



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:08 PM UTC

PDB ID : 6XQD / pdb_00006xqd
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with sarecycline, UUC-mRNA, and deacylated P-site tRNA at 2.80Å resolution
Authors : Batool, Z.; Lomakin, I.B.; Bunick, C.G.; Polikanov, Y.S.
Deposited on : 2020-07-09
Resolution : 2.80 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

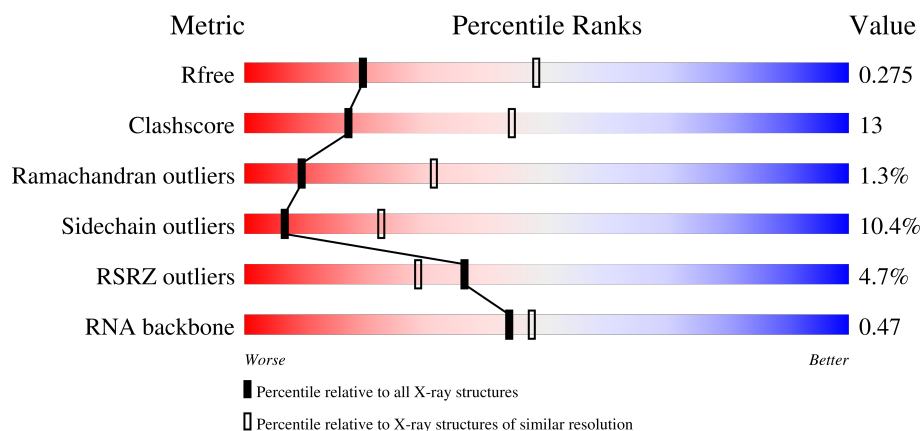
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



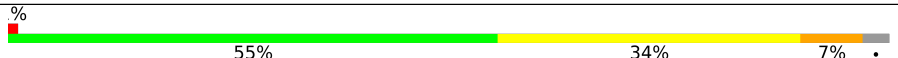
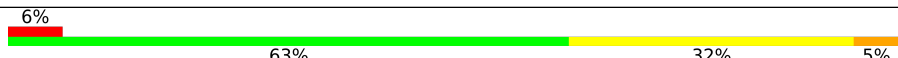
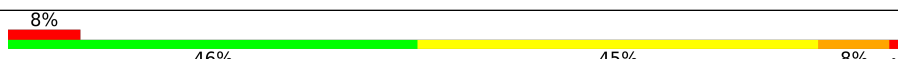
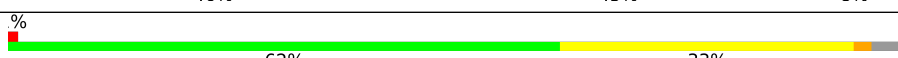
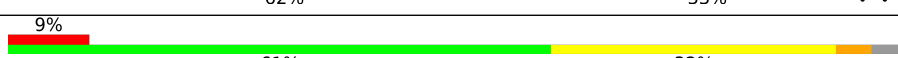
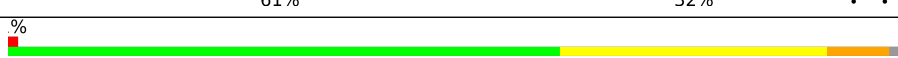
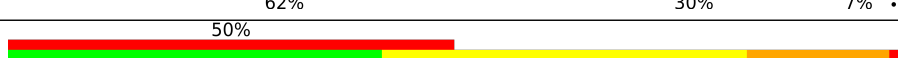
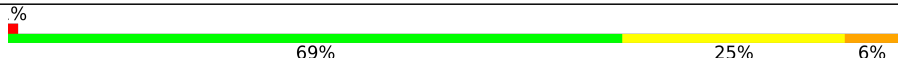
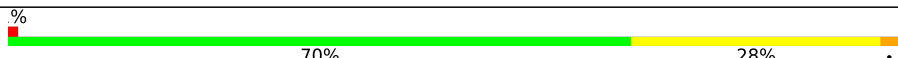
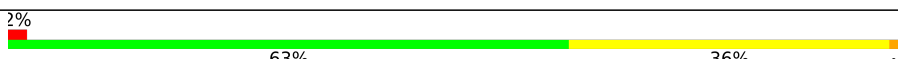
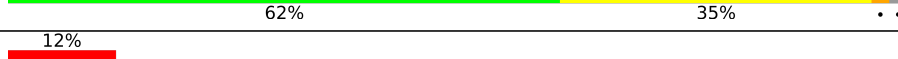
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	2% 50% 40% 9% .
1	2A	2915	3% 45% 42% 9% .
2	1B	121	% 60% 33% 6% .
2	2B	121	5% 39% 47% 13% .

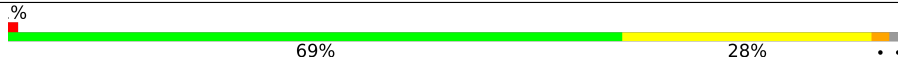
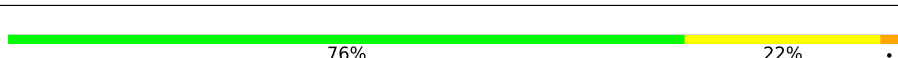
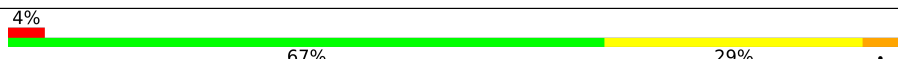
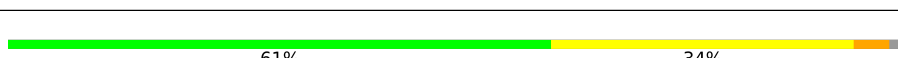
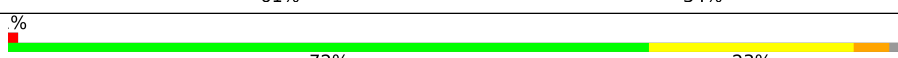
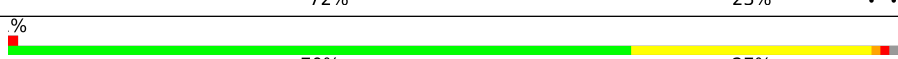
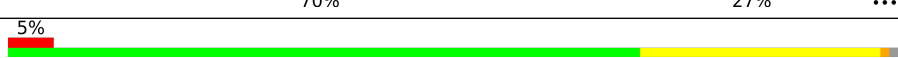
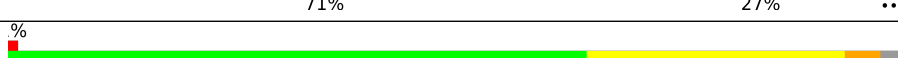
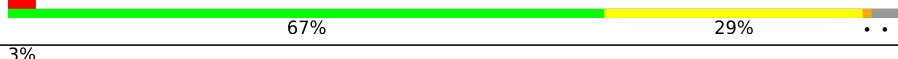
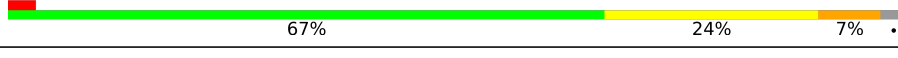
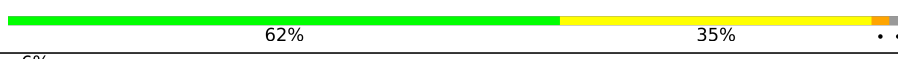
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
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	3541	-	-	-	X
55	MG	1B	229	-	-	-	X
55	MG	1U	207	-	-	-	X
55	MG	1a	1662	-	-	-	X
55	MG	2A	3484	-	-	-	X
55	MG	2a	3092	-	-	-	X
55	MG	2i	201	-	-	-	X
58	SF4	1d	501	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292670 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
			213	96	39	68	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	1117	Total	Mg	0	0
			1117	1117		
55	1B	35	Total	Mg	0	0
			35	35		
55	1D	13	Total	Mg	0	0
			13	13		
55	1E	11	Total	Mg	0	0
			11	11		
55	1F	11	Total	Mg	0	0
			11	11		
55	1G	4	Total	Mg	0	0
			4	4		
55	1N	4	Total	Mg	0	0
			4	4		
55	1O	4	Total	Mg	0	0
			4	4		
55	1P	3	Total	Mg	0	0
			3	3		
55	1Q	7	Total	Mg	0	0
			7	7		
55	1R	2	Total	Mg	0	0
			2	2		
55	1S	1	Total	Mg	0	0
			1	1		
55	1T	3	Total	Mg	0	0
			3	3		
55	1U	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1V	4	Total 4	Mg 4	0	0
55	1W	5	Total 5	Mg 5	0	0
55	1X	6	Total 6	Mg 6	0	0
55	1Y	4	Total 4	Mg 4	0	0
55	1Z	2	Total 2	Mg 2	0	0
55	10	5	Total 5	Mg 5	0	0
55	11	4	Total 4	Mg 4	0	0
55	12	2	Total 2	Mg 2	0	0
55	13	3	Total 3	Mg 3	0	0
55	15	5	Total 5	Mg 5	0	0
55	16	1	Total 1	Mg 1	0	0
55	17	4	Total 4	Mg 4	0	0
55	18	6	Total 6	Mg 6	0	0
55	19	1	Total 1	Mg 1	0	0
55	1a	234	Total 234	Mg 234	0	0
55	1b	1	Total 1	Mg 1	0	0
55	1e	2	Total 2	Mg 2	0	0
55	1f	2	Total 2	Mg 2	0	0
55	1l	4	Total 4	Mg 4	0	0
55	1n	2	Total 2	Mg 2	0	0
55	1t	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1v	2	Total 2	Mg 2	0	0
55	1x	13	Total 13	Mg 13	0	0
55	2A	862	Total 862	Mg 862	0	0
55	2B	19	Total 19	Mg 19	0	0
55	2D	3	Total 3	Mg 3	0	0
55	2E	9	Total 9	Mg 9	0	0
55	2F	6	Total 6	Mg 6	0	0
55	2G	1	Total 1	Mg 1	0	0
55	2N	2	Total 2	Mg 2	0	0
55	2O	2	Total 2	Mg 2	0	0
55	2P	2	Total 2	Mg 2	0	0
55	2Q	4	Total 4	Mg 4	0	0
55	2R	2	Total 2	Mg 2	0	0
55	2T	3	Total 3	Mg 3	0	0
55	2U	2	Total 2	Mg 2	0	0
55	2V	3	Total 3	Mg 3	0	0
55	2W	2	Total 2	Mg 2	0	0
55	2X	2	Total 2	Mg 2	0	0
55	2Z	1	Total 1	Mg 1	0	0
55	20	1	Total 1	Mg 1	0	0
55	23	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	25	2	Total 2	Mg 2	0	0
55	26	1	Total 1	Mg 1	0	0
55	27	1	Total 1	Mg 1	0	0
55	28	3	Total 3	Mg 3	0	0
55	2a	209	Total 209	Mg 209	0	0
55	2d	2	Total 2	Mg 2	0	0
55	2e	1	Total 1	Mg 1	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	2l	3	Total 3	Mg 3	0	0
55	2p	1	Total 1	Mg 1	0	0
55	2q	1	Total 1	Mg 1	0	0
55	2r	1	Total 1	Mg 1	0	0
55	2t	1	Total 1	Mg 1	0	0
55	2x	5	Total 5	Mg 5	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

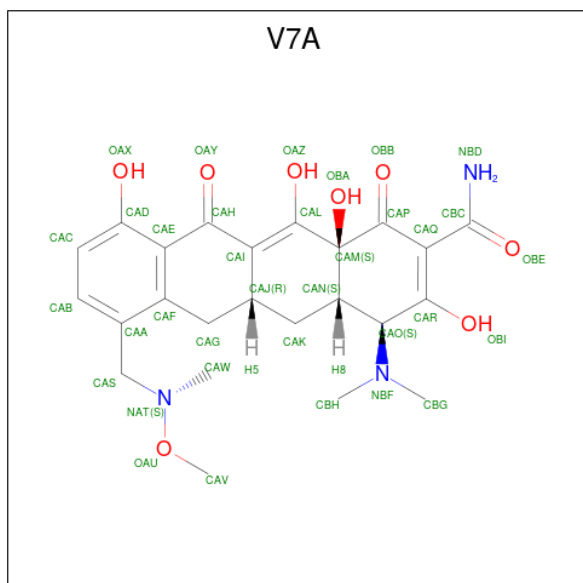
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Zn 1	0	0
56	14	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	15	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		
56	19	1	Total	Zn	0	0
			1	1		
56	1n	1	Total	Zn	0	0
			1	1		
56	2Y	1	Total	Zn	0	0
			1	1		
56	24	1	Total	Zn	0	0
			1	1		
56	25	1	Total	Zn	0	0
			1	1		
56	26	1	Total	Zn	0	0
			1	1		
56	29	1	Total	Zn	0	0
			1	1		
56	2n	1	Total	Zn	0	0
			1	1		

- Molecule 57 is Sarecycline (CCD ID: V7A) (formula: $C_{24}H_{29}N_3O_8$).



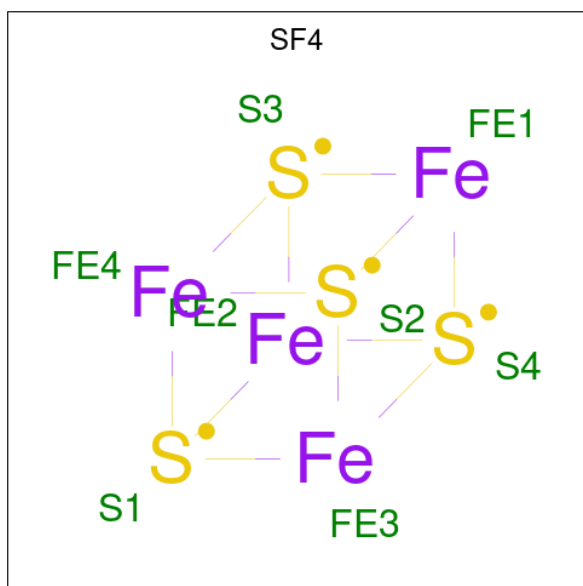
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1a	1	Total	C	N	O	0	0
			35	24	3	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	2a	1	Total	C	N	O	0	0
			35	24	3	8		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1716	Total	O	0	0
			1716	1716		
59	1B	47	Total	O	0	0
			47	47		
59	1D	21	Total	O	0	0
			21	21		
59	1E	25	Total	O	0	0
			25	25		
59	1F	13	Total	O	0	0
			13	13		
59	1G	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1H	2	Total	O	0	0
			2	2		
59	1I	2	Total	O	0	0
			2	2		
59	1N	3	Total	O	0	0
			3	3		
59	1O	7	Total	O	0	0
			7	7		
59	1P	17	Total	O	0	0
			17	17		
59	1Q	6	Total	O	0	0
			6	6		
59	1R	9	Total	O	0	0
			9	9		
59	1S	1	Total	O	0	0
			1	1		
59	1T	8	Total	O	0	0
			8	8		
59	1U	13	Total	O	0	0
			13	13		
59	1V	9	Total	O	0	0
			9	9		
59	1W	8	Total	O	0	0
			8	8		
59	1X	6	Total	O	0	0
			6	6		
59	1Y	2	Total	O	0	0
			2	2		
59	10	8	Total	O	0	0
			8	8		
59	11	7	Total	O	0	0
			7	7		
59	12	1	Total	O	0	0
			1	1		
59	13	4	Total	O	0	0
			4	4		
59	15	7	Total	O	0	0
			7	7		
59	16	2	Total	O	0	0
			2	2		
59	17	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	18	9	Total 9	O 9	0	0
59	1a	294	Total 294	O 294	0	0
59	1b	1	Total 1	O 1	0	0
59	1d	3	Total 3	O 3	0	0
59	1e	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1l	4	Total 4	O 4	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	1	Total 1	O 1	0	0
59	1q	2	Total 2	O 2	0	0
59	1v	4	Total 4	O 4	0	0
59	1x	17	Total 17	O 17	0	0
59	2A	867	Total 867	O 867	0	0
59	2B	14	Total 14	O 14	0	0
59	2D	16	Total 16	O 16	0	0
59	2E	8	Total 8	O 8	0	0
59	2F	13	Total 13	O 13	0	0
59	2I	1	Total 1	O 1	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2P	4	Total 4	O 4	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	2	Total 2	O 2	0	0
59	2T	4	Total 4	O 4	0	0
59	2U	3	Total 3	O 3	0	0
59	2W	5	Total 5	O 5	0	0
59	2X	2	Total 2	O 2	0	0
59	2Z	1	Total 1	O 1	0	0
59	20	3	Total 3	O 3	0	0
59	21	8	Total 8	O 8	0	0
59	22	1	Total 1	O 1	0	0
59	25	1	Total 1	O 1	0	0
59	27	1	Total 1	O 1	0	0
59	28	3	Total 3	O 3	0	0
59	29	1	Total 1	O 1	0	0
59	2a	146	Total 146	O 146	0	0
59	2g	1	Total 1	O 1	0	0
59	2j	2	Total 2	O 2	0	0
59	2l	4	Total 4	O 4	0	0
59	2p	1	Total 1	O 1	0	0
59	2r	1	Total 1	O 1	0	0

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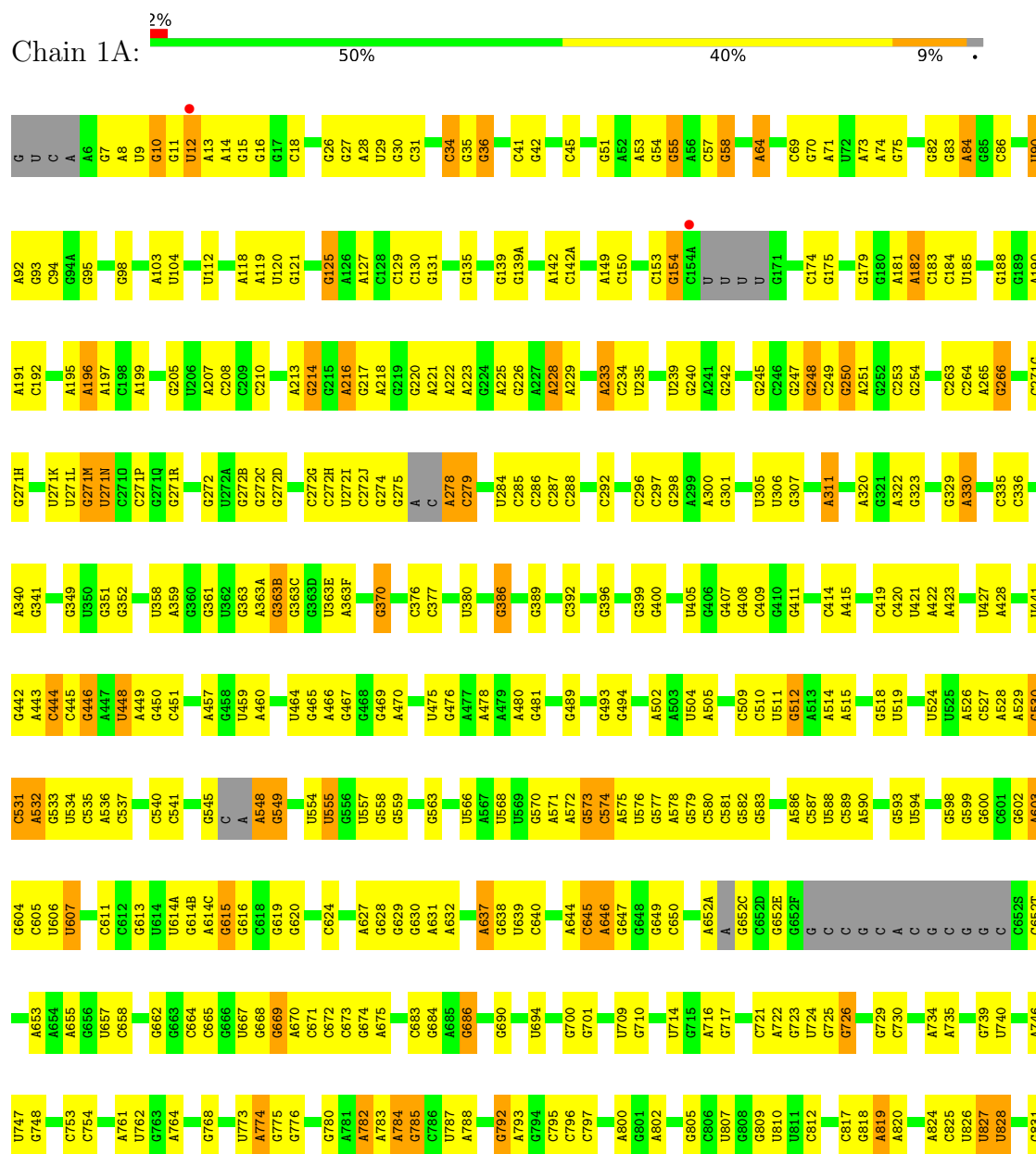
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2t	1	Total	O	0	0
			1	1		
59	2v	1	Total	O	0	0
			1	1		
59	2x	6	Total	O	0	0
			6	6		

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.

