MG	1A	3188	1/1	0.98	0.04	22,22,22,22	0
55	MG	1A	3579	1/1	0.98	0.11	15,15,15,15	0
55	MG	1A	3065	1/1	0.98	0.10	16,16,16,16	0
55	MG	1A	4002	1/1	0.98	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3384	1/1	0.98	0.07	21,21,21,21	0
55	MG	1R	205	1/1	0.98	0.03	30,30,30,30	0
55	MG	1A	3132	1/1	0.98	0.08	35,35,35,35	0
55	MG	1A	3447	1/1	0.98	0.14	33,33,33,33	0
55	MG	1A	3387	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3028	1/1	0.98	0.07	39,39,39,39	0
55	MG	1A	3042	1/1	0.98	0.04	18,18,18,18	0
55	MG	1A	3886	1/1	0.98	0.12	36,36,36,36	0
55	MG	2A	3556	1/1	0.98	0.05	26,26,26,26	0
55	MG	1A	3092	1/1	0.98	0.13	22,22,22,22	0
55	MG	2A	3003	1/1	0.98	0.15	29,29,29,29	0
55	MG	1A	3674	1/1	0.98	0.08	32,32,32,32	0
55	MG	1A	3093	1/1	0.98	0.05	18,18,18,18	0
55	MG	2A	3006	1/1	0.98	0.10	38,38,38,38	0
55	MG	2A	3782	1/1	0.98	0.04	37,37,37,37	0
55	MG	2A	3563	1/1	0.98	0.18	27,27,27,27	0
55	MG	2A	3564	1/1	0.98	0.08	25,25,25,25	0
55	MG	1A	3009	1/1	0.98	0.05	32,32,32,32	0
55	MG	1U	205	1/1	0.98	0.15	27,27,27,27	0
55	MG	1A	3891	1/1	0.98	0.06	42,42,42,42	0
55	MG	1A	3114	1/1	0.98	0.05	10,10,10,10	0
55	MG	1A	3592	1/1	0.98	0.04	27,27,27,27	0
55	MG	2A	3369	1/1	0.98	0.07	19,19,19,19	0
55	MG	1A	4019	1/1	0.98	0.04	41,41,41,41	0
55	MG	1A	3679	1/1	0.98	0.04	23,23,23,23	0
55	MG	2A	3573	1/1	0.98	0.04	23,23,23,23	0
55	MG	2A	3014	1/1	0.98	0.04	21,21,21,21	0
55	MG	2A	3192	1/1	0.98	0.12	25,25,25,25	0
55	MG	1A	3396	1/1	0.98	0.15	22,22,22,22	0
55	MG	1A	3346	1/1	0.98	0.03	15,15,15,15	0
55	MG	2A	3799	1/1	0.98	0.13	29,29,29,29	0
55	MG	1A	3398	1/1	0.98	0.33	29,29,29,29	0
55	MG	2A	3018	1/1	0.98	0.13	10,10,10,10	0
55	MG	1A	3399	1/1	0.98	0.05	17,17,17,17	0
55	MG	2A	3581	1/1	0.98	0.09	33,33,33,33	0
55	MG	2A	3582	1/1	0.98	0.05	33,33,33,33	0
55	MG	1A	4027	1/1	0.98	0.11	11,11,11,11	0
55	MG	1A	4028	1/1	0.98	0.11	17,17,17,17	0
55	MG	1A	3899	1/1	0.98	0.09	22,22,22,22	0
55	MG	1A	3785	1/1	0.98	0.13	14,14,14,14	0
55	MG	2A	3811	1/1	0.98	0.14	10,10,10,10	0
55	MG	2A	3812	1/1	0.98	0.04	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3901	1/1	0.98	0.06	28,28,28,28	0
55	MG	1A	4032	1/1	0.98	0.12	39,39,39,39	0
55	MG	1A	3597	1/1	0.98	0.04	34,34,34,34	0