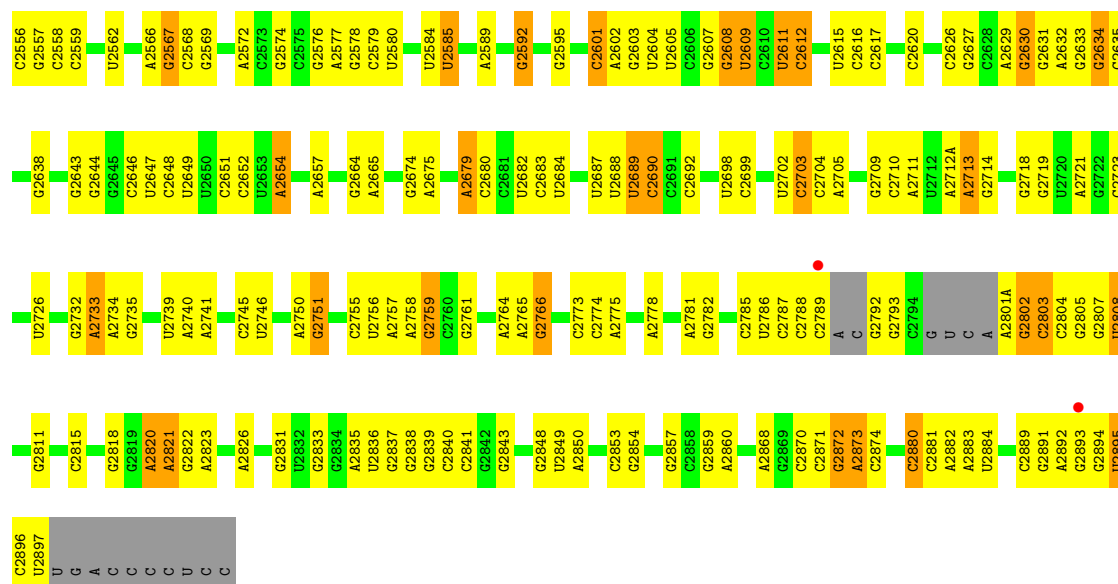
• Molecule 1: 23S Ribosomal RNA



C1999	U1915	A1810	G1702	A1603	C1511	A1419	G1324	G1235	G1139	C1075	A1010	U922	G832
A1916	A1916	G1811	G1703	C1604	U1512	U1420	G1328	G1236	C1140	C1076	G1011	C923	U833
A1918	A1918	A1812	C1711	C1604	C1513	G1421	G1328	A1237	U1142	A1077	U1012	C928	G836
A1919	A1919	A1815	C1712	C1607	G1517	G1424	G1332	G1238	U1143	C1079	U1013	G928	C837
C1920	C1920	G1816	G1721	A1608	U1518	G1425	C1333	G1239	A1143	C1080	U1014	G932	C838
G1921	G1921	G1817	A1722	A1609	G1519	G1426	G1334	U1240	G1144	U1081	C1018	U839	U839
G1922	G1922	A1818	A1723	A1616	G1525	A1427	U1335	A1241	G1149	U1082	U1019	G938	G848
U1923	U1923	A1819	A1724	C1617	G1528	C1428	G1339	A1242	G1149	A1084	A1020	U943	A849
C1924	C1924	A1823	A1741	C1617	A1528	C1430	G1339	G1243	C1152	A1084	G1022	G944	G857
G2023	G2023	A1825	G1746	G1627	A1528A	U1431	A1342	G1244	C1153	A1088	G1025	A945	U858
G2029	G2029	G1826	G1746	G1635	G1529	C1432	G1343	A1246	G1154	A1088	U1026	A946	G859
A2030	A2030	C1827	G1750	C1636	C1530	U1433	G1344	A1247	A1155	A1088	U1027	G947	U860
A2031	A2031	G1828	C1751	A1637	C1531	G1441	G1348	G1248	G1165	A1089	A1028	G949	A861
G2032	G2032	A1829	G1756	C1638	C1532	G1442	G1352	C1251	C1166	G1091	A1029	G952	G862
A2033	A2033	U1833	G1759	A1641	U	A1445	U1352	G1252	G1170	C1092	G1030	A953	A863
C2036	C2036	G1843	A1759	G1642	A	A1445	A1353	A1253	G1171	G1093	G1031	A954	G864
G2037	G1935	C1844	A1762	C1647	C	G1448	G1355	G1256	G1173	U1094	A1032	C955	C865
C2038	A1936	C1844	G1763	G1647	G1537	A1449	G1356	G1257	U1175	U1095	U1033	G956	A866
C2039	A1937	G1847	G1764	C1648	G1541	G1450	U1357	C1257	A1174	A1096	U1034	A957	C867
A1938	A1938	A1847	G1765	G1651	A1542	U1453	G1358	G1260	G1176	G1099	U1035	U958	U868
U1939	U1939	A1853	U1766	A1652	G1546	G1455	A1359	C1261	A1177	C1100	G1036	A959	G869
C1942	C1942	G1858	C1767	G1653	C1547	G1456	A1360	A1262	C1178	U1101	C1038	C961	C876
A2051	A1952	A1859	A1773	A1655	C1548	G1466	G1364	G1263	G1179	C1102	G1039	G962	U877
C2055	A1953	G1860	C1774	C1656	A1553	G1467	A1365	G1264	C1180	A1103	C1040	U963	G880
G2056	G1954	G1861	U1775	C1657	G1554	A1472	A1367	G1267	A1182	U1105	C1041	C964	G881
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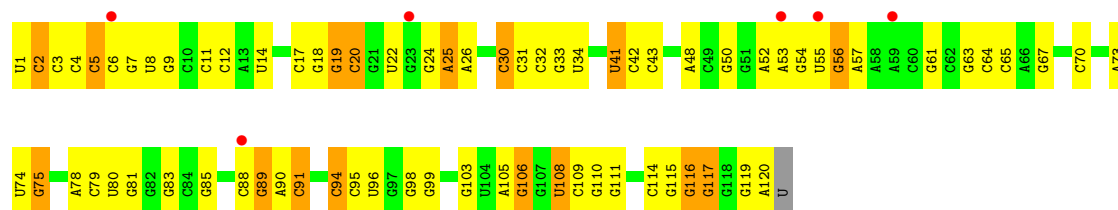
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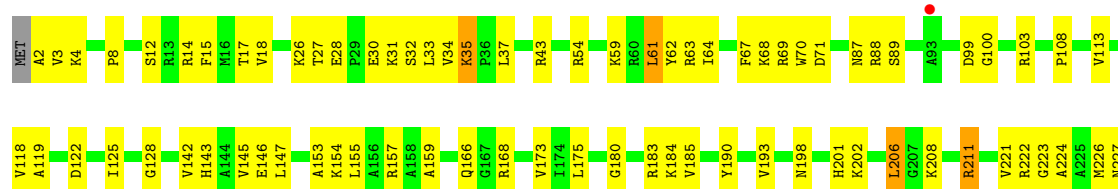
- Molecule 2: 5S Ribosomal RNA

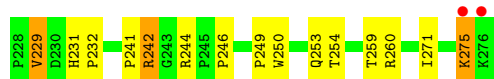


- Molecule 2: 5S Ribosomal RNA

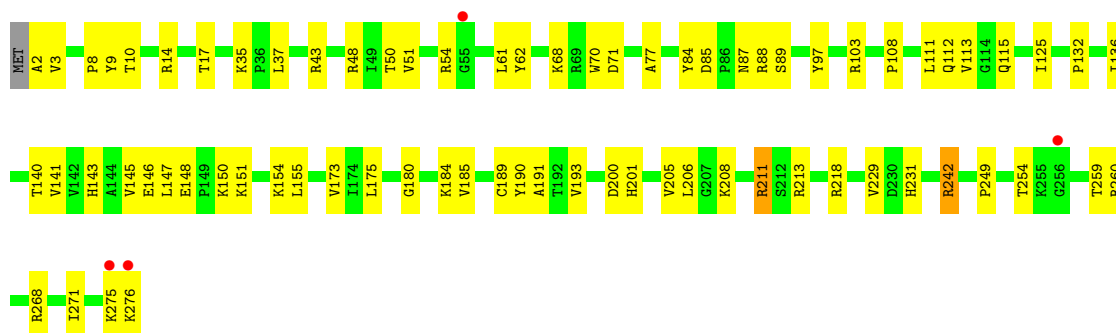
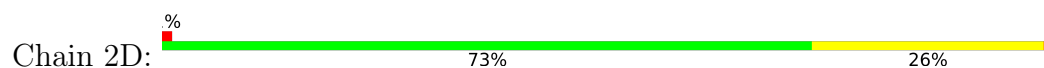


- Molecule 3: 50S ribosomal protein L2

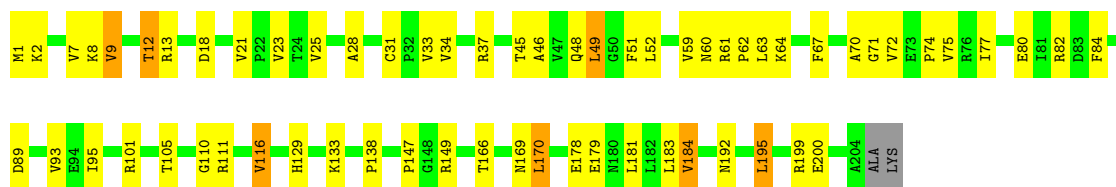




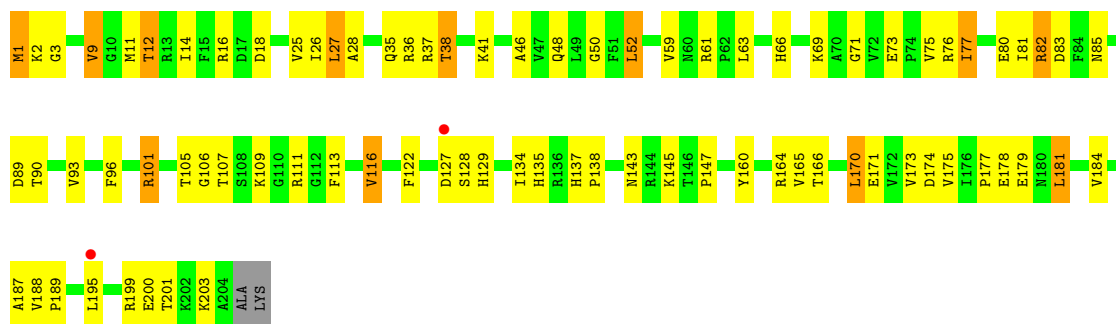
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

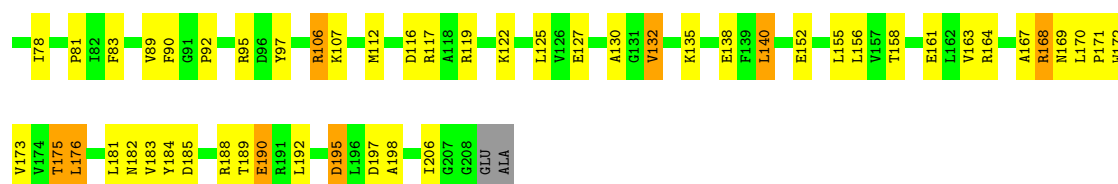


- Molecule 4: 50S ribosomal protein L3

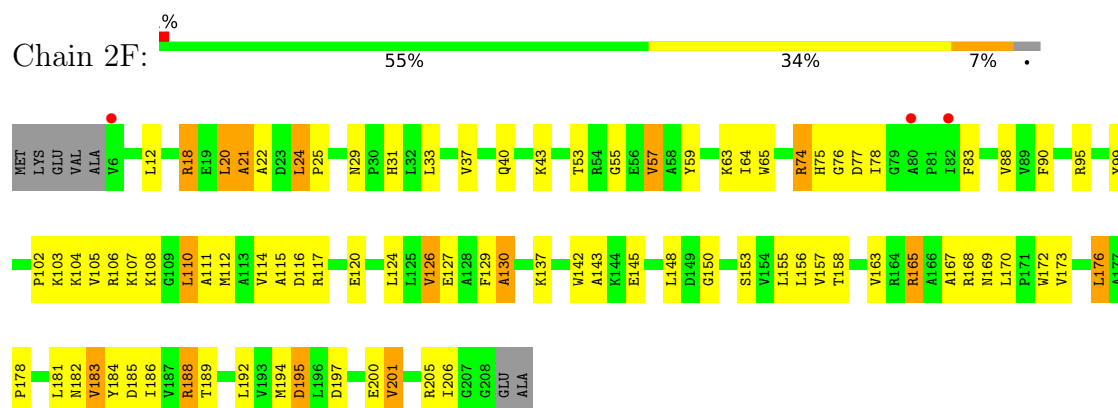


- Molecule 5: 50S ribosomal protein L4

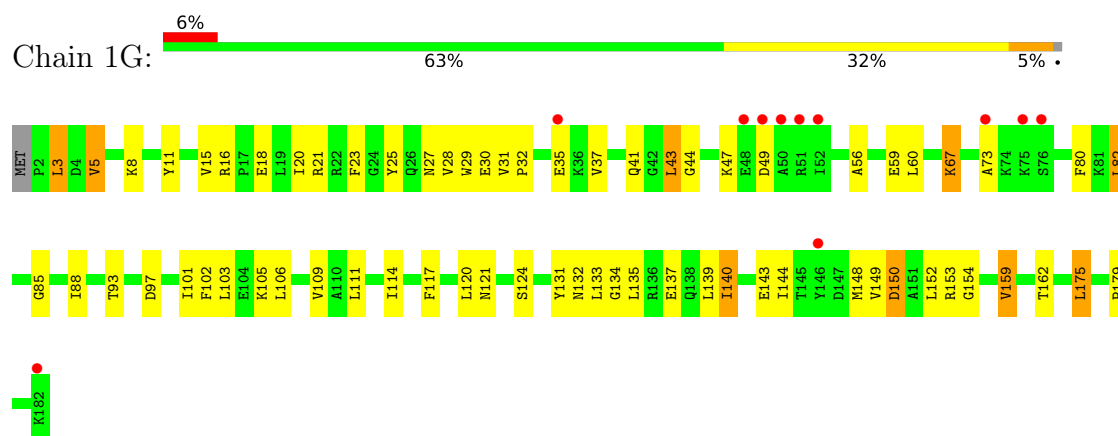




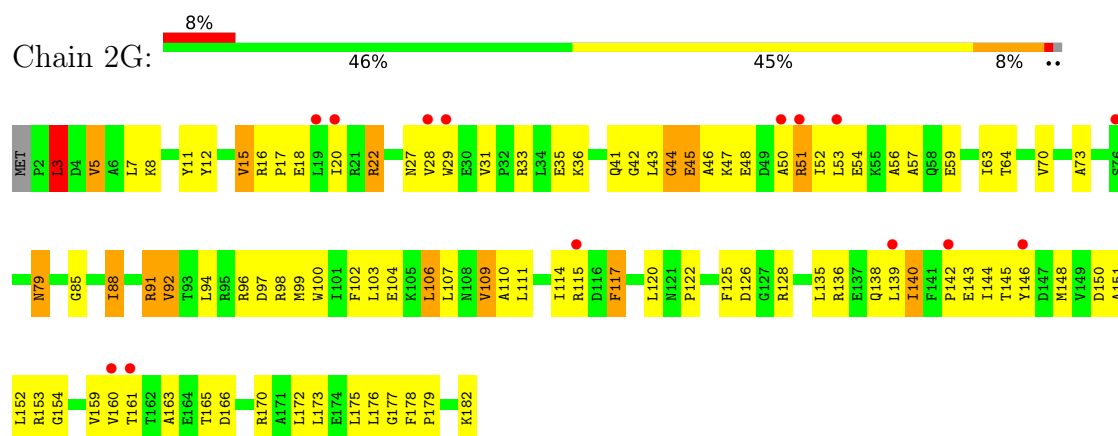
- Molecule 5: 50S ribosomal protein L4



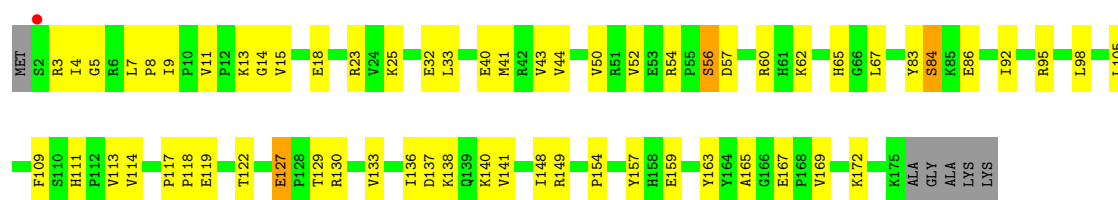
- Molecule 6: 50S ribosomal protein L5



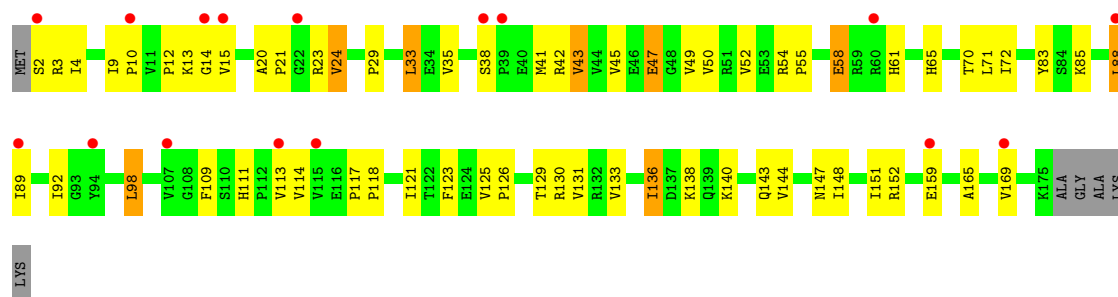
- Molecule 6: 50S ribosomal protein L5



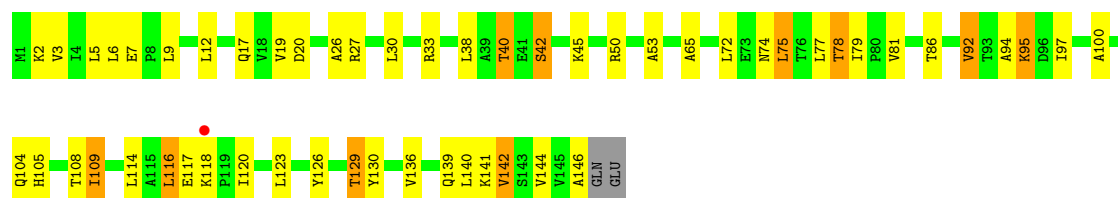
- Molecule 7: 50S ribosomal protein L6



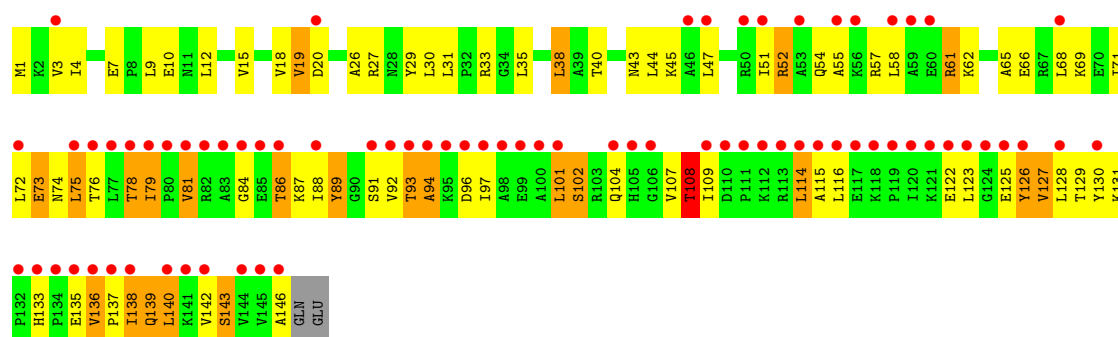
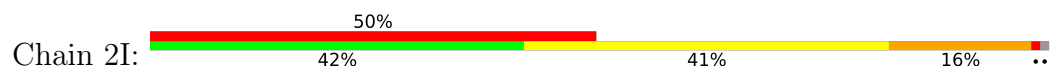
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9

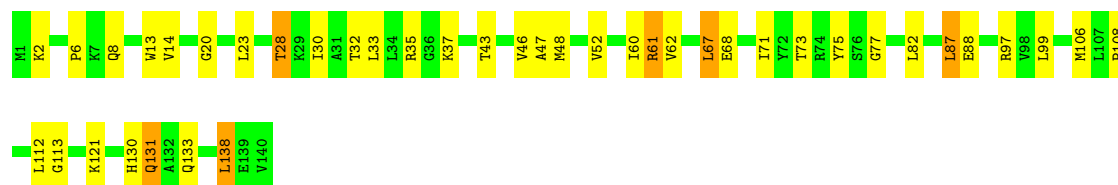


• Molecule 8: 50S ribosomal protein L9

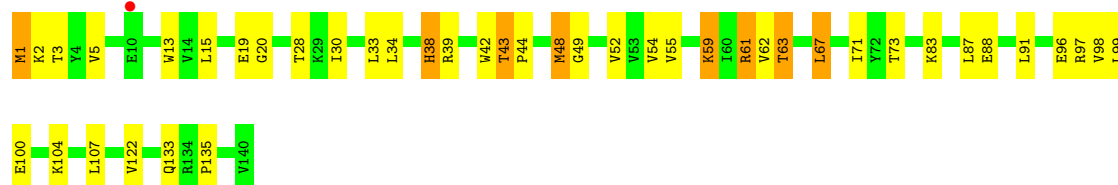


• Molecule 9: 50S ribosomal protein L13

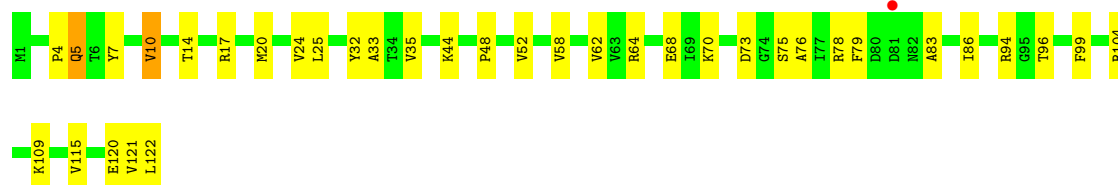




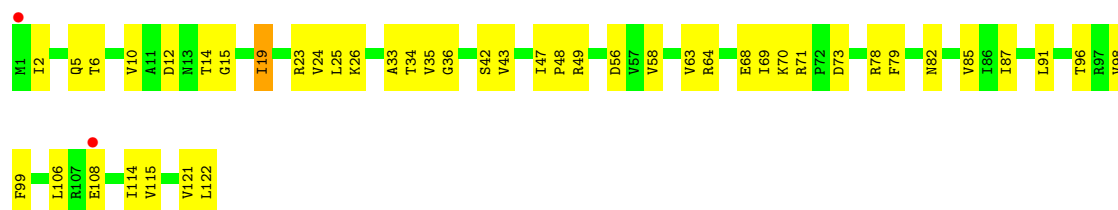
• Molecule 9: 50S ribosomal protein L13



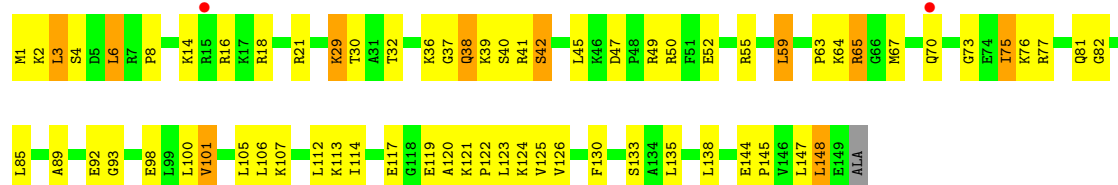
• Molecule 10: 50S ribosomal protein L14



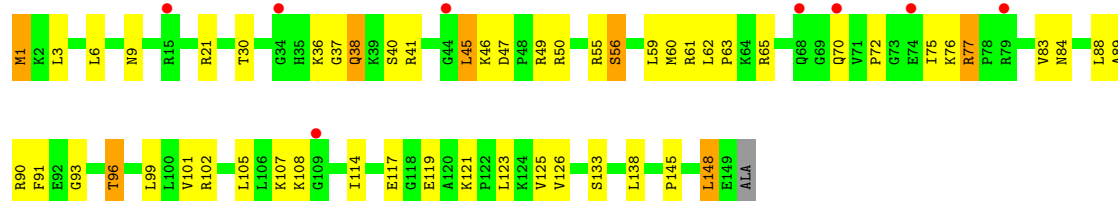
• Molecule 10: 50S ribosomal protein L14



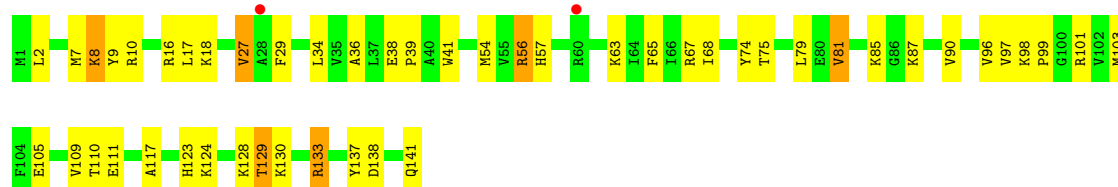
• Molecule 11: 50S ribosomal protein L15



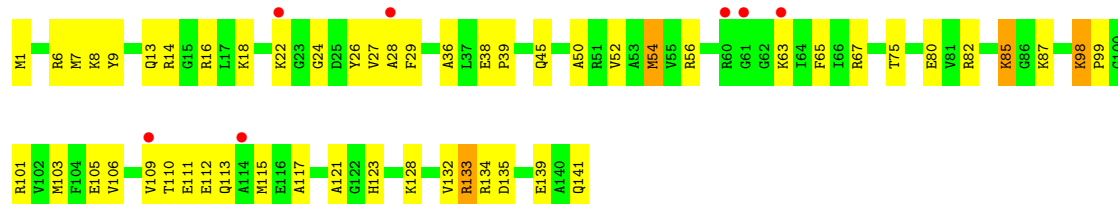
• Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17



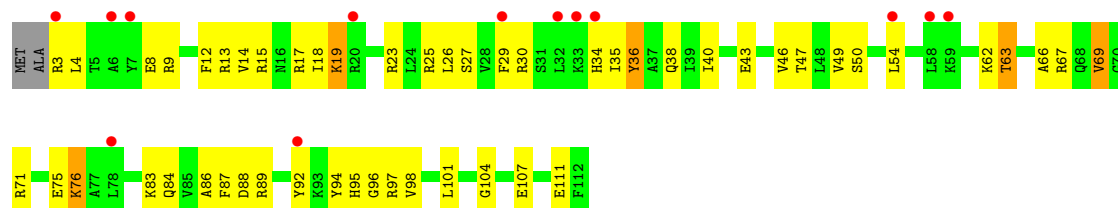
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  62% 35% ..



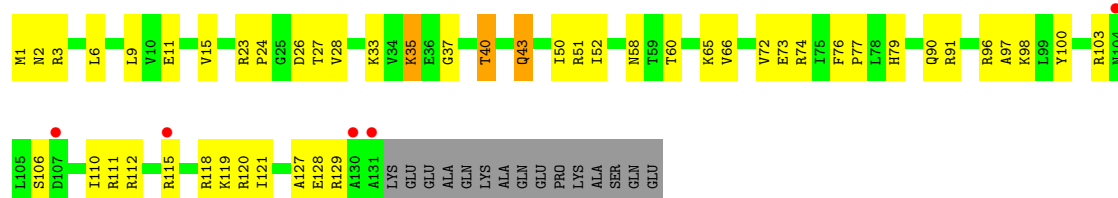
• Molecule 14: 50S ribosomal protein L18

Chain 2S:  12% 52% 42% ..



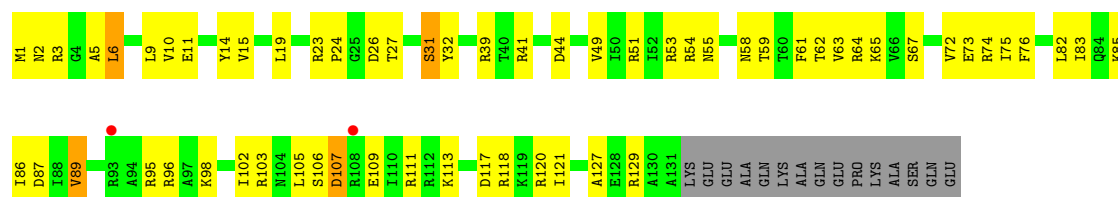
• Molecule 15: 50S ribosomal protein L19

Chain 1T:  3% 56% 32% 10%



• Molecule 15: 50S ribosomal protein L19

Chain 2T:  % 48% 39% 10%

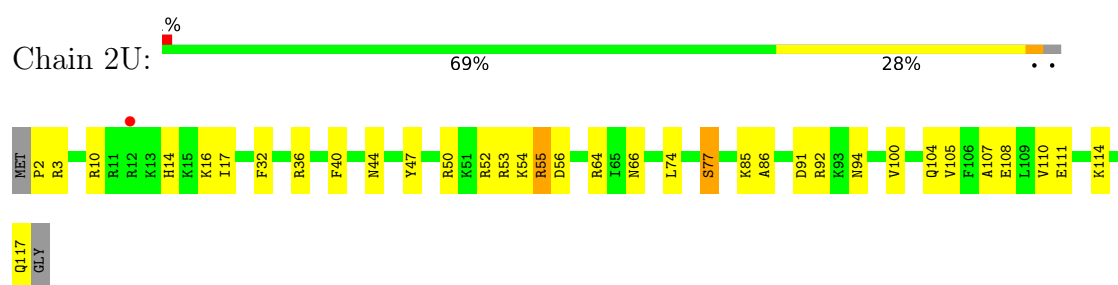


• Molecule 16: 50S ribosomal protein L20

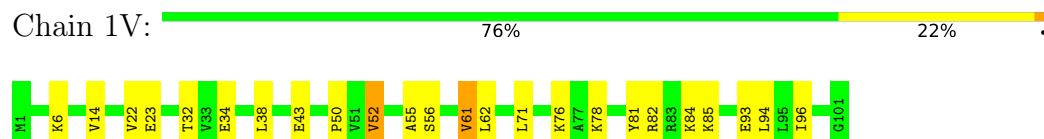
Chain 1U:  % 75% 20%



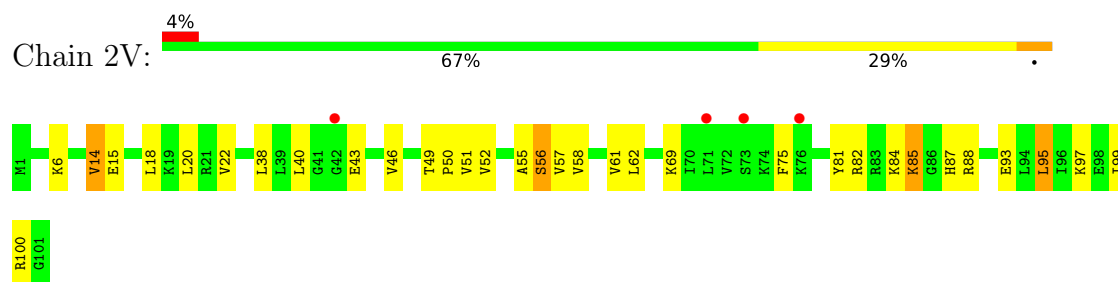
• Molecule 16: 50S ribosomal protein L20



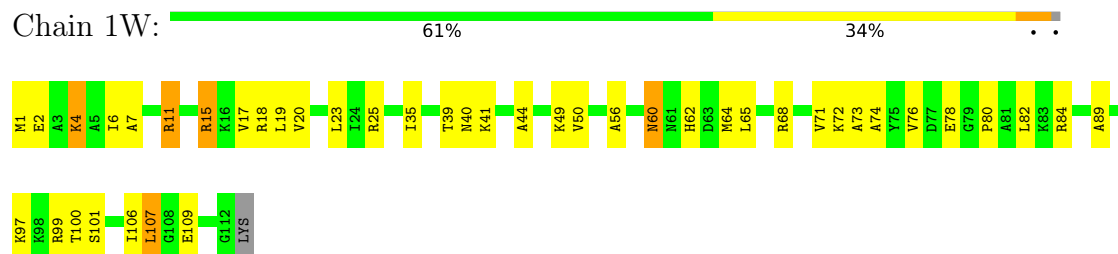
- Molecule 17: 50S ribosomal protein L21



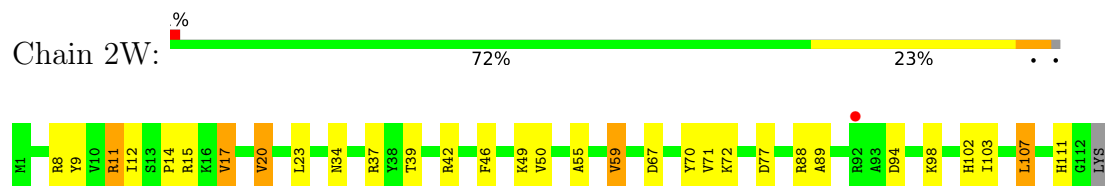
- Molecule 17: 50S ribosomal protein L21



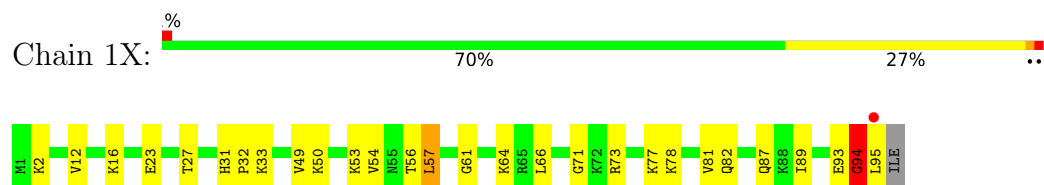
- Molecule 18: 50S ribosomal protein L22



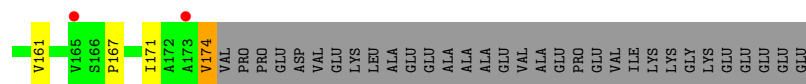
- Molecule 18: 50S ribosomal protein L22



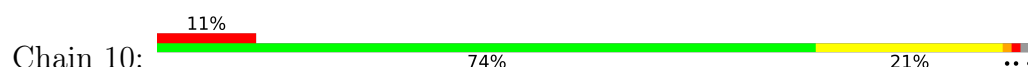
- Molecule 19: 50S ribosomal protein L23



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|--|-----|-----|------|------|--|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|--|------|--|------|
| S92 | E93 | D94 | | M98 | Y99 | V100 | P101 | | V105 | G106 | THR | PRO | ALA | GLY | VAL | ARG | ALA | GLY | GLY | VAL | LEU | GLN | GLU | I1E | H121 | R122 | D123 | I124 | L125 | K126 | V127 | V128 | S129 | P130 | R131 | | P134 | | E138 | V139 | D140 | V141 | S142 | L143 | L144 | F145 | L146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | K156 | L157 |
|-----|-----|-----|--|-----|-----|------|------|--|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|--|------|--|------|



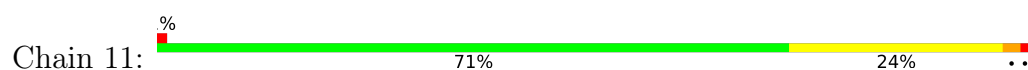
- Molecule 22: 50S ribosomal protein L27



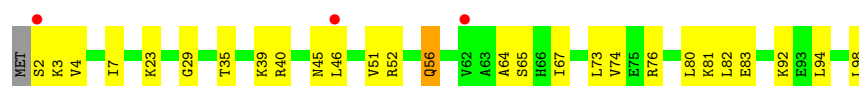
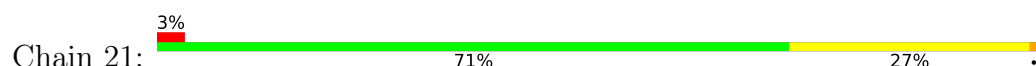
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



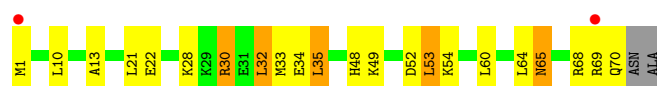
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



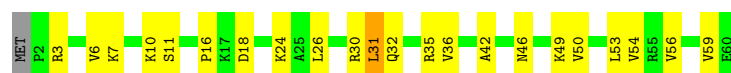
- Molecule 25: 50S ribosomal protein L30

Chain 13:  53% 40% 5% .



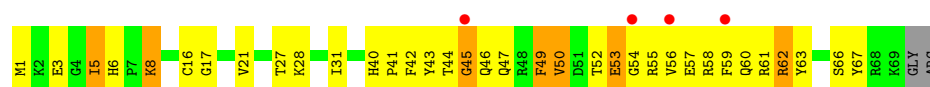
- Molecule 25: 50S ribosomal protein L30

Chain 23:  62% 35% ..



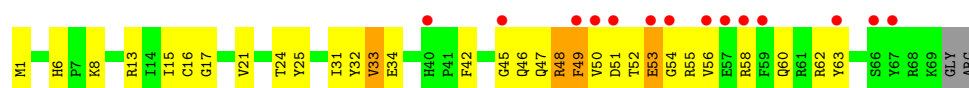
- Molecule 26: 50S ribosomal protein L31

Chain 14:  6% 48% 39% 10% .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  20% 54% 38% 6% .



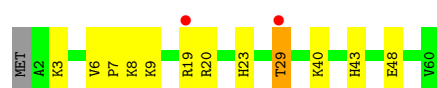
- Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 75% 20% ..



- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 78% 18% ..



- Molecule 28: 50S ribosomal protein L33

Chain 16:  59% 28% 11% .