55	MG	1A	3140	1/1	0.98	0.09	33,33,33,33	0
55	MG	1a	3106	1/1	0.98	0.10	10,10,10,10	0
55	MG	1A	4035	1/1	0.98	0.17	15,15,15,15	0
55	MG	1X	104	1/1	0.98	0.05	22,22,22,22	0
55	MG	1A	3788	1/1	0.98	0.08	35,35,35,35	0
55	MG	2A	3822	1/1	0.98	0.03	28,28,28,28	0
55	MG	1A	3302	1/1	0.98	0.05	26,26,26,26	0
55	MG	1a	3111	1/1	0.98	0.10	25,25,25,25	0
55	MG	1A	3462	1/1	0.98	0.12	30,30,30,30	0
55	MG	1A	3525	1/1	0.98	0.16	25,25,25,25	0
55	MG	1Z	303	1/1	0.98	0.04	28,28,28,28	0
55	MG	1A	3303	1/1	0.98	0.07	37,37,37,37	0
55	MG	1A	3527	1/1	0.98	0.10	17,17,17,17	0
55	MG	2A	3830	1/1	0.98	0.14	31,31,31,31	0
55	MG	10	103	1/1	0.98	0.04	25,25,25,25	0
55	MG	1A	3115	1/1	0.98	0.07	20,20,20,20	0
55	MG	2A	3219	1/1	0.98	0.05	24,24,24,24	0
55	MG	2a	1738	1/1	0.98	0.03	59,59,59,59	0
55	MG	1A	3305	1/1	0.98	0.04	23,23,23,23	0
55	MG	2A	3606	1/1	0.98	0.12	34,34,34,34	0
55	MG	2A	3221	1/1	0.98	0.07	33,33,33,33	0
55	MG	2A	3404	1/1	0.98	0.06	12,12,12,12	0
55	MG	1A	3231	1/1	0.98	0.10	22,22,22,22	0
55	MG	1A	3799	1/1	0.98	0.09	51,51,51,51	0
55	MG	11	101	1/1	0.98	0.23	32,32,32,32	0
55	MG	1A	3468	1/1	0.98	0.12	34,34,34,34	0
55	MG	2A	3047	1/1	0.98	0.04	33,33,33,33	0
55	MG	1A	3116	1/1	0.98	0.04	29,29,29,29	0
55	MG	2A	3049	1/1	0.98	0.04	21,21,21,21	0
55	MG	1a	3125	1/1	0.98	0.03	21,21,21,21	0
55	MG	1A	3609	1/1	0.98	0.09	17,17,17,17	0
55	MG	1A	3081	1/1	0.98	0.09	15,15,15,15	0
55	MG	2A	3415	1/1	0.98	0.06	36,36,36,36	0
55	MG	1A	3309	1/1	0.98	0.16	25,25,25,25	0
55	MG	2A	3417	1/1	0.98	0.07	16,16,16,16	0
55	MG	1B	210	1/1	0.98	0.04	30,30,30,30	0
55	MG	1a	3130	1/1	0.98	0.19	38,38,38,38	0
55	MG	1A	3807	1/1	0.98	0.10	31,31,31,31	0
55	MG	2A	3421	1/1	0.98	0.21	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3626	1/1	0.98	0.06	21,21,21,21	0
55	MG	2A	3627	1/1	0.98	0.16	23,23,23,23	0
55	MG	1A	3118	1/1	0.98	0.09	24,24,24,24	0
55	MG	1A	3613	1/1	0.98	0.08	19,19,19,19	0
55	MG	2a	1765	1/1	0.98	0.07	42,42,42,42	0
55	MG	1A	3614	1/1	0.98	0.12	14,14,14,14	0
55	MG	1a	3136	1/1	0.98	0.07	32,32,32,32	0
55	MG	2A	3426	1/1	0.98	0.09	55,55,55,55	0
55	MG	1A	3119	1/1	0.98	0.05	34,34,34,34	0
55	MG	2A	3635	1/1	0.98	0.04	31,31,31,31	0
55	MG	2A	3636	1/1	0.98	0.12	28,28,28,28	0
55	MG	2A	3062	1/1	0.98	0.03	17,17,17,17	0
55	MG	15	104	1/1	0.98	0.02	17,17,17,17	0
55	MG	1A	3925	1/1	0.98	0.04	20,20,20,20	0
55	MG	2A	3640	1/1	0.98	0.04	39,39,39,39	0
55	MG	1A	3537	1/1	0.98	0.08	30,30,30,30	0
55	MG	2a	1777	1/1	0.98	0.06	38,38,38,38	0
55	MG	1A	3813	1/1	0.98	0.04	44,44,44,44	0
55	MG	1A	3060	1/1	0.98	0.09	21,21,21,21	0
55	MG	2A	3645	1/1	0.98	0.08	49,49,49,49	0
55	MG	2D	303	1/1	0.98	0.04	40,40,40,40	0
55	MG	17	102	1/1	0.98	0.06	18,18,18,18	0
55	MG	1A	3061	1/1	0.98	0.03	37,37,37,37	0
55	MG	1A	3619	1/1	0.98	0.04	23,23,23,23	0
55	MG	2D	307	1/1	0.98	0.08	25,25,25,25	0
55	MG	1A	3817	1/1	0.98	0.11	40,40,40,40	0
55	MG	2A	3072	1/1	0.98	0.11	26,26,26,26	0
55	MG	2A	3073	1/1	0.98	0.09	30,30,30,30	0
55	MG	2A	3652	1/1	0.98	0.04	31,31,31,31	0
55	MG	1A	3621	1/1	0.98	0.08	36,36,36,36	0
55	MG	1A	3414	1/1	0.98	0.12	26,26,26,26	0
55	MG	1a	3151	1/1	0.98	0.10	28,28,28,28	0
55	MG	2F	302	1/1	0.98	0.07	32,32,32,32	0
55	MG	18	101	1/1	0.98	0.20	27,27,27,27	0
55	MG	2A	3445	1/1	0.98	0.09	32,32,32,32	0
55	MG	2A	3078	1/1	0.98	0.06	41,41,41,41	0
55	MG	1A	3174	1/1	0.98	0.10	23,23,23,23	0
55	MG	1A	3713	1/1	0.98	0.05	40,40,40,40	0
55	MG	2A	3260	1/1	0.98	0.05	23,23,23,23	0
55	MG	1A	3054	1/1	0.98	0.13	21,21,21,21	0
55	MG	1A	3625	1/1	0.98	0.05	20,20,20,20	0
55	MG	2A	3083	1/1	0.98	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3241	1/1	0.98	0.07	34,34,34,34	0
55	MG	2Q	203	1/1	0.98	0.09	49,49,49,49	0
55	MG	2A	3454	1/1	0.98	0.20	28,28,28,28	0
55	MG	2R	201	1/1	0.98	0.08	17,17,17,17	0
55	MG	2A	3667	1/1	0.98	0.06	32,32,32,32	0
55	MG	2A	3668	1/1	0.98	0.03	29,29,29,29	0
55	MG	1A	3940	1/1	0.98	0.12	22,22,22,22	0
55	MG	1A	3627	1/1	0.98	0.12	10,10,10,10	0
55	MG	1A	3942	1/1	0.98	0.05	35,35,35,35	0
55	MG	2U	202	1/1	0.98	0.04	23,23,23,23	0
55	MG	1A	3149	1/1	0.98	0.11	23,23,23,23	0
55	MG	1A	3482	1/1	0.98	0.10	28,28,28,28	0
55	MG	2A	3674	1/1	0.98	0.05	36,36,36,36	0
55	MG	1A	3945	1/1	0.98	0.17	24,24,24,24	0
55	MG	1A	3946	1/1	0.98	0.03	30,30,30,30	0
55	MG	1A	3947	1/1	0.98	0.06	25,25,25,25	0
55	MG	1a	3008	1/1	0.98	0.07	54,54,54,54	0
55	MG	2I	102	1/1	0.98	0.05	40,40,40,40	0
55	MG	2I	103	1/1	0.98	0.08	18,18,18,18	0
55	MG	1A	3018	1/1	0.98	0.05	16,16,16,16	0