- Molecule 28: 50S ribosomal protein L33



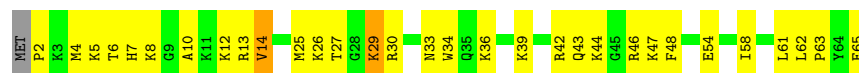
- Molecule 29: 50S ribosomal protein L34



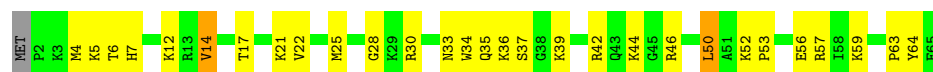
- Molecule 29: 50S ribosomal protein L34



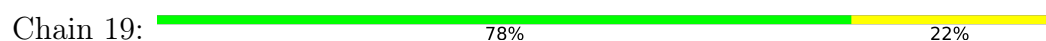
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

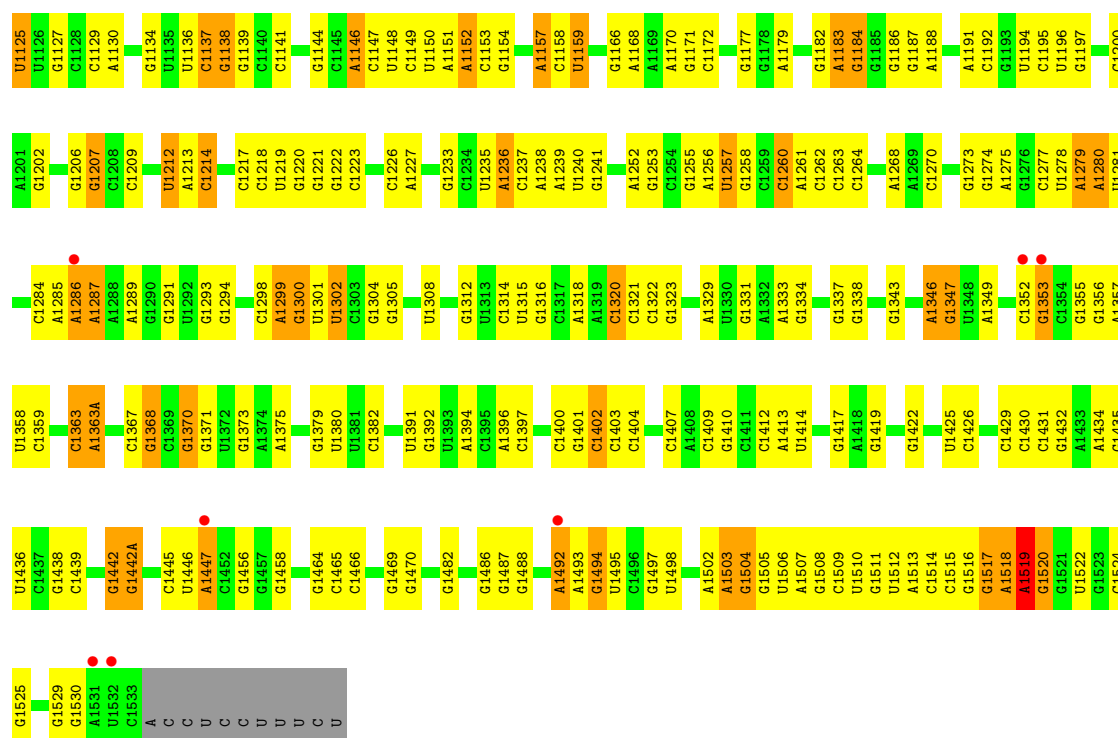


- Molecule 31: 50S ribosomal protein L36

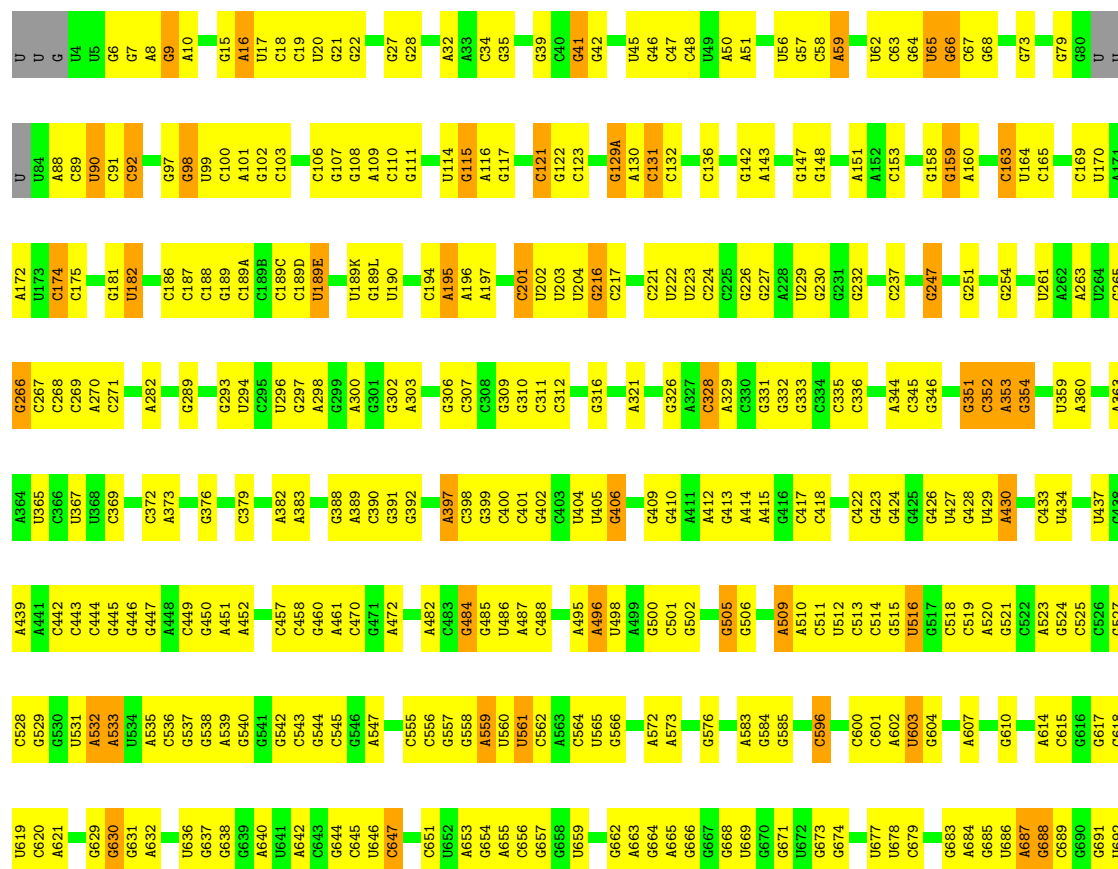


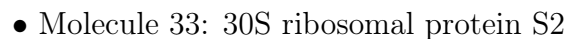
- Molecule 32: 16S Ribosomal RNA

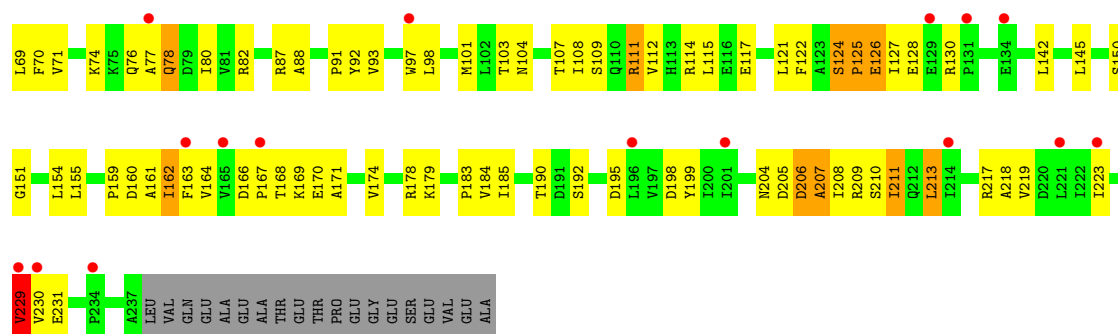




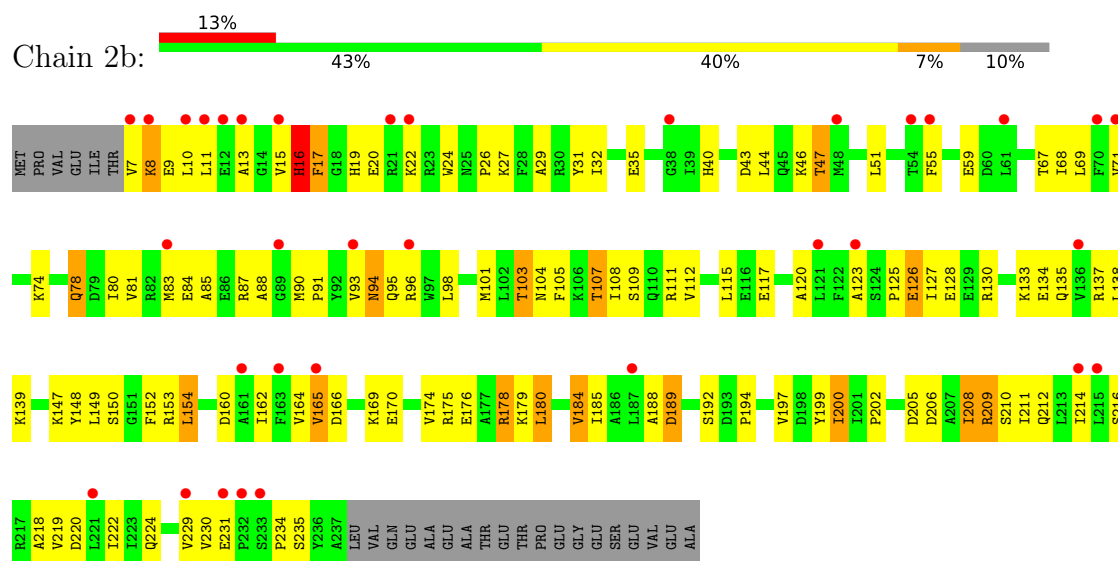
Molecule 32: 16S Ribosomal RNA



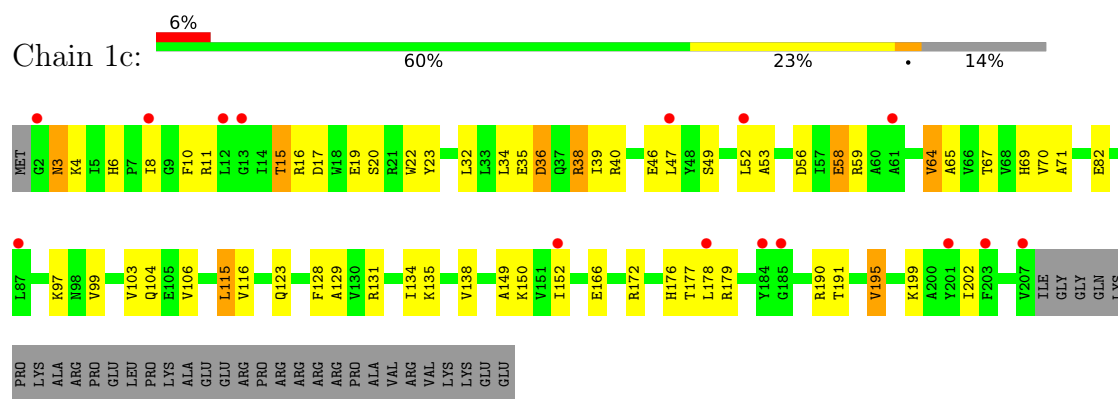




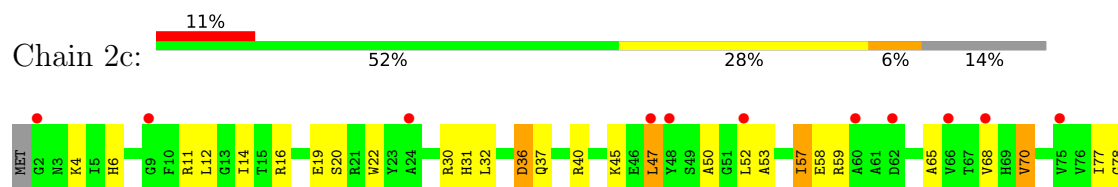
• Molecule 33: 30S ribosomal protein S2

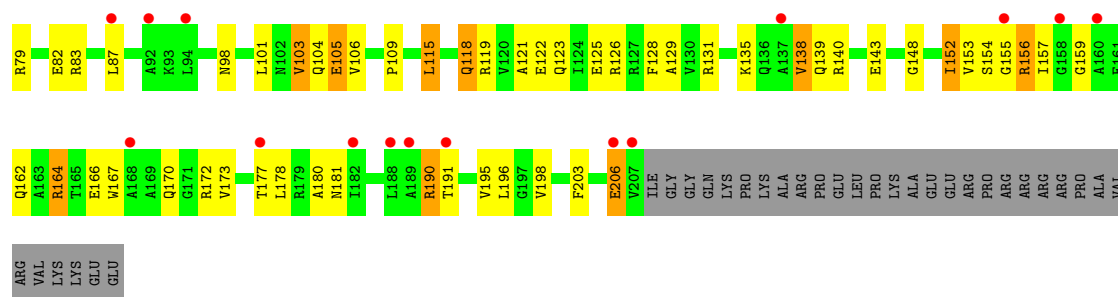


• Molecule 34: 30S ribosomal protein S3

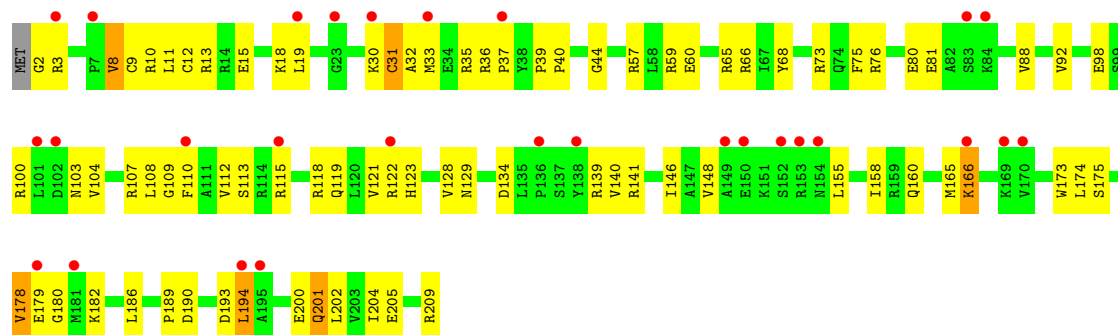


• Molecule 34: 30S ribosomal protein S3

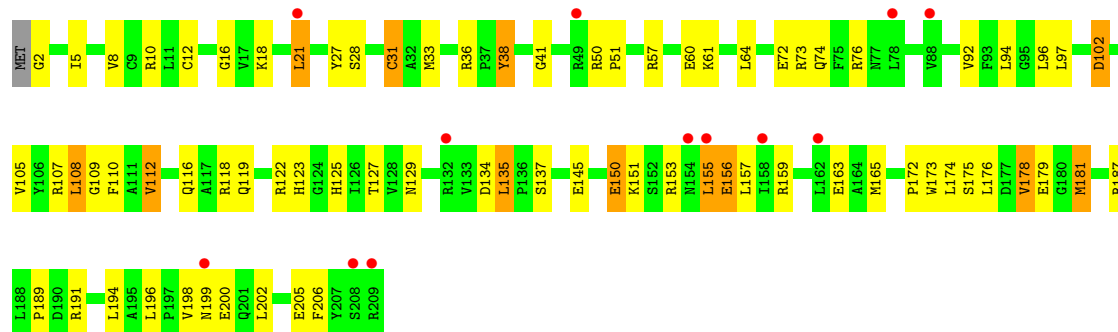




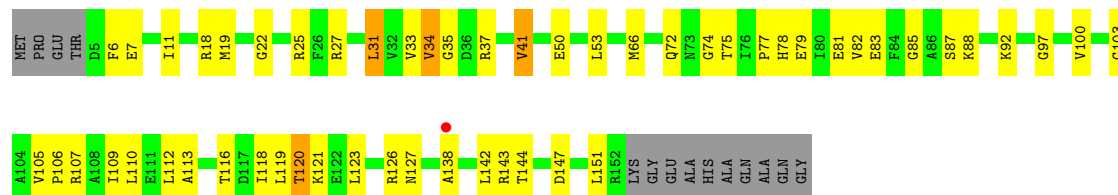
• Molecule 35: 30S ribosomal protein S4



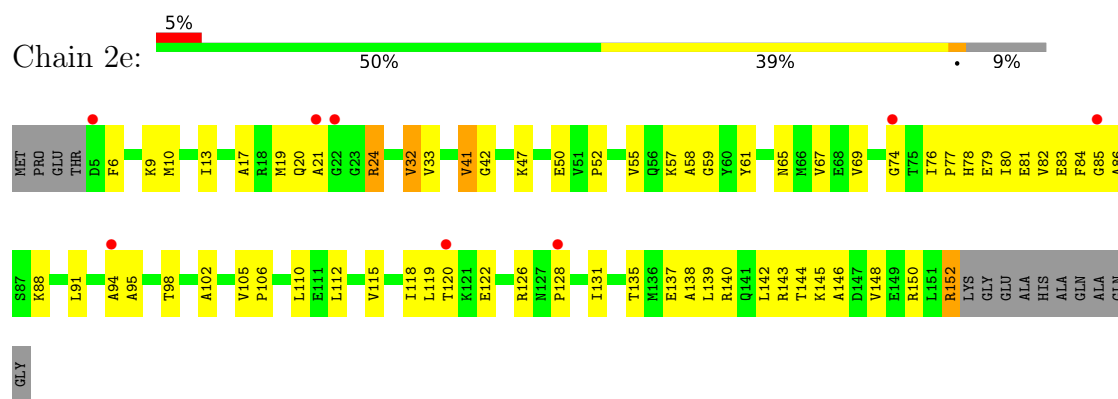
• Molecule 35: 30S ribosomal protein S4



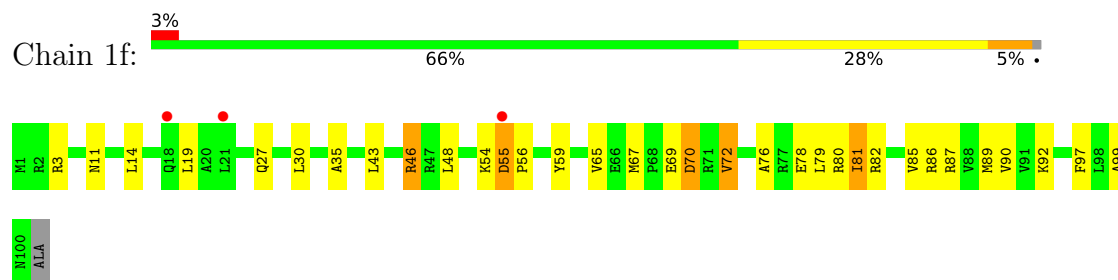
• Molecule 36: 30S ribosomal protein S5



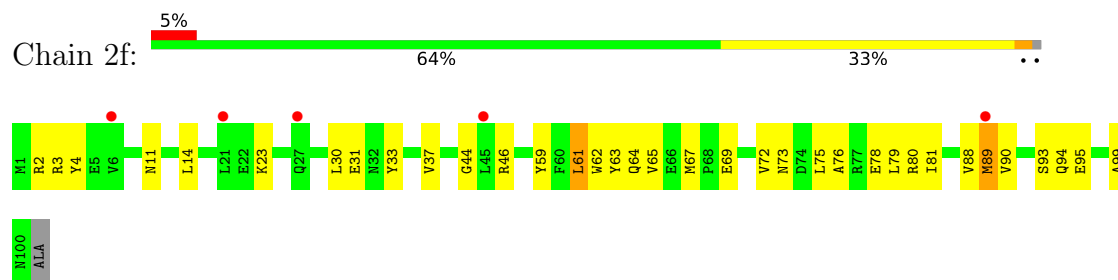
• Molecule 36: 30S ribosomal protein S5



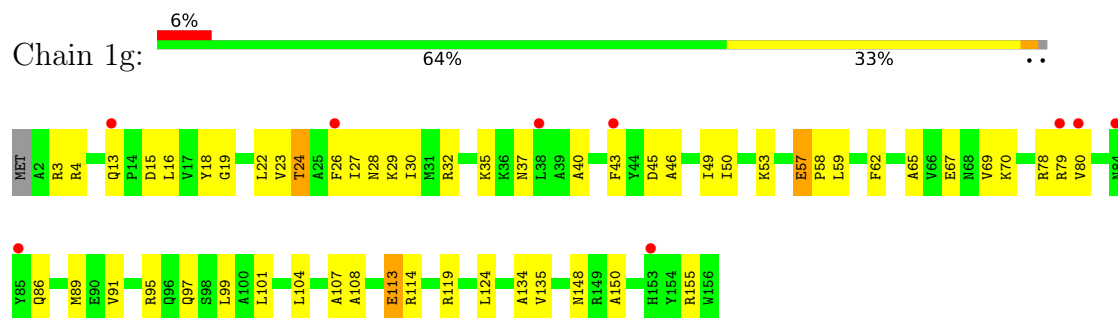
- Molecule 37: 30S ribosomal protein S6



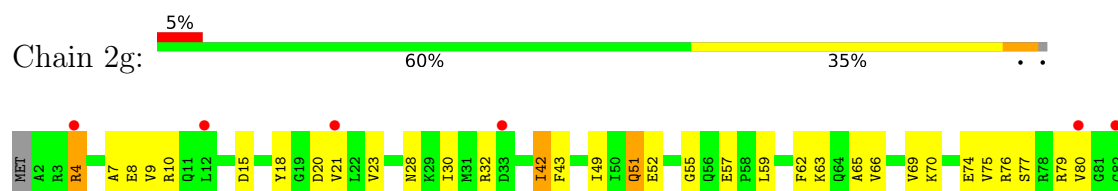
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