55	MG	1A	3949	1/1	0.98	0.03	31,31,31,31	0
55	MG	1A	3950	1/1	0.98	0.12	27,27,27,27	0
55	MG	2A	3467	1/1	0.98	0.20	34,34,34,34	0
55	MG	1A	3278	1/1	0.98	0.05	32,32,32,32	0
55	MG	1A	3724	1/1	0.98	0.06	20,20,20,20	0
55	MG	2A	3100	1/1	0.98	0.14	22,22,22,22	0
55	MG	2I	202	1/1	0.98	0.03	42,42,42,42	0
55	MG	1D	310	1/1	0.98	0.04	36,36,36,36	0
55	MG	25	103	1/1	0.98	0.06	27,27,27,27	0
55	MG	1A	3244	1/1	0.98	0.18	20,20,20,20	0
55	MG	1A	3125	1/1	0.98	0.09	29,29,29,29	0
55	MG	2A	3104	1/1	0.98	0.06	28,28,28,28	0
55	MG	1A	3551	1/1	0.98	0.08	19,19,19,19	0
55	MG	2A	3476	1/1	0.98	0.11	24,24,24,24	0
55	MG	1E	304	1/1	0.98	0.08	24,24,24,24	0
55	MG	2a	1601	1/1	0.98	0.04	23,23,23,23	0
55	MG	2a	1602	1/1	0.98	0.04	51,51,51,51	0
55	MG	2A	3107	1/1	0.98	0.10	39,39,39,39	0
55	MG	1E	305	1/1	0.98	0.04	34,34,34,34	0
55	MG	1A	3838	1/1	0.98	0.08	26,26,26,26	0
55	MG	2A	3481	1/1	0.98	0.18	39,39,39,39	0
55	MG	1A	3552	1/1	0.98	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3012	1/1	0.98	0.16	27,27,27,27	0
57	ZN	2Y	203	1/1	0.98	0.05	98,98,98,98	0
55	MG	1A	3554	1/1	0.98	0.06	18,18,18,18	0
55	MG	2A	3485	1/1	0.98	0.03	22,22,22,22	0
55	MG	1A	3247	1/1	0.98	0.05	37,37,37,37	0
55	MG	2A	3293	1/1	0.98	0.10	16,16,16,16	0
55	MG	2A	3299	1/1	0.99	0.04	46,46,46,46	0
55	MG	1A	3135	1/1	0.99	0.05	23,23,23,23	0
55	MG	1A	3978	1/1	0.99	0.12	21,21,21,21	0
55	MG	1A	3796	1/1	0.99	0.03	10,10,10,10	0
55	MG	1A	3797	1/1	0.99	0.04	20,20,20,20	0
55	MG	1A	3745	1/1	0.99	0.05	32,32,32,32	0
55	MG	1A	3375	1/1	0.99	0.14	29,29,29,29	0
55	MG	1A	3335	1/1	0.99	0.04	19,19,19,19	0
55	MG	2A	3767	1/1	0.99	0.07	40,40,40,40	0
55	MG	1A	3802	1/1	0.99	0.03	38,38,38,38	0
55	MG	1A	3010	1/1	0.99	0.07	33,33,33,33	0
55	MG	13	101	1/1	0.99	0.04	30,30,30,30	0
55	MG	2A	3771	1/1	0.99	0.11	26,26,26,26	0
55	MG	1A	3337	1/1	0.99	0.05	16,16,16,16	0
55	MG	1A	3107	1/1	0.99	0.06	14,14,14,14	0
55	MG	2A	3400	1/1	0.99	0.10	13,13,13,13	0
55	MG	1A	3404	1/1	0.99	0.03	21,21,21,21	0
55	MG	1A	3432	1/1	0.99	0.09	20,20,20,20	0
55	MG	1A	3234	1/1	0.99	0.05	28,28,28,28	0
55	MG	1A	3667	1/1	0.99	0.08	18,18,18,18	0
55	MG	2a	1763	1/1	0.99	0.10	31,31,31,31	0
55	MG	1a	3135	1/1	0.99	0.08	26,26,26,26	0