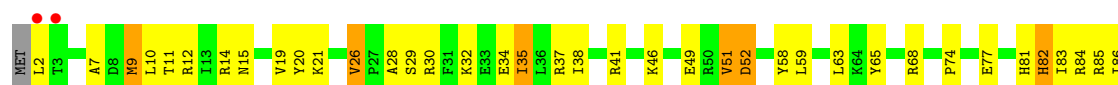


- Molecule 38: 30S ribosomal protein S7

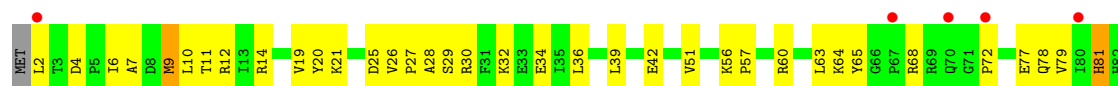




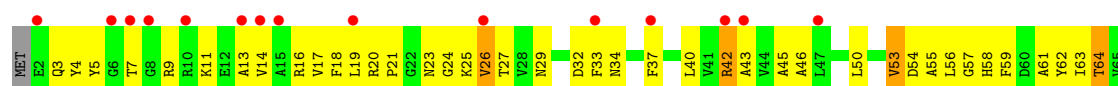
• Molecule 39: 30S ribosomal protein S8



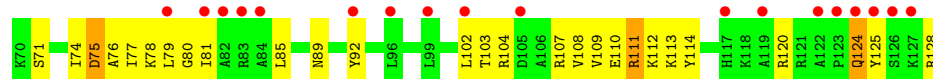
• Molecule 39: 30S ribosomal protein S8



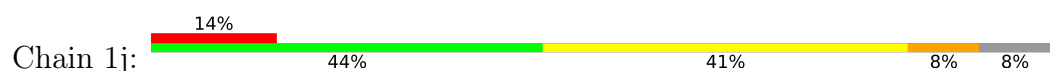
• Molecule 40: 30S ribosomal protein S9



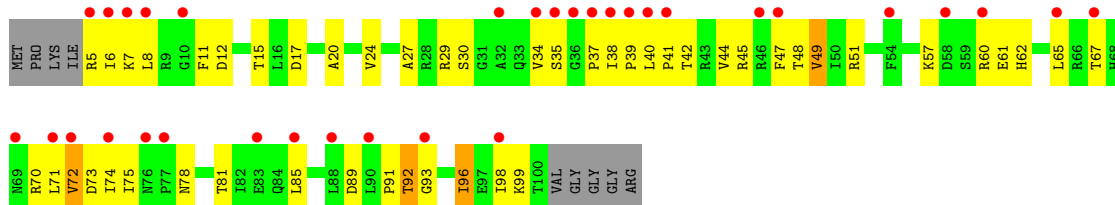
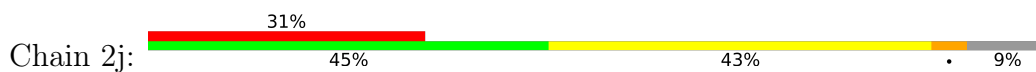
• Molecule 40: 30S ribosomal protein S9



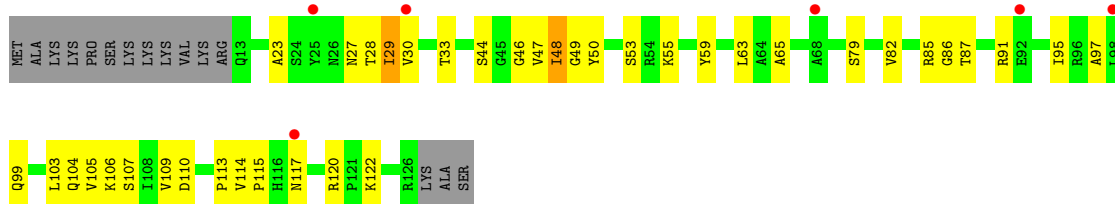
• Molecule 41: 30S ribosomal protein S10



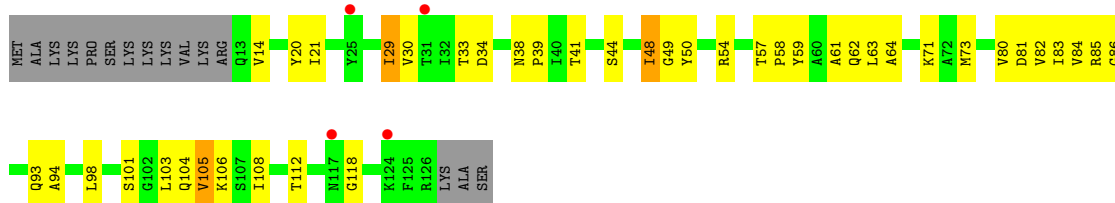
- Molecule 41: 30S ribosomal protein S10



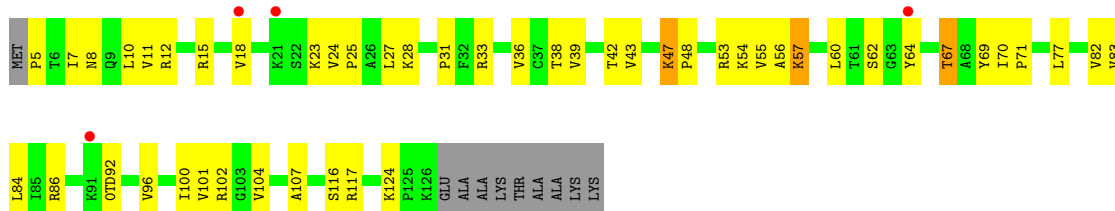
- Molecule 42: 30S ribosomal protein S11



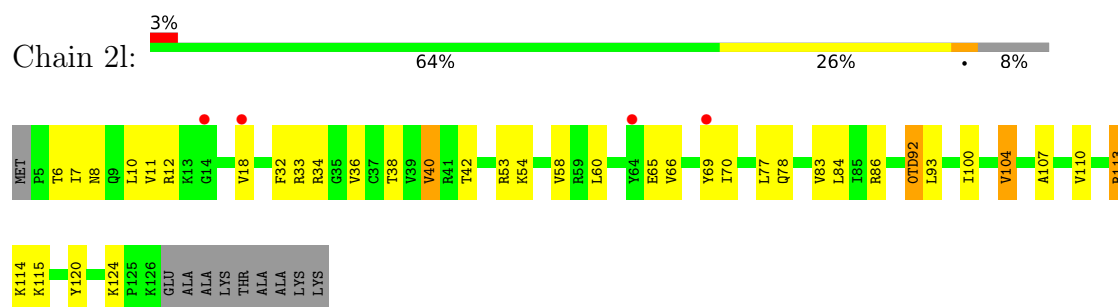
- Molecule 42: 30S ribosomal protein S11



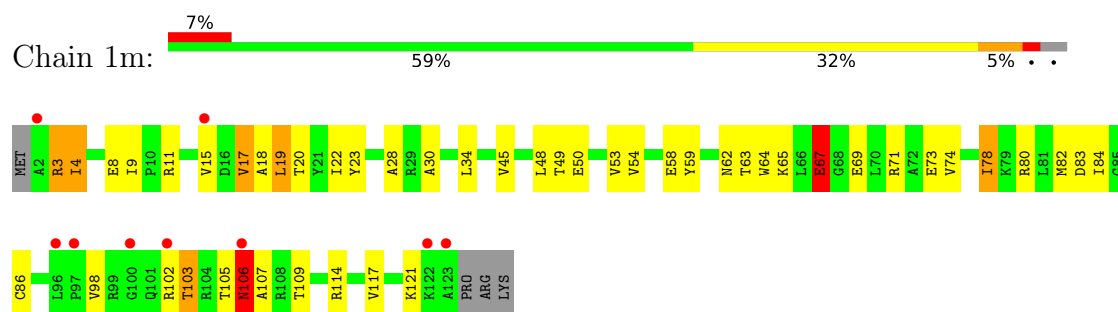
- Molecule 43: 30S ribosomal protein S12



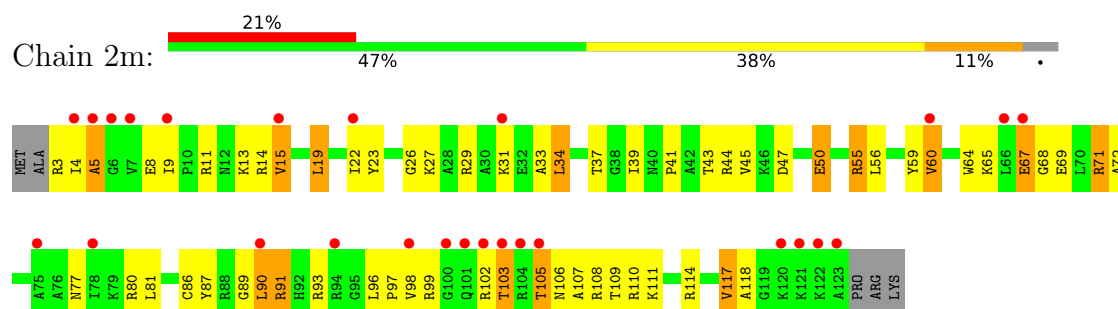
- Molecule 43: 30S ribosomal protein S12



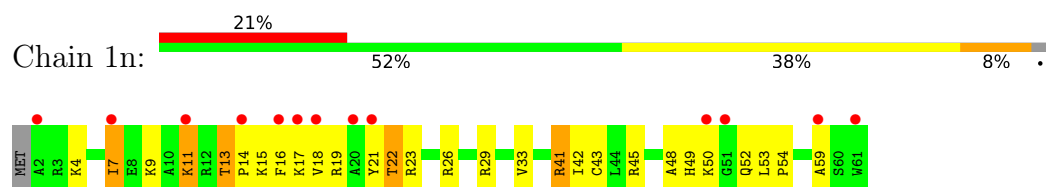
- Molecule 44: 30S ribosomal protein S13



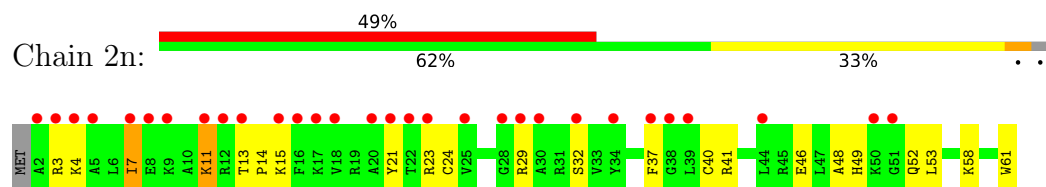
- Molecule 44: 30S ribosomal protein S13



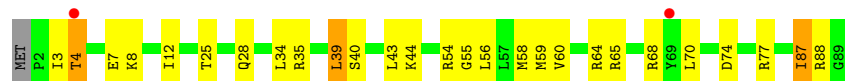
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



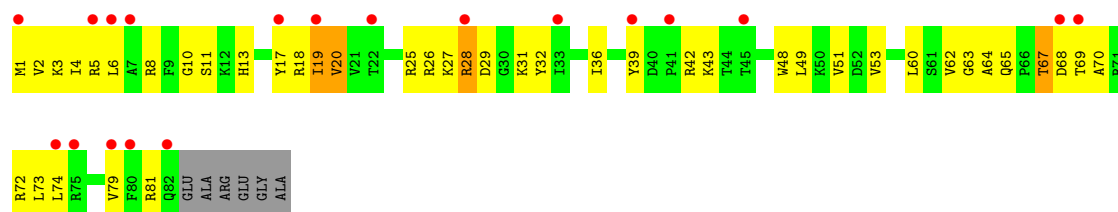
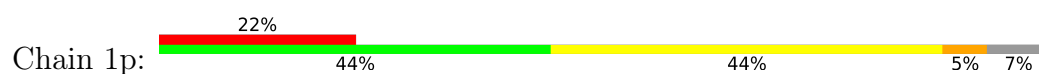
- Molecule 46: 30S ribosomal protein S15



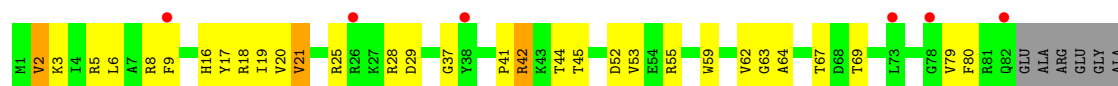
- Molecule 46: 30S ribosomal protein S15



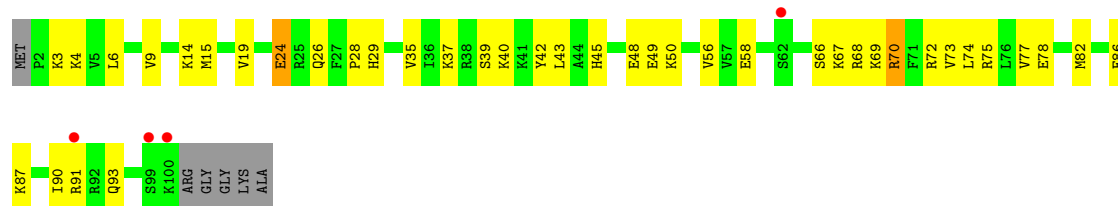
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

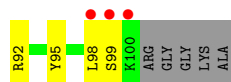


- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17





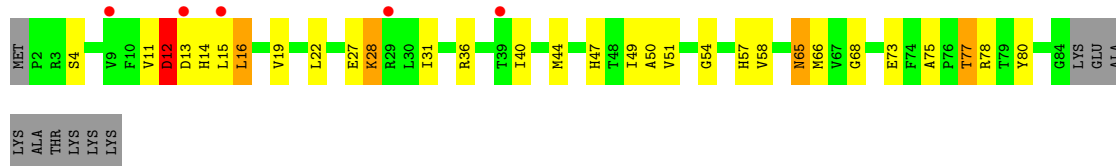
- Molecule 49: 30S ribosomal protein S18



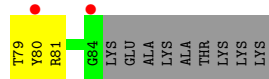
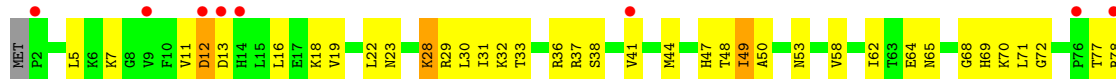
- Molecule 49: 30S ribosomal protein S18



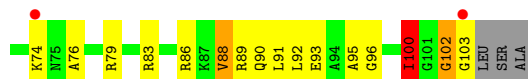
- Molecule 50: 30S ribosomal protein S19



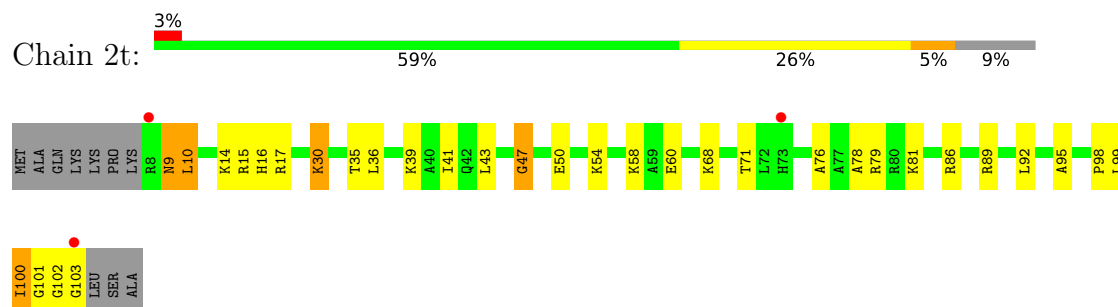
- Molecule 50: 30S ribosomal protein S19



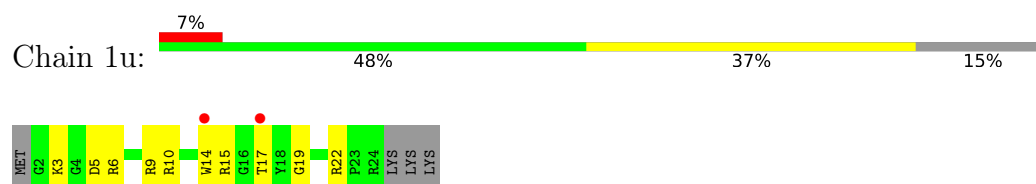
- Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



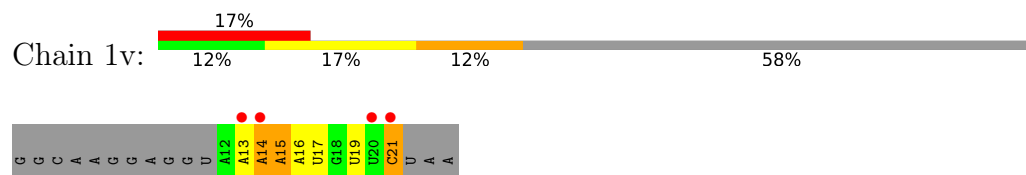
• Molecule 52: 30S ribosomal protein Thx