55	MG	15	102	1/1	0.99	0.06	33,33,33,33	0
55	MG	1A	3929	1/1	0.99	0.07	18,18,18,18	0
55	MG	1A	3494	1/1	0.99	0.18	10,10,10,10	0
55	MG	1a	3139	1/1	0.99	0.02	30,30,30,30	0
55	MG	1A	3631	1/1	0.99	0.05	42,42,42,42	0
55	MG	1A	3708	1/1	0.99	0.04	26,26,26,26	0
55	MG	2F	305	1/1	0.99	0.06	27,27,27,27	0
55	MG	1A	3709	1/1	0.99	0.03	28,28,28,28	0
55	MG	1A	3075	1/1	0.99	0.13	10,10,10,10	0
55	MG	2A	3325	1/1	0.99	0.04	22,22,22,22	0
55	MG	2A	3691	1/1	0.99	0.08	24,24,24,24	0
55	MG	2P	202	1/1	0.99	0.06	29,29,29,29	0
55	MG	1A	3711	1/1	0.99	0.07	10,10,10,10	0
55	MG	2A	3791	1/1	0.99	0.02	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3109	1/1	0.99	0.07	21,21,21,21	0
55	MG	2a	1672	1/1	0.99	0.08	21,21,21,21	0
55	MG	1a	3146	1/1	0.99	0.14	29,29,29,29	0
55	MG	1A	3465	1/1	0.99	0.04	22,22,22,22	0
55	MG	1B	227	1/1	0.99	0.04	31,31,31,31	0
55	MG	1A	3022	1/1	0.99	0.07	29,29,29,29	0
55	MG	1A	3819	1/1	0.99	0.05	22,22,22,22	0
55	MG	2A	3699	1/1	0.99	0.07	20,20,20,20	0
55	MG	1A	3120	1/1	0.99	0.08	30,30,30,30	0
55	MG	2A	3800	1/1	0.99	0.07	20,20,20,20	0
55	MG	1A	3500	1/1	0.99	0.07	34,34,34,34	0
55	MG	1A	3717	1/1	0.99	0.08	25,25,25,25	0
55	MG	1A	3823	1/1	0.99	0.05	16,16,16,16	0
55	MG	1A	3385	1/1	0.99	0.04	26,26,26,26	0
55	MG	18	106	1/1	0.99	0.03	10,10,10,10	0
55	MG	2A	3518	1/1	0.99	0.03	34,34,34,34	0
55	MG	1A	4008	1/1	0.99	0.03	24,24,24,24	0
55	MG	1B	236	1/1	0.99	0.08	21,21,21,21	0
55	MG	1A	3177	1/1	0.99	0.04	26,26,26,26	0
55	MG	1A	3178	1/1	0.99	0.03	17,17,17,17	0
55	MG	2A	3084	1/1	0.99	0.07	28,28,28,28	0
55	MG	1A	3388	1/1	0.99	0.04	19,19,19,19	0
55	MG	1A	3828	1/1	0.99	0.07	28,28,28,28	0
55	MG	1A	3153	1/1	0.99	0.12	30,30,30,30	0
55	MG	2A	3816	1/1	0.99	0.03	25,25,25,25	0
55	MG	1A	3723	1/1	0.99	0.03	36,36,36,36	0
55	MG	1A	4015	1/1	0.99	0.05	19,19,19,19	0
55	MG	1a	3084	1/1	0.99	0.10	10,10,10,10	0
55	MG	1D	308	1/1	0.99	0.07	42,42,42,42	0
55	MG	1A	3327	1/1	0.99	0.07	26,26,26,26	0
55	MG	1U	204	1/1	0.99	0.03	17,17,17,17	0
55	MG	1A	3725	1/1	0.99	0.09	26,26,26,26	0
55	MG	1A	3391	1/1	0.99	0.04	37,37,37,37	0
55	MG	1A	3834	1/1	0.99	0.04	11,11,11,11	0
55	MG	1A	3573	1/1	0.99	0.07	24,24,24,24	0
55	MG	28	102	1/1	0.99	0.11	29,29,29,29	0