• Molecule 52: 30S ribosomal protein Thx



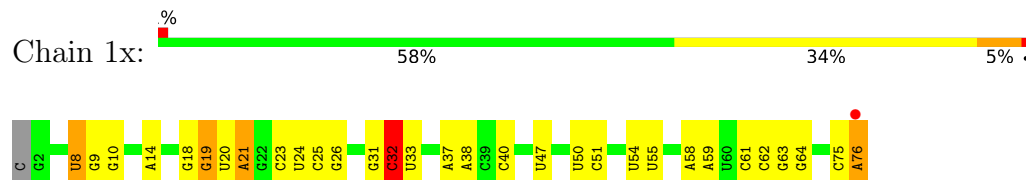
• Molecule 53: mRNA



• Molecule 53: mRNA



• Molecule 54: 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	208.33Å 447.60Å 612.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.46 – 2.80 75.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (75.46-2.80) 98.3 (75.46-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.225 , 0.276 0.226 , 0.275	Depositor DCC
R_{free} test set	68487 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292670	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 2MA, OMG, 4OC, UR3, MG, V7A, 0TD, 5MC, MA6, SF4, ZN, M2G, 2MG, 5MU, 7MG, 2MU, 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	0.30	0/69009	0.46	1/107712 (0.0%)
1	2A	0.23	0/67293	0.41	2/105034 (0.0%)
2	1B	0.25	0/2882	0.41	0/4494
2	2B	0.19	0/2879	0.39	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.24	0/2186	0.46	0/2944
4	1E	0.27	0/1592	0.52	0/2149
4	2E	0.22	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.22	0/1448	0.45	0/1957
6	2G	0.20	0/1453	0.46	0/1963
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.22	0/1112	0.44	0/1514
8	2I	2.31	2/1079 (0.2%)	0.77	4/1475 (0.3%)
9	1N	0.26	0/1144	0.46	0/1543
9	2N	0.18	0/1144	0.40	0/1543
10	1O	0.26	0/943	0.51	0/1269
10	2O	0.23	0/943	0.47	0/1269
11	1P	0.28	0/1152	0.56	0/1533
11	2P	0.22	0/1152	0.50	0/1533
12	1Q	0.27	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.42	0/1527
13	1R	0.28	0/982	0.48	0/1312
13	2R	0.20	0/982	0.44	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.23	0/1097	0.44	0/1468
16	1U	0.31	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.43	0/1301
17	1V	0.24	0/782	0.46	0/1049
17	2V	0.19	0/782	0.40	0/1049
18	1W	0.28	0/897	0.45	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.27	0/764	0.52	2/1025 (0.2%)
19	2X	0.20	0/764	0.49	2/1025 (0.2%)
20	1Y	0.25	0/819	0.47	0/1095
20	2Y	0.19	0/819	0.41	0/1095
21	1Z	0.23	0/1267	0.48	0/1717
21	2Z	0.20	0/1299	0.46	0/1763
22	10	0.28	0/662	0.49	0/881
22	20	0.22	0/662	0.48	0/881
23	11	0.26	0/762	0.46	0/1014
23	21	0.25	0/762	0.44	0/1014
24	12	0.25	0/590	0.44	0/781
24	22	0.19	0/590	0.37	0/781
25	13	0.26	0/474	0.46	0/635
25	23	0.25	0/469	0.46	0/630
26	14	0.27	0/565	0.58	0/761
26	24	0.27	0/545	0.65	1/737 (0.1%)
27	15	0.32	0/469	0.53	0/635
27	25	0.23	0/469	0.41	0/635
28	16	0.29	0/460	0.51	0/613
28	26	0.20	0/456	0.42	0/608
29	17	0.30	0/426	0.53	0/561
29	27	0.24	0/426	0.48	0/561
30	18	0.29	0/525	0.53	0/691
30	28	0.22	0/525	0.42	0/691
31	19	0.25	0/310	0.50	0/407
31	29	0.20	0/310	0.45	0/407
32	1a	0.35	10/35795 (0.0%)	0.40	2/55864 (0.0%)
32	2a	0.19	0/35886	0.38	0/56005
33	1b	0.22	0/1881	0.50	0/2542
33	2b	0.23	0/1860	0.48	0/2518
34	1c	0.18	0/1572	0.39	0/2126
34	2c	0.21	0/1566	0.48	1/2119 (0.0%)
35	1d	0.21	0/1685	0.46	0/2262
35	2d	0.20	0/1704	0.42	0/2284
36	1e	0.21	0/1145	0.44	0/1543
36	2e	0.21	0/1149	0.47	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.19	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.43	0/1679
38	2g	0.18	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.17	0/1108	0.40	0/1494
40	1i	0.22	0/1002	0.48	0/1346
40	2i	0.21	0/997	0.50	0/1343
41	1j	0.19	0/722	0.42	0/982
41	2j	0.20	0/727	0.44	0/988
42	1k	0.20	0/844	0.49	0/1145
42	2k	0.19	0/848	0.47	1/1149 (0.1%)
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.20	0/937	0.42	0/1260
44	1m	0.23	0/961	0.49	0/1290
44	2m	0.21	0/953	0.55	1/1279 (0.1%)
45	1n	0.19	0/501	0.44	0/664
45	2n	0.20	0/501	0.46	0/664
46	1o	0.19	0/739	0.40	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.21	0/697	0.44	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.19	0/836	0.45	0/1117
48	2q	0.20	0/836	0.41	0/1117
49	1r	0.20	0/560	0.42	0/746
49	2r	0.19	0/560	0.41	0/746
50	1s	0.20	0/667	0.48	0/900
50	2s	0.23	0/661	0.55	0/893
51	1t	0.20	0/730	0.45	0/965
51	2t	0.21	0/729	0.49	0/965
52	1u	0.19	0/203	0.47	0/266
52	2u	0.23	0/203	0.49	0/266
53	1v	0.23	0/238	0.38	0/368
53	2v	0.27	0/126	0.41	0/195
54	1x	0.26	0/1725	0.41	0/2689
54	2x	0.24	0/1725	0.39	0/2689
All	All	0.29	12/310063 (0.0%)	0.43	19/463821 (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
21	1Z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	1a	0	1
33	1b	0	2
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2I	89	TYR	CE1-CZ	55.02	2.70	1.38
8	2I	89	TYR	CD2-CE2	51.24	2.92	1.38
32	1a	55	A	C5-C4	35.15	2.09	1.38
32	1a	55	A	N7-C5	15.61	1.70	1.39
32	1a	55	A	C8-N7	15.23	1.62	1.31

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2I	89	TYR	CZ-CE2-CD2	-11.38	99.12	119.60
8	2I	89	TYR	CD1-CE1-CZ	10.32	138.18	119.60
26	24	54	GLY	N-CA-C	-9.43	103.85	115.08
8	2I	89	TYR	CG-CD2-CE2	8.93	134.59	121.20
32	1a	357	G	OP1-P-O3'	-8.67	81.98	108.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	136	PHE	Peptide
32	1a	55	A	Sidechain
33	1b	122	PHE	Peptide
33	1b	126	GLU	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	31187	997	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	60322	0	30423	1063	0
2	1B	2577	0	1305	39	0
2	2B	2575	0	1303	60	0
3	1D	2136	0	2218	69	0
3	2D	2136	0	2218	66	0
4	1E	1559	0	1618	37	0
4	2E	1559	0	1618	62	0
5	1F	1584	0	1625	61	0
5	2F	1580	0	1619	59	0
6	1G	1423	0	1436	42	0
6	2G	1428	0	1438	70	0
7	1H	1330	0	1407	35	0
7	2H	1330	0	1407	33	0
8	1I	1097	0	1140	38	0
8	2I	1064	0	1082	60	12
9	1N	1117	0	1184	21	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	24	0
10	2O	933	0	996	38	0
11	1P	1135	0	1212	61	0
11	2P	1135	0	1212	46	0
12	1Q	1122	0	1179	39	0
12	2Q	1122	0	1179	37	0
13	1R	968	0	1033	23	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	36	0
14	2S	870	0	923	41	0
15	1T	1091	0	1151	33	0
15	2T	1083	0	1136	45	0
16	1U	959	0	1019	22	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	12	0
17	2V	771	0	830	22	0
18	1W	886	0	940	28	0
18	2W	886	0	940	22	0
19	1X	750	0	814	17	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	21	0
20	2Y	806	0	881	21	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	52	0
22	10	653	0	674	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	21	0
23	11	755	0	826	19	0
23	21	755	0	826	17	0
24	12	588	0	643	11	0
24	22	588	0	643	14	0
25	13	469	0	518	17	0
25	23	464	0	514	12	0
26	14	552	0	533	26	0
26	24	532	0	503	24	0
27	15	455	0	465	10	0
27	25	455	0	465	9	0
28	16	453	0	473	16	0
28	26	449	0	469	9	0
29	17	418	0	467	13	0
29	27	418	0	467	13	0
30	18	517	0	582	34	0
30	28	517	0	582	25	0
31	19	307	0	335	5	0
31	29	307	0	335	11	0
32	1a	32246	0	16295	626	12
32	2a	32327	0	16339	656	0
33	1b	1846	0	1867	77	0
33	2b	1825	0	1828	70	0
34	1c	1548	0	1535	45	0
34	2c	1542	0	1517	50	0
35	1d	1655	0	1672	67	0
35	2d	1674	0	1714	59	0
36	1e	1129	0	1185	42	0
36	2e	1133	0	1191	48	0
37	1f	810	0	804	26	0
37	2f	816	0	808	20	0
38	1g	1231	0	1238	38	0
38	2g	1235	0	1249	42	0
39	1h	1088	0	1126	44	0
39	2h	1088	0	1126	44	0
40	1i	983	0	986	50	0
40	2i	978	0	966	54	0
41	1j	709	0	650	44	0
41	2j	714	0	672	37	0
42	1k	829	0	825	25	0
42	2k	833	0	836	23	0
43	1l	932	0	981	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	23	0
44	1m	951	0	995	30	0
44	2m	943	0	981	49	0
45	1n	492	0	529	28	0
45	2n	492	0	529	17	0
46	1o	728	0	760	19	0
46	2o	728	0	760	24	0
47	1p	681	0	697	32	0
47	2p	677	0	686	22	0
48	1q	823	0	891	28	0
48	2q	823	0	891	26	0
49	1r	555	0	618	15	0
49	2r	555	0	618	9	0
50	1s	652	0	662	28	0
50	2s	646	0	644	28	0
51	1t	728	0	798	28	0
51	2t	727	0	796	25	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	213	0	108	5	0
53	2v	113	0	54	1	0
54	1x	1625	0	829	19	0
54	2x	1625	0	829	21	0
55	10	5	0	0	0	0
55	11	4	0	0	0	0
55	12	2	0	0	0	0
55	13	3	0	0	0	0
55	15	5	0	0	0	0
55	16	1	0	0	0	0
55	17	4	0	0	0	0
55	18	6	0	0	0	0
55	19	1	0	0	0	0
55	1A	1117	0	0	0	0
55	1B	35	0	0	0	0
55	1D	13	0	0	0	0
55	1E	11	0	0	0	0
55	1F	11	0	0	0	0
55	1G	4	0	0	0	0
55	1N	4	0	0	0	0
55	1O	4	0	0	0	0
55	1P	3	0	0	0	0
55	1Q	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1R	2	0	0	0	0
55	1S	1	0	0	0	0
55	1T	3	0	0	0	0
55	1U	7	0	0	0	0
55	1V	4	0	0	0	0
55	1W	5	0	0	0	0
55	1X	6	0	0	0	0
55	1Y	4	0	0	0	0
55	1Z	2	0	0	0	0
55	1a	234	0	0	0	0
55	1b	1	0	0	0	0
55	1e	2	0	0	0	0
55	1f	2	0	0	0	0
55	1l	4	0	0	0	0
55	1n	2	0	0	0	0
55	1t	1	0	0	0	0
55	1v	2	0	0	0	0
55	1x	13	0	0	0	0
55	20	1	0	0	0	0
55	23	1	0	0	0	0
55	25	2	0	0	0	0
55	26	1	0	0	0	0
55	27	1	0	0	0	0
55	28	3	0	0	0	0
55	2A	862	0	0	0	0
55	2B	19	0	0	0	0
55	2D	3	0	0	0	0
55	2E	9	0	0	0	0
55	2F	6	0	0	0	0
55	2G	1	0	0	0	0
55	2N	2	0	0	0	0
55	2O	2	0	0	0	0
55	2P	2	0	0	0	0
55	2Q	4	0	0	0	0
55	2R	2	0	0	0	0
55	2T	3	0	0	0	0
55	2U	2	0	0	0	0
55	2V	3	0	0	0	0
55	2W	2	0	0	0	0
55	2X	2	0	0	0	0
55	2Z	1	0	0	0	0
55	2a	209	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	2d	2	0	0	0	0
55	2e	1	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	2l	3	0	0	0	0
55	2p	1	0	0	0	0
55	2q	1	0	0	0	0
55	2r	1	0	0	0	0
55	2t	1	0	0	0	0
55	2x	5	0	0	0	0
56	14	1	0	0	0	0
56	15	1	0	0	0	0
56	16	1	0	0	0	0
56	19	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1n	1	0	0	0	0
56	24	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	29	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2n	1	0	0	0	0
57	1a	35	0	0	2	0
57	2a	35	0	0	4	0
58	1d	8	0	0	3	0
58	2d	8	0	0	1	0
59	10	8	0	0	1	0
59	11	7	0	0	1	0
59	12	1	0	0	0	0
59	13	4	0	0	0	0
59	15	7	0	0	0	0
59	16	2	0	0	0	0
59	17	6	0	0	3	0
59	18	9	0	0	1	0
59	1A	1716	0	0	124	0
59	1B	47	0	0	1	0
59	1D	21	0	0	3	0
59	1E	25	0	0	1	0
59	1F	13	0	0	0	0
59	1G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1H	2	0	0	0	0
59	1I	2	0	0	0	0
59	1N	3	0	0	1	0
59	1O	7	0	0	0	0
59	1P	17	0	0	1	0
59	1Q	6	0	0	0	0
59	1R	9	0	0	0	0
59	1S	1	0	0	0	0
59	1T	8	0	0	0	0
59	1U	13	0	0	1	0
59	1V	9	0	0	0	0
59	1W	8	0	0	0	0
59	1X	6	0	0	0	0
59	1Y	2	0	0	1	0
59	1a	294	0	0	23	0
59	1b	1	0	0	0	0
59	1d	3	0	0	0	0
59	1e	1	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1l	4	0	0	0	0
59	1m	1	0	0	0	0
59	1o	1	0	0	0	0
59	1q	2	0	0	0	0
59	1v	4	0	0	0	0
59	1x	17	0	0	2	0
59	20	3	0	0	0	0
59	21	8	0	0	0	0
59	22	1	0	0	0	0
59	25	1	0	0	0	0
59	27	1	0	0	0	0
59	28	3	0	0	0	0
59	29	1	0	0	0	0
59	2A	867	0	0	80	0
59	2B	14	0	0	3	0
59	2D	16	0	0	0	0
59	2E	8	0	0	1	0
59	2F	13	0	0	0	0
59	2I	1	0	0	0	0
59	2N	1	0	0	0	0
59	2O	1	0	0	0	0
59	2P	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2Q	2	0	0	0	0
59	2R	2	0	0	0	0
59	2T	4	0	0	0	0
59	2U	3	0	0	1	0
59	2W	5	0	0	1	0
59	2X	2	0	0	0	0
59	2Z	1	0	0	0	0
59	2a	146	0	0	11	0
59	2g	1	0	0	0	0
59	2j	2	0	0	0	0
59	2l	4	0	0	1	0
59	2p	1	0	0	0	0
59	2r	1	0	0	0	0
59	2t	1	0	0	0	0
59	2v	1	0	0	0	0
59	2x	6	0	0	0	0
All	All	292670	0	193346	5696	12

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 13.

The worst 5 of 5696 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)
32:1a:55:A:C5	32:1a:55:A:N7	1.70	1.56
32:1a:55:A:C5	32:1a:55:A:C4	2.09	1.39
1:1A:1082:U:H3	1:1A:1086:A:N6	1.39	1.17
1:2A:2138:C:N4	1:2A:2153:G:H1	1.51	1.07
1:1A:1059:G:H1	1:1A:1079:C:N4	1.56	1.03

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:55:A:C5	8:2I:89:TYR:CZ[2_655]	1.80	0.40
32:1a:55:A:C4	8:2I:89:TYR:CZ[2_655]	1.82	0.38
32:1a:55:A:C4	8:2I:89:TYR:CE2[2_655]	1.95	0.25
32:1a:55:A:C5	8:2I:89:TYR:CE2[2_655]	1.98	0.22
32:1a:55:A:C8	8:2I:89:TYR:CE1[2_655]	2.01	0.19

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
3	2D	273/276 (99%)	251 (92%)	21 (8%)	1 (0%)	30	60
4	1E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	12	38
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	12	38
5	1F	201/210 (96%)	194 (96%)	4 (2%)	3 (2%)	8	28
5	2F	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	24	55
6	1G	179/182 (98%)	162 (90%)	13 (7%)	4 (2%)	5	19
6	2G	179/182 (98%)	148 (83%)	24 (13%)	7 (4%)	2	8
7	1H	172/180 (96%)	158 (92%)	14 (8%)	0	100	100
7	2H	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	18
8	1I	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	9	30
8	2I	144/148 (97%)	112 (78%)	26 (18%)	6 (4%)	2	7
9	1N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	47
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	47
10	1O	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	16	44
10	2O	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	16	44
11	1P	147/150 (98%)	134 (91%)	10 (7%)	3 (2%)	6	21
11	2P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	30
12	1Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	47
12	2Q	139/141 (99%)	124 (89%)	15 (11%)	0	100	100
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14	41
14	1S	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	14	41
14	2S	108/112 (96%)	101 (94%)	4 (4%)	3 (3%)	4	14
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	38
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	1W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	14	41
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	5	19
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	36
20	1Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
20	2Y	105/110 (96%)	93 (89%)	11 (10%)	1 (1%)	12	38
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	30
21	2Z	156/206 (76%)	128 (82%)	24 (15%)	4 (3%)	4	15
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	34
22	20	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	34
23	11	95/98 (97%)	91 (96%)	2 (2%)	2 (2%)	5	20
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	60 (88%)	8 (12%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	23
26	14	67/71 (94%)	56 (84%)	7 (10%)	4 (6%)	1	3
26	24	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	28
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	58 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	3	13
33	1b	229/256 (90%)	193 (84%)	29 (13%)	7 (3%)	3	12
33	2b	229/256 (90%)	199 (87%)	21 (9%)	9 (4%)	2	8
34	1c	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	24	55
34	2c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	8	28
35	1d	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	24	55
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	9	30
36	2e	146/162 (90%)	126 (86%)	18 (12%)	2 (1%)	9	30
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	9	31
38	2g	153/156 (98%)	132 (86%)	18 (12%)	3 (2%)	6	21
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	106 (85%)	17 (14%)	2 (2%)	7	27
40	2i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	44
41	1j	95/105 (90%)	77 (81%)	13 (14%)	5 (5%)	1	5
41	2j	94/105 (90%)	82 (87%)	8 (8%)	4 (4%)	2	7
42	1k	112/129 (87%)	101 (90%)	7 (6%)	4 (4%)	2	10
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	6	23
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	105 (88%)	14 (12%)	0	100	100
44	1m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	7	25
44	2m	119/126 (94%)	105 (88%)	11 (9%)	3 (2%)	4	16
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	25
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
47	1p	80/88 (91%)	68 (85%)	9 (11%)	3 (4%)	2	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	12	38
49	1r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	28
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	10	34
50	2s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	16
51	1t	94/106 (89%)	82 (87%)	7 (7%)	5 (5%)	1	5
51	2t	94/106 (89%)	82 (87%)	7 (7%)	5 (5%)	1	5
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	6
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
All	All	11368/12128 (94%)	10282 (90%)	942 (8%)	144 (1%)	9	31

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
5	1F	130	ALA
11	1P	36	LYS
11	1P	38	GLN
12	1Q	27	VAL

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%)	200 (93%)	15 (7%)	14	40
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26	61
4	1E	164/166 (99%)	152 (93%)	12 (7%)	13	38
4	2E	164/166 (99%)	148 (90%)	16 (10%)	7	25
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3	12
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	17
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	8
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	28
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	20
8	1I	113/124 (91%)	98 (87%)	15 (13%)	4	14
8	2I	105/124 (85%)	73 (70%)	32 (30%)	0	1
9	1N	118/119 (99%)	103 (87%)	15 (13%)	4	15
9	2N	118/119 (99%)	103 (87%)	15 (13%)	4	15
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	54
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	47
11	1P	115/116 (99%)	99 (86%)	16 (14%)	3	12
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	22
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	28
12	2Q	111/111 (100%)	99 (89%)	12 (11%)	6	21
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	21
13	2R	101/101 (100%)	93 (92%)	8 (8%)	11	35
14	1S	86/88 (98%)	82 (95%)	4 (5%)	23	57
14	2S	85/88 (97%)	72 (85%)	13 (15%)	3	10
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	46
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	34
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	51
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	37
17	1V	80/82 (98%)	75 (94%)	5 (6%)	16	45
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	24
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	35
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	29
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	64
19	2X	77/78 (99%)	69 (90%)	8 (10%)	7	22
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	17
20	2Y	85/91 (93%)	75 (88%)	10 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	119 (88%)	16 (12%)	5	17
21	2Z	137/179 (76%)	119 (87%)	18 (13%)	4	14
22	10	65/67 (97%)	61 (94%)	4 (6%)	16	45
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	45
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	54
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	29
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	16
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	21
25	13	51/52 (98%)	43 (84%)	8 (16%)	2	9
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	34
26	14	59/63 (94%)	46 (78%)	13 (22%)	1	3
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	10
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	17
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	34
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	13
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	34
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	38
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	38
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	65
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	37
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	73
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	48
33	1b	192/220 (87%)	170 (88%)	22 (12%)	5	18
33	2b	187/220 (85%)	151 (81%)	36 (19%)	1	5
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	22
34	2c	140/188 (74%)	115 (82%)	25 (18%)	2	6
35	1d	169/181 (93%)	153 (90%)	16 (10%)	8	26
35	2d	173/181 (96%)	153 (88%)	20 (12%)	5	18
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	45
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6	22
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8	27
38	1g	119/127 (94%)	115 (97%)	4 (3%)	32	68
38	2g	120/127 (94%)	105 (88%)	15 (12%)	4	15
39	1h	114/119 (96%)	99 (87%)	15 (13%)	4	14
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	16
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	24
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	19
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	10
41	2j	69/92 (75%)	63 (91%)	6 (9%)	9	30
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	20
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	32
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	22
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	27
44	1m	92/101 (91%)	78 (85%)	14 (15%)	3	10
44	2m	91/101 (90%)	76 (84%)	15 (16%)	2	8
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	11
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	16
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	44
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7	23
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	23
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	17
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	26
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	37
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	31
49	2r	59/77 (77%)	50 (85%)	9 (15%)	3	10
50	1s	69/80 (86%)	64 (93%)	5 (7%)	13	39
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	17
51	1t	70/82 (85%)	63 (90%)	7 (10%)	7	24
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9301/10064 (92%)	8332 (90%)	969 (10%)	7 22