55	MG	1A	3728	1/1	0.99	0.03	24,24,24,24	0
55	MG	2A	3538	1/1	0.99	0.05	35,35,35,35	0
55	MG	1A	4022	1/1	0.99	0.09	27,27,27,27	0
55	MG	1A	3646	1/1	0.99	0.05	16,16,16,16	0
55	MG	2A	3633	1/1	0.99	0.13	30,30,30,30	0
55	MG	1E	307	1/1	0.99	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3032	1/1	0.99	0.05	16,16,16,16	0
55	MG	1a	3097	1/1	0.99	0.14	23,23,23,23	0
55	MG	1A	3731	1/1	0.99	0.06	25,25,25,25	0
55	MG	2A	3190	1/1	0.99	0.03	42,42,42,42	0
55	MG	1a	3099	1/1	0.99	0.19	18,18,18,18	0
55	MG	1A	4026	1/1	0.99	0.04	26,26,26,26	0
55	MG	1A	3960	1/1	0.99	0.09	14,14,14,14	0
55	MG	2A	3642	1/1	0.99	0.12	12,12,12,12	0
55	MG	1A	3112	1/1	0.99	0.08	16,16,16,16	0
55	MG	1A	3211	1/1	0.99	0.03	37,37,37,37	0
55	MG	1W	207	1/1	0.99	0.08	23,23,23,23	0
55	MG	1A	3783	1/1	0.99	0.09	21,21,21,21	0
55	MG	1A	3784	1/1	0.99	0.05	24,24,24,24	0
55	MG	1A	3020	1/1	0.99	0.08	24,24,24,24	0
55	MG	2A	3030	1/1	0.99	0.25	33,33,33,33	0
55	MG	1A	3845	1/1	0.99	0.05	19,19,19,19	0
55	MG	2A	3557	1/1	0.99	0.09	15,15,15,15	0
55	MG	1A	3197	1/1	0.99	0.11	16,16,16,16	0
55	MG	1A	3906	1/1	0.99	0.04	21,21,21,21	0
55	MG	1A	3450	1/1	0.99	0.04	14,14,14,14	0
55	MG	1A	3422	1/1	0.99	0.06	36,36,36,36	0
55	MG	2a	1627	1/1	0.99	0.12	27,27,27,27	0
55	MG	1A	3099	1/1	0.99	0.07	23,23,23,23	0
57	ZN	1Y	203	1/1	0.99	0.03	62,62,62,62	0
55	MG	2A	3121	1/1	0.99	0.04	29,29,29,29	0
55	MG	1A	3739	1/1	0.99	0.08	34,34,34,34	0
57	ZN	16	104	1/1	0.99	0.02	36,36,36,36	0
57	ZN	1n	104	1/1	0.99	0.03	68,68,68,68	0
55	MG	1A	3424	1/1	0.99	0.03	21,21,21,21	0
55	MG	1A	3549	1/1	0.99	0.08	16,16,16,16	0
55	MG	2B	208	1/1	0.99	0.03	22,22,22,22	0
57	ZN	26	102	1/1	0.99	0.03	40,40,40,40	0
57	ZN	29	501	1/1	0.99	0.05	60,60,60,60	0
55	MG	1A	3584	1/1	0.99	0.04	31,31,31,31	0
55	MG	1A	3743	1/1	0.99	0.10	10,10,10,10	0
59	SF4	1d	302	8/8	0.99	0.03	47,72,75,78	0
59	SF4	2d	303	8/8	0.99	0.03	45,64,72,73	0
55	MG	1A	3620	1/1	1.00	0.03	15,15,15,15	0
57	ZN	2n	102	1/1	1.00	0.02	52,52,52,52	0
55	MG	1A	3801	1/1	1.00	0.06	10,10,10,10	0
55	MG	2A	3803	1/1	1.00	0.06	32,32,32,32	0
55	MG	2Y	202	1/1	1.00	0.11	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	ZN	19	103	1/1	1.00	0.01	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.