5 of 969 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2E	170	LEU
42	2k	14	VAL
9	2N	99	LEU
40	2i	114	TYR
49	2r	25	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
44	1m	12	ASN
40	2i	3	GLN
8	2I	133	HIS
38	2g	153	HIS
46	2o	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	481 (16%)	37 (1%)
1	2A	2791/2915 (95%)	530 (18%)	25 (0%)
2	1B	120/121 (99%)	12 (10%)	1 (0%)
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1497/1521 (98%)	286 (19%)	0
32	2a	1501/1521 (98%)	262 (17%)	0
53	1v	9/24 (37%)	4 (44%)	0
53	2v	4/24 (16%)	0	0
54	1x	75/77 (97%)	8 (10%)	0
54	2x	75/77 (97%)	11 (14%)	0
All	All	9054/9316 (97%)	1625 (17%)	63 (0%)

5 of 1625 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U

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Mol	Chain	Res	Type
1	1A	13	A
1	1A	14	A
1	1A	15	G

5 of 63 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2156	G
1	2A	1530	C
1	1A	2601	C
1	2A	1442	G
1	2A	1992	G

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
1	5MU	1A	1939	1,55	19,22,23	1.40	5 (26%)	27,32,35	2.29	6 (22%)
1	5MC	2A	1962	1,55	19,22,23	1.55	3 (15%)	26,32,35	1.15	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.08	2 (7%)
32	PSU	2a	516	32,55	18,21,22	1.35	2 (11%)	21,30,33	1.94	4 (19%)
32	5MC	2a	1400	54,32	19,22,23	1.71	3 (15%)	26,32,35	1.30	3 (11%)
1	2MA	2A	2503	1,55	22,25,26	1.47	5 (22%)	32,37,40	2.22	9 (28%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.78	3 (11%)
1	OMG	1A	2251	54,1,55	23,26,27	1.24	3 (13%)	32,38,41	1.98	6 (18%)
1	5MU	2A	1915	1	19,22,23	1.56	5 (26%)	27,32,35	2.03	7 (25%)
54	5MC	2x	32	54	19,22,23	1.75	3 (15%)	26,32,35	1.21	3 (11%)
1	2MU	1A	2552	1,55	19,22,24	1.18	1 (5%)	25,31,36	2.05	6 (24%)
32	PSU	1a	516	32,55	18,21,22	1.40	2 (11%)	21,30,33	1.94	4 (19%)
32	4OC	1a	1402	32	20,23,24	0.79	0	25,32,35	0.97	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.13	2 (7%)
54	4SU	2x	8	54	18,21,22	2.03	6 (33%)	25,30,33	1.50	4 (16%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.00	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.51	3 (15%)	26,32,35	1.14	2 (7%)
32	MA6	1a	1519	32	23,26,27	1.58	5 (21%)	33,38,41	2.21	13 (39%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.76	3 (11%)
1	4OC	1A	1920	1	19,22,24	0.79	0	25,31,35	1.00	1 (4%)
1	2MA	1A	2503	1,55	22,25,26	1.47	5 (22%)	32,37,40	2.17	9 (28%)
32	M2G	2a	966	32,55	24,27,28	1.35	4 (16%)	33,40,43	1.95	5 (15%)
43	0TD	2l	92	43	8,9,10	4.58	1 (12%)	6,11,13	6.85	3 (50%)
54	5MU	1x	54	54,55	19,22,23	1.39	5 (26%)	27,32,35	1.84	7 (25%)
32	MA6	1a	1518	32	23,26,27	1.48	6 (26%)	33,38,41	2.37	13 (39%)
1	4OC	2A	1920	1	19,22,24	0.77	0	25,31,35	1.05	2 (8%)
54	4SU	1x	8	54	18,21,22	2.12	4 (22%)	25,30,33	1.59	5 (20%)
32	5MC	1a	1404	32	19,22,23	1.86	3 (15%)	26,32,35	1.17	3 (11%)
32	MA6	2a	1518	32	23,26,27	1.55	5 (21%)	33,38,41	2.27	13 (39%)
32	5MC	2a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.16	3 (11%)
54	PSU	1x	55	54	18,21,22	1.32	2 (11%)	21,30,33	1.98	4 (19%)
1	5MC	1A	1962	1,55	19,22,23	1.57	3 (15%)	26,32,35	1.06	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.03	3 (14%)
1	PSU	1A	1911	1	18,21,22	1.33	2 (11%)	21,30,33	1.99	3 (14%)
1	2MU	2A	2552	1,55	19,22,24	1.27	3 (15%)	25,31,36	1.86	5 (20%)
1	PSU	1A	1917	1	18,21,22	1.35	3 (16%)	21,30,33	2.08	4 (19%)
32	7MG	1a	527	32,55	23,26,27	1.35	3 (13%)	27,39,42	2.64	7 (25%)
32	2MG	1a	1207	32,55	23,26,27	1.23	2 (8%)	33,38,41	2.18	8 (24%)
54	5MC	1x	32	54	19,22,23	1.64	3 (15%)	26,32,35	1.26	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.44	5 (26%)	27,32,35	2.40	6 (22%)
32	4OC	2a	1402	32,55	20,23,24	0.80	0	25,32,35	0.98	1 (4%)
32	MA6	2a	1519	32	23,26,27	1.57	4 (17%)	33,38,41	2.29	11 (33%)
1	PSU	2A	1917	1,55	18,21,22	1.41	2 (11%)	21,30,33	1.91	3 (14%)
32	5MC	1a	967	32	19,22,23	1.53	3 (15%)	26,32,35	1.23	4 (15%)
1	5MU	1A	1915	1	19,22,23	1.42	5 (26%)	27,32,35	2.08	7 (25%)
1	5MC	1A	1942	1,55	19,22,23	1.46	3 (15%)	26,32,35	1.16	2 (7%)
1	OMG	2A	2251	54,1,55	23,26,27	1.22	3 (13%)	32,38,41	1.93	6 (18%)
43	0TD	1l	92	43	8,9,10	4.46	1 (12%)	6,11,13	4.35	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	2605	1	18,21,22	1.41	4 (22%)	21,30,33	2.00	4 (19%)
54	5MU	2x	54	54	19,22,23	1.39	5 (26%)	27,32,35	2.05	7 (25%)
32	5MC	1a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.55	3 (15%)	26,32,35	1.11	2 (7%)
32	M2G	1a	966	32,55	24,27,28	1.33	4 (16%)	33,40,43	1.85	5 (15%)
32	7MG	2a	527	32,55	23,26,27	1.38	4 (17%)	27,39,42	2.54	5 (18%)
54	PSU	2x	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.00	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.26	4 (17%)	33,38,41	2.13	8 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1939	1,55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	54,32	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	1,55	-	0/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	54,1,55	-	0/9/27/28	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,55	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32,55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
1	2MA	1A	2503	1,55	-	1/7/25/26	0/3/3/3
32	M2G	2a	966	32,55	-	0/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
54	5MU	1x	54	54,55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,55	-	0/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,55	-	1/7/37/38	0/3/3/3
32	2MG	1a	1207	32,55	-	0/9/27/28	0/3/3/3
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,55	-	2/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
1	PSU	2A	1917	1,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	1,55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	54,1,55	-	0/9/27/28	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32,55	-	0/11/29/30	0/3/3/3
32	7MG	2a	527	32,55	-	2/7/37/38	0/3/3/3
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.61	1.69	1.82
43	1l	92	0TD	CB-SB	-12.16	1.70	1.82
32	1a	1404	5MC	C5-C4	6.96	1.49	1.44
54	2x	32	5MC	C5-C4	6.25	1.48	1.44
32	1a	1400	5MC	C5-C4	6.20	1.48	1.44

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-16.09	73.45	102.36
43	1l	92	0TD	CSB-SB-CB	-9.64	85.04	102.36
32	1a	527	7MG	N9-C4-N3	8.98	138.62	125.46
32	2a	527	7MG	N9-C4-N3	8.54	137.97	125.46
1	2A	2503	2MA	C5-C4-N3	-7.80	118.96	127.18

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

32 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	5MU	1	0
1	2A	1962	5MC	1	0
32	2a	516	PSU	2	0
32	2a	1400	5MC	1	0
1	2A	2503	2MA	2	0
1	1A	2251	OMG	1	0
1	2A	1915	5MU	1	0
54	2x	32	5MC	1	0
1	1A	2552	2MU	2	0
32	1a	1402	4OC	1	0
1	2A	1942	5MC	2	0
54	2x	8	4SU	2	0
32	1a	1519	MA6	2	0
1	1A	1920	4OC	1	0
43	2l	92	0TD	2	0
32	1a	1518	MA6	2	0
1	2A	1920	4OC	2	0
54	1x	8	4SU	3	0
32	2a	1518	MA6	3	0
32	2a	967	5MC	1	0
1	2A	1911	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2552	2MU	3	0
1	1A	1917	PSU	1	0
32	1a	1207	2MG	1	0
54	1x	32	5MC	1	0
1	2A	1939	5MU	1	0
32	2a	1402	4OC	2	0
32	2a	1519	MA6	3	0
32	1a	967	5MC	2	0
1	2A	2251	OMG	1	0
32	2a	1404	5MC	2	0
32	1a	966	M2G	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2715 ligands modelled in this entry, 2711 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	$\# Z > 2$
57	V7A	2a	3210	55	37,38,38	3.93	11 (29%)	43,60,60	1.65	9 (20%)
58	SF4	2d	303	35	0,12,12	-	-	-		
57	V7A	1a	1835	55	37,38,38	4.19	12 (32%)	43,60,60	1.77	9 (20%)
58	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	V7A	2a	3210	55	-	4/13/72/72	0/4/4/4
58	SF4	2d	303	35	-	-	0/6/5/5
57	V7A	1a	1835	55	-	4/13/72/72	0/4/4/4
58	SF4	1d	501	35	-	-	0/6/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1a	1835	V7A	CAM-CAL	-14.48	1.39	1.52
57	2a	3210	V7A	CAM-CAL	-12.85	1.40	1.52
57	1a	1835	V7A	CAM-CAP	-11.58	1.39	1.55
57	1a	1835	V7A	CAJ-CAI	-11.22	1.40	1.51
57	2a	3210	V7A	CAJ-CAI	-10.67	1.40	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1a	1835	V7A	CAJ-CAK-CAN	-3.90	103.74	110.38
57	1a	1835	V7A	OAZ-CAL-CAI	-3.74	116.27	123.52
57	2a	3210	V7A	OBI-CAR-CAQ	-3.73	116.69	122.93
57	1a	1835	V7A	OBI-CAR-CAQ	-3.62	116.88	122.93
57	2a	3210	V7A	OAZ-CAL-CAI	-3.61	116.51	123.52

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

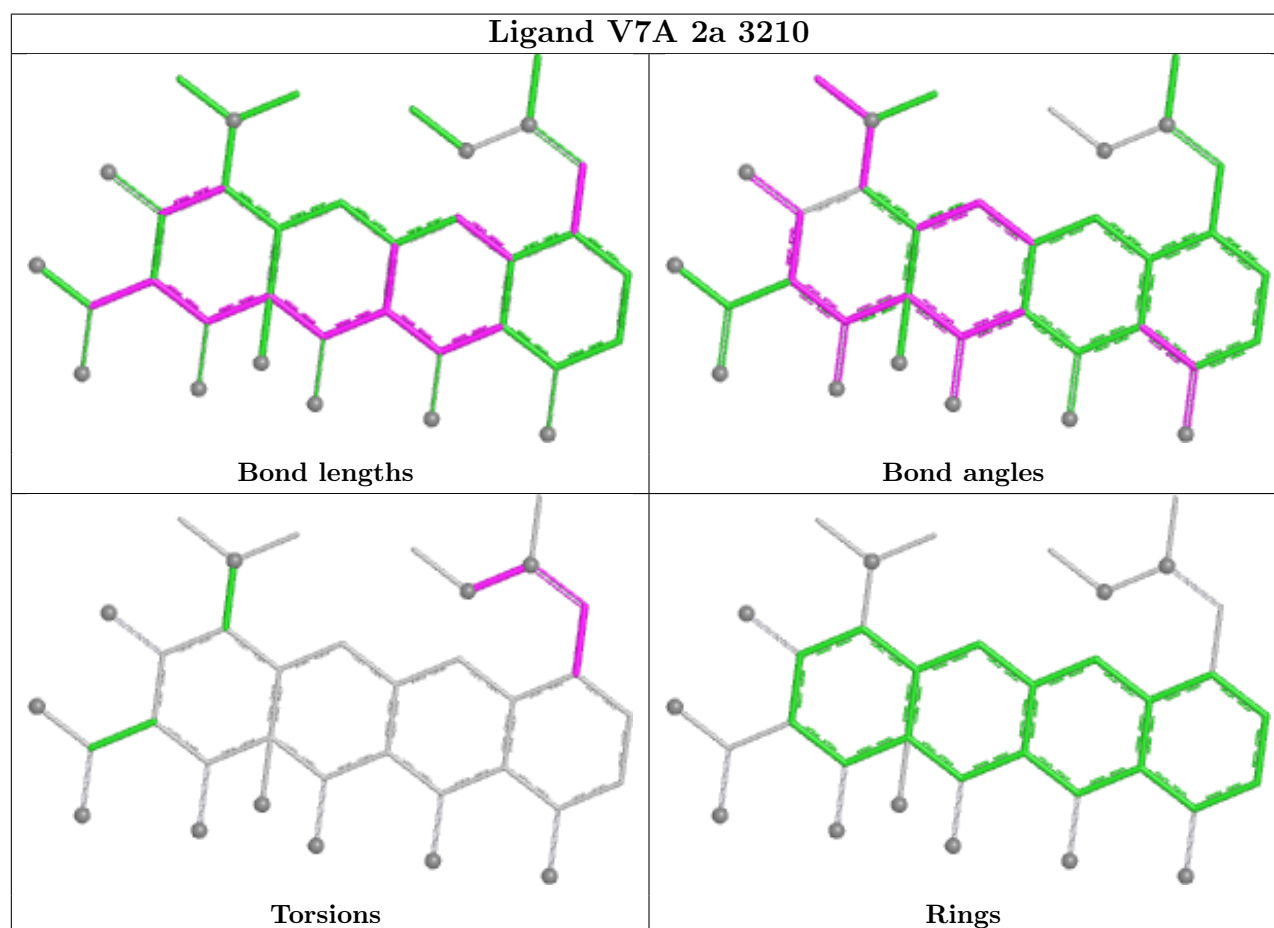
Mol	Chain	Res	Type	Atoms
57	1a	1835	V7A	CAN-CAO-NBF-CBH
57	1a	1835	V7A	CAA-CAS-NAT-CAW
57	1a	1835	V7A	CAA-CAS-NAT-OAU
57	1a	1835	V7A	CAW-NAT-OAU-CAV
57	2a	3210	V7A	CAA-CAS-NAT-CAW

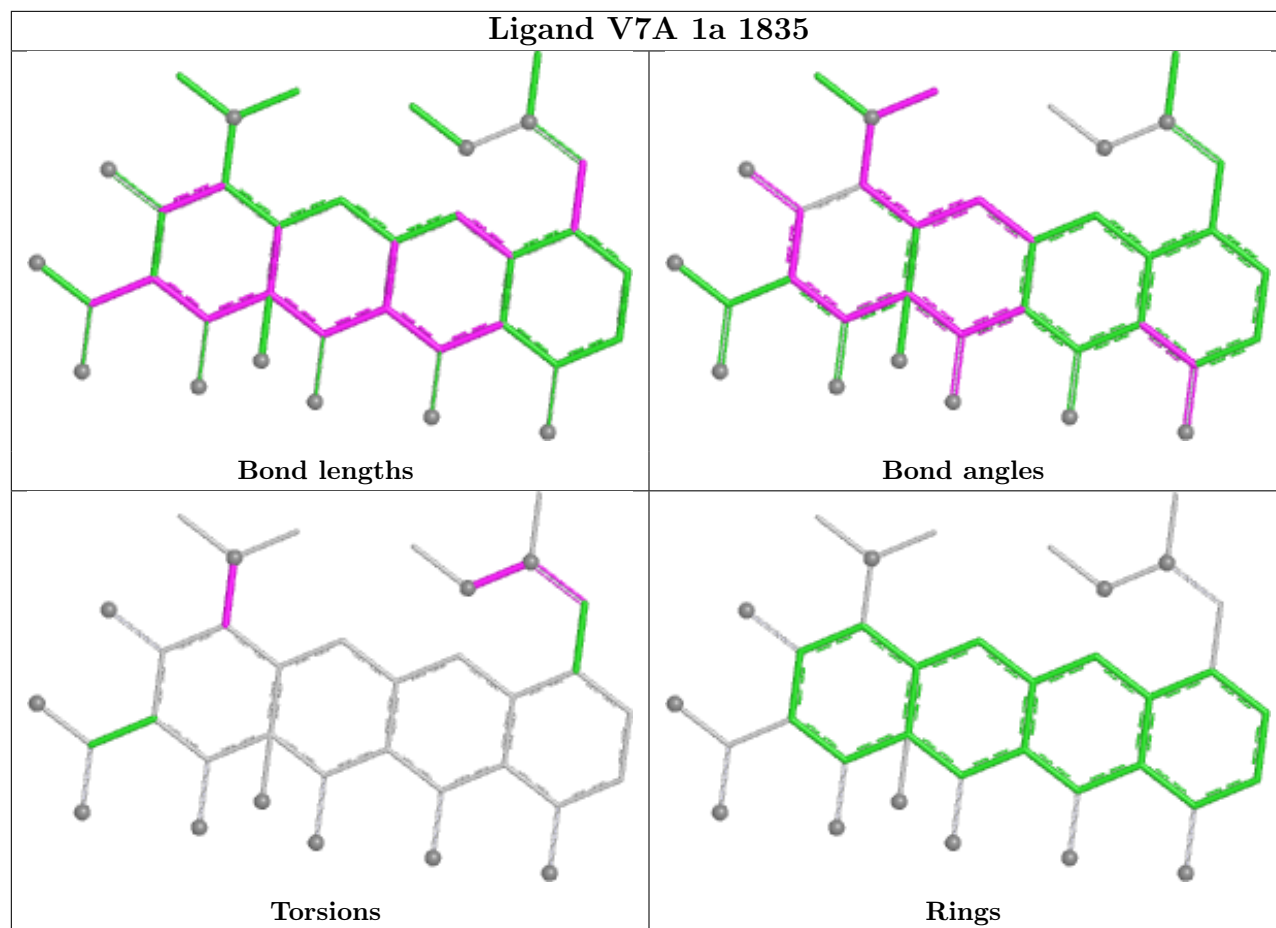
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2a	3210	V7A	4	0
58	2d	303	SF4	1	0
57	1a	1835	V7A	2	0
58	1d	501	SF4	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.





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%)	-0.41	71 (2%) 58 48	17, 35, 97, 110	0
1	2A	2789/2915 (95%)	-0.06	82 (2%) 53 43	28, 55, 93, 117	0
2	1B	120/121 (99%)	-0.41	1 (0%) 82 75	25, 50, 67, 89	0
2	2B	120/121 (99%)	0.60	6 (5%) 34 26	58, 79, 89, 99	0
3	1D	275/276 (99%)	-0.05	3 (1%) 78 70	19, 36, 50, 75	0
3	2D	275/276 (99%)	0.17	4 (1%) 72 63	28, 48, 62, 79	0
4	1E	204/206 (99%)	-0.25	0 100 100	18, 38, 58, 75	0
4	2E	204/206 (99%)	0.21	2 (0%) 79 72	32, 53, 69, 78	0
5	1F	203/210 (96%)	-0.15	0 100 100	19, 40, 65, 83	0
5	2F	203/210 (96%)	0.43	3 (1%) 72 63	33, 64, 80, 88	0
6	1G	181/182 (99%)	0.51	11 (6%) 27 20	37, 58, 72, 86	0
6	2G	181/182 (99%)	1.06	14 (7%) 19 14	63, 79, 86, 94	0
7	1H	174/180 (96%)	-0.05	1 (0%) 85 80	35, 51, 64, 72	0
7	2H	174/180 (96%)	0.95	16 (9%) 14 10	67, 80, 89, 95	0
8	1I	146/148 (98%)	0.43	1 (0%) 84 77	40, 70, 78, 83	0
8	2I	146/148 (98%)	2.22	74 (50%) 0 0	52, 87, 98, 104	0
9	1N	140/140 (100%)	-0.18	0 100 100	22, 38, 60, 71	0
9	2N	140/140 (100%)	0.29	1 (0%) 84 77	44, 63, 78, 87	0
10	1O	122/122 (100%)	-0.12	1 (0%) 82 75	28, 40, 55, 60	0
10	2O	122/122 (100%)	0.11	2 (1%) 70 61	40, 52, 64, 72	0
11	1P	149/150 (99%)	0.04	2 (1%) 75 66	18, 43, 64, 71	0
11	2P	149/150 (99%)	0.52	8 (5%) 31 24	37, 65, 80, 88	0
12	1Q	141/141 (100%)	0.04	2 (1%) 73 64	28, 39, 54, 69	0
12	2Q	141/141 (100%)	0.64	7 (4%) 34 26	46, 62, 74, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.15	0 100 100	24, 32, 47, 60	0
13	2R	118/118 (100%)	-0.04	0 100 100	37, 49, 61, 66	0
14	1S	110/112 (98%)	-0.03	0 100 100	35, 48, 58, 63	0
14	2S	110/112 (98%)	0.96	13 (11%) 9 7	59, 72, 80, 87	0
15	1T	131/146 (89%)	-0.05	5 (3%) 44 35	30, 44, 68, 78	0
15	2T	131/146 (89%)	0.41	2 (1%) 72 63	47, 57, 73, 82	0
16	1U	116/118 (98%)	-0.35	1 (0%) 81 74	20, 29, 43, 63	0
16	2U	116/118 (98%)	0.32	1 (0%) 81 74	40, 59, 72, 80	0
17	1V	101/101 (100%)	-0.34	0 100 100	21, 36, 58, 67	0
17	2V	101/101 (100%)	0.41	4 (3%) 42 33	40, 68, 79, 84	0
18	1W	112/113 (99%)	-0.44	0 100 100	19, 29, 46, 82	0
18	2W	112/113 (99%)	0.24	1 (0%) 81 74	39, 49, 66, 86	0
19	1X	95/96 (98%)	-0.10	1 (1%) 78 70	24, 36, 56, 75	0
19	2X	95/96 (98%)	0.56	5 (5%) 32 24	47, 59, 75, 81	0
20	1Y	107/110 (97%)	0.22	1 (0%) 81 74	33, 47, 69, 79	0
20	2Y	107/110 (97%)	0.91	9 (8%) 17 12	56, 70, 80, 92	0
21	1Z	154/206 (74%)	0.33	4 (2%) 57 47	38, 56, 70, 78	0
21	2Z	160/206 (77%)	0.99	17 (10%) 11 8	63, 74, 86, 94	0
22	10	83/85 (97%)	0.26	9 (10%) 11 8	25, 35, 69, 86	0
22	20	83/85 (97%)	0.86	11 (13%) 7 5	50, 61, 79, 89	0
23	11	97/98 (98%)	0.13	1 (1%) 79 72	23, 41, 68, 75	0
23	21	97/98 (98%)	0.54	3 (3%) 51 41	40, 54, 73, 81	0
24	12	70/72 (97%)	0.23	2 (2%) 53 43	35, 47, 57, 76	0
24	22	70/72 (97%)	0.54	2 (2%) 53 43	56, 69, 80, 85	0
25	13	59/60 (98%)	-0.28	0 100 100	23, 35, 54, 72	0
25	23	59/60 (98%)	0.43	0 100 100	47, 58, 75, 83	0
26	14	69/71 (97%)	0.58	4 (5%) 29 22	56, 74, 88, 94	0
26	24	69/71 (97%)	1.17	14 (20%) 3 2	75, 86, 93, 98	0
27	15	59/60 (98%)	-0.35	1 (1%) 69 60	18, 32, 51, 67	0
27	25	59/60 (98%)	0.09	2 (3%) 48 39	35, 50, 66, 83	0
28	16	53/54 (98%)	-0.11	0 100 100	28, 38, 51, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.83	3 (5%) 29 22	49, 58, 69, 71	0
29	17	48/49 (97%)	0.03	4 (8%) 17 12	22, 26, 55, 59	0
29	27	48/49 (97%)	0.17	3 (6%) 26 19	31, 41, 62, 75	0
30	18	64/65 (98%)	-0.07	0 100 100	25, 31, 39, 53	0
30	28	64/65 (98%)	0.45	0 100 100	44, 54, 61, 73	0
31	19	37/37 (100%)	-0.03	0 100 100	28, 38, 56, 62	0
31	29	37/37 (100%)	0.86	2 (5%) 31 24	53, 64, 75, 77	0
32	1a	1488/1521 (97%)	0.28	25 (1%) 69 60	37, 71, 95, 109	0
32	2a	1491/1521 (98%)	0.32	32 (2%) 63 54	44, 75, 96, 111	0
33	1b	231/256 (90%)	0.92	24 (10%) 11 8	64, 78, 90, 97	0
33	2b	231/256 (90%)	1.09	34 (14%) 6 4	67, 83, 90, 100	0
34	1c	206/239 (86%)	0.86	15 (7%) 21 15	64, 76, 85, 90	0
34	2c	206/239 (86%)	1.16	26 (12%) 8 6	71, 82, 90, 93	0
35	1d	208/209 (99%)	0.97	28 (13%) 7 5	59, 74, 87, 97	0
35	2d	208/209 (99%)	0.75	12 (5%) 29 22	58, 70, 80, 85	0
36	1e	148/162 (91%)	0.41	1 (0%) 84 77	54, 66, 74, 77	0
36	2e	148/162 (91%)	0.68	8 (5%) 31 24	60, 71, 81, 85	0
37	1f	100/101 (99%)	0.56	3 (3%) 52 42	55, 69, 76, 79	0
37	2f	100/101 (99%)	0.54	5 (5%) 34 26	63, 71, 79, 82	0
38	1g	155/156 (99%)	0.61	9 (5%) 29 22	63, 73, 86, 90	0
38	2g	155/156 (99%)	0.68	8 (5%) 33 25	69, 80, 91, 96	0
39	1h	137/138 (99%)	0.49	3 (2%) 62 52	56, 68, 76, 82	0
39	2h	137/138 (99%)	0.64	6 (4%) 39 31	61, 74, 80, 87	0
40	1i	127/128 (99%)	1.37	25 (19%) 3 2	61, 78, 84, 86	0
40	2i	127/128 (99%)	1.55	33 (25%) 1 1	70, 85, 92, 94	0
41	1j	97/105 (92%)	1.32	15 (15%) 5 4	64, 80, 90, 91	0
41	2j	96/105 (91%)	1.70	33 (34%) 1 1	75, 85, 93, 95	0
42	1k	114/129 (88%)	0.41	6 (5%) 32 24	44, 67, 78, 80	0
42	2k	114/129 (88%)	0.58	4 (3%) 47 38	55, 73, 80, 84	0
43	1l	121/132 (91%)	0.45	4 (3%) 49 39	49, 61, 70, 76	0
43	2l	121/132 (91%)	0.55	4 (3%) 49 39	53, 63, 73, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	122/126 (96%)	0.82	9 (7%) 20 15	61, 72, 82, 84	0
44	2m	121/126 (96%)	1.45	26 (21%) 2 2	73, 82, 87, 93	0
45	1n	60/61 (98%)	1.47	13 (21%) 2 2	67, 74, 80, 81	0
45	2n	60/61 (98%)	2.03	30 (50%) 0 0	72, 83, 87, 90	0
46	1o	88/89 (98%)	0.38	2 (2%) 61 51	48, 63, 76, 86	0
46	2o	88/89 (98%)	0.52	2 (2%) 61 51	56, 69, 76, 81	0
47	1p	82/88 (93%)	1.44	19 (23%) 2 1	62, 75, 84, 87	0
47	2p	82/88 (93%)	0.81	6 (7%) 21 15	58, 68, 77, 82	0
48	1q	99/105 (94%)	0.71	4 (4%) 42 33	56, 65, 74, 79	0
48	2q	99/105 (94%)	0.78	6 (6%) 27 20	55, 68, 78, 84	0
49	1r	68/88 (77%)	0.44	2 (2%) 53 43	59, 69, 77, 81	0
49	2r	68/88 (77%)	0.46	2 (2%) 53 43	62, 70, 79, 83	0
50	1s	83/93 (89%)	0.81	5 (6%) 27 21	63, 76, 85, 89	0
50	2s	83/93 (89%)	1.25	10 (12%) 9 6	75, 83, 91, 94	0
51	1t	96/106 (90%)	0.92	12 (12%) 8 6	61, 71, 80, 84	0
51	2t	96/106 (90%)	0.53	3 (3%) 51 41	58, 68, 76, 79	0
52	1u	23/27 (85%)	1.04	2 (8%) 16 11	66, 72, 77, 80	0
52	2u	23/27 (85%)	2.02	13 (56%) 0 0	75, 80, 82, 85	0
53	1v	10/24 (41%)	1.47	4 (40%) 1 0	54, 92, 98, 99	0
53	2v	6/24 (25%)	0.76	1 (16%) 4 3	67, 72, 86, 96	0
54	1x	72/77 (93%)	-0.03	1 (1%) 73 64	38, 64, 78, 89	0
54	2x	72/77 (93%)	0.23	2 (2%) 55 45	49, 77, 89, 93	0
All	All	20598/21444 (96%)	0.28	974 (4%) 36 29	17, 63, 89, 117	0

The worst 5 of 974 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2147	G	9.5
1	1A	2145	C	8.9
1	2A	2111	C	7.8
8	2I	111	PRO	7.8
1	2A	2148	G	7.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.73	0.12	74,81,86,91	0
54	PSU	2x	55	20/21	0.78	0.12	72,78,85,91	0
32	PSU	2a	516	20/21	0.86	0.12	70,76,79,84	0
32	5MC	2a	1400	21/22	0.86	0.15	65,72,79,81	0
54	4SU	2x	8	20/21	0.86	0.11	72,83,87,87	0
1	5MU	1A	1915	21/22	0.86	0.11	58,70,76,89	0
32	2MG	2a	1207	24/25	0.87	0.11	77,83,89,92	0
43	0TD	2l	92	10/11	0.87	0.15	57,66,71,84	0
54	PSU	1x	55	20/21	0.88	0.10	61,67,75,78	0
54	5MC	2x	32	21/22	0.89	0.15	61,79,80,82	0
32	PSU	1a	516	20/21	0.89	0.10	65,70,76,78	0
32	7MG	2a	527	24/25	0.90	0.11	59,66,71,72	0
54	5MC	1x	32	21/22	0.90	0.13	52,64,68,76	0
1	PSU	2A	1911	20/21	0.90	0.10	57,65,72,79	0
32	4OC	2a	1402	22/23	0.90	0.13	55,63,68,75	0
32	M2G	2a	966	25/26	0.91	0.14	63,69,81,83	0
32	2MG	1a	1207	24/25	0.91	0.09	60,76,82,87	0
43	0TD	1l	92	10/11	0.91	0.11	52,57,60,75	0
54	5MU	2x	54	21/22	0.91	0.09	72,79,82,87	0
54	4SU	1x	8	20/21	0.91	0.10	58,68,74,78	0
54	5MU	1x	54	21/22	0.92	0.10	64,69,77,83	0
32	5MC	2a	967	21/22	0.93	0.14	67,72,79,80	0
1	PSU	2A	1917	20/21	0.93	0.08	60,70,75,77	0
32	M2G	1a	966	25/26	0.93	0.13	51,59,65,73	0
1	5MC	2A	1962	21/22	0.94	0.09	40,53,61,65	0
1	2MA	2A	2503	23/24	0.94	0.10	30,34,39,42	0
32	5MC	2a	1404	21/22	0.94	0.09	45,57,67,68	0
32	UR3	2a	1498	21/22	0.94	0.10	52,59,63,70	0
32	MA6	2a	1518	24/25	0.94	0.12	55,62,66,67	0
32	5MC	1a	1404	21/22	0.94	0.10	34,46,49,51	0
1	PSU	1A	1917	20/21	0.94	0.08	50,59,68,74	0
32	7MG	1a	527	24/25	0.94	0.10	51,57,63,66	0
1	4OC	2A	1920	21/23	0.94	0.10	53,65,68,71	0
1	5MU	2A	1939	21/22	0.94	0.10	39,43,47,50	0
32	5MC	1a	967	21/22	0.95	0.10	54,62,71,74	0
1	OMG	2A	2251	24/25	0.95	0.10	30,40,46,46	0
32	5MC	1a	1407	21/22	0.95	0.09	41,43,48,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	1A	1911	20/21	0.95	0.08	42,49,56,58	0
32	4OC	1a	1402	22/23	0.95	0.10	49,53,59,62	0
1	5MC	2A	1942	21/22	0.95	0.08	47,55,60,63	0
32	5MC	2a	1407	21/22	0.96	0.09	51,57,62,64	0
1	5MC	1A	1942	21/22	0.96	0.08	28,34,40,43	0
1	4OC	1A	1920	21/23	0.96	0.08	34,46,49,54	0
32	MA6	2a	1519	24/25	0.96	0.11	56,60,65,67	0
32	5MC	1a	1400	21/22	0.96	0.09	36,57,61,62	0
32	MA6	1a	1518	24/25	0.96	0.10	35,43,48,52	0
1	2MU	2A	2552	21/23	0.96	0.07	34,38,44,47	0
1	PSU	2A	2605	20/21	0.96	0.09	28,38,44,46	0
32	MA6	1a	1519	24/25	0.96	0.10	38,43,48,51	0
32	UR3	1a	1498	21/22	0.97	0.07	39,46,49,52	0
1	5MU	1A	1939	21/22	0.97	0.07	22,27,32,34	0
1	OMG	1A	2251	24/25	0.97	0.08	23,29,33,35	0
1	PSU	1A	2605	20/21	0.97	0.07	20,27,29,31	0
1	2MA	1A	2503	23/24	0.98	0.06	14,21,24,25	0
1	2MU	1A	2552	21/23	0.98	0.07	26,29,34,37	0
1	5MC	1A	1962	21/22	0.98	0.07	28,37,44,54	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	2a	3173	1/1	0.30	0.26	76,76,76,76	0
55	MG	1B	232	1/1	0.43	0.27	65,65,65,65	0
55	MG	1a	1765	1/1	0.45	0.17	90,90,90,90	0
55	MG	1B	230	1/1	0.56	0.24	82,82,82,82	0
55	MG	1a	1678	1/1	0.56	0.23	85,85,85,85	0
55	MG	2A	3464	1/1	0.58	0.30	77,77,77,77	0
55	MG	2A	3741	1/1	0.58	0.22	72,72,72,72	0
55	MG	1A	3624	1/1	0.58	0.29	81,81,81,81	0
55	MG	1B	229	1/1	0.59	0.42	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3735	1/1	0.59	0.17	60,60,60,60	0
55	MG	2a	3024	1/1	0.60	0.35	77,77,77,77	0
55	MG	1A	3541	1/1	0.61	0.58	67,67,67,67	0
55	MG	2A	3270	1/1	0.62	0.27	70,70,70,70	0
55	MG	2B	213	1/1	0.62	0.31	76,76,76,76	0
55	MG	1a	1677	1/1	0.62	0.30	75,75,75,75	0
55	MG	1x	113	1/1	0.62	0.16	68,68,68,68	0
55	MG	2A	3854	1/1	0.63	0.28	68,68,68,68	0
55	MG	2a	3128	1/1	0.64	0.17	90,90,90,90	0
55	MG	2a	3139	1/1	0.64	0.21	69,69,69,69	0
55	MG	2A	3222	1/1	0.64	0.21	68,68,68,68	0
55	MG	2A	3377	1/1	0.67	0.13	65,65,65,65	0
55	MG	1a	1662	1/1	0.67	0.45	69,69,69,69	0
55	MG	1a	1638	1/1	0.68	0.17	55,55,55,55	0
55	MG	1A	3347	1/1	0.68	0.31	60,60,60,60	0
55	MG	2a	3082	1/1	0.68	0.26	75,75,75,75	0
55	MG	2A	3289	1/1	0.68	0.34	75,75,75,75	0
55	MG	2A	3830	1/1	0.68	0.16	76,76,76,76	0
55	MG	1U	207	1/1	0.68	0.43	54,54,54,54	0
55	MG	2A	3653	1/1	0.69	0.20	72,72,72,72	0
55	MG	2a	3083	1/1	0.69	0.12	64,64,64,64	0
55	MG	2A	3690	1/1	0.69	0.12	64,64,64,64	0
55	MG	1a	1681	1/1	0.69	0.21	76,76,76,76	0
55	MG	1a	1789	1/1	0.69	0.19	79,79,79,79	0
55	MG	1a	1715	1/1	0.70	0.15	53,53,53,53	0
55	MG	2A	3294	1/1	0.70	0.22	61,61,61,61	0
55	MG	2A	3317	1/1	0.70	0.12	78,78,78,78	0
55	MG	2a	3180	1/1	0.70	0.27	63,63,63,63	0
55	MG	1a	1769	1/1	0.71	0.19	71,71,71,71	0
55	MG	1a	1718	1/1	0.71	0.33	68,68,68,68	0
55	MG	2a	3050	1/1	0.71	0.33	79,79,79,79	0
55	MG	2a	3040	1/1	0.72	0.15	55,55,55,55	0
55	MG	1a	1719	1/1	0.73	0.36	61,61,61,61	0
55	MG	1a	1612	1/1	0.73	0.12	57,57,57,57	0
55	MG	2d	302	1/1	0.73	0.19	73,73,73,73	0
55	MG	2B	216	1/1	0.74	0.21	65,65,65,65	0
55	MG	1A	3219	1/1	0.74	0.29	68,68,68,68	0
55	MG	2a	3029	1/1	0.74	0.37	78,78,78,78	0
55	MG	1A	3248	1/1	0.74	0.22	66,66,66,66	0
55	MG	2i	201	1/1	0.74	0.57	82,82,82,82	0
55	MG	2x	101	1/1	0.74	0.21	84,84,84,84	0
55	MG	2A	3498	1/1	0.75	0.39	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	3174	1/1	0.75	0.20	75,75,75,75	0
55	MG	1A	3499	1/1	0.75	0.35	65,65,65,65	0
55	MG	2a	3206	1/1	0.75	0.23	78,78,78,78	0
55	MG	2a	3092	1/1	0.75	0.42	68,68,68,68	0
55	MG	1A	4023	1/1	0.75	0.10	73,73,73,73	0
55	MG	2j	202	1/1	0.75	0.18	74,74,74,74	0
55	MG	2T	201	1/1	0.75	0.31	65,65,65,65	0
55	MG	2A	3252	1/1	0.76	0.10	50,50,50,50	0
55	MG	2a	3190	1/1	0.76	0.22	66,66,66,66	0
55	MG	2a	3130	1/1	0.76	0.35	69,69,69,69	0
55	MG	1A	3926	1/1	0.76	0.11	45,45,45,45	0
55	MG	2a	3158	1/1	0.76	0.19	70,70,70,70	0
55	MG	1A	3851	1/1	0.76	0.15	49,49,49,49	0
55	MG	2A	3229	1/1	0.76	0.17	59,59,59,59	0
55	MG	2A	3092	1/1	0.77	0.29	62,62,62,62	0
55	MG	2A	3163	1/1	0.77	0.22	64,64,64,64	0
55	MG	2a	3105	1/1	0.77	0.22	80,80,80,80	0
55	MG	2a	3117	1/1	0.77	0.31	49,49,49,49	0
55	MG	2A	3760	1/1	0.77	0.10	76,76,76,76	0
55	MG	2A	3346	1/1	0.77	0.11	67,67,67,67	0
55	MG	2A	3359	1/1	0.77	0.20	63,63,63,63	0
55	MG	2B	204	1/1	0.77	0.20	75,75,75,75	0
55	MG	2A	3361	1/1	0.77	0.19	64,64,64,64	0
55	MG	1a	1702	1/1	0.77	0.25	60,60,60,60	0
55	MG	2A	3441	1/1	0.77	0.14	63,63,63,63	0
55	MG	1A	3947	1/1	0.77	0.12	23,23,23,23	0
55	MG	2a	3205	1/1	0.77	0.22	59,59,59,59	0
55	MG	1A	3450	1/1	0.77	0.18	74,74,74,74	0
55	MG	1A	3741	1/1	0.77	0.10	56,56,56,56	0
55	MG	2A	3089	1/1	0.77	0.20	72,72,72,72	0
55	MG	2a	3061	1/1	0.77	0.23	68,68,68,68	0
55	MG	2A	3715	1/1	0.77	0.14	66,66,66,66	0
55	MG	2x	104	1/1	0.77	0.17	70,70,70,70	0
55	MG	2A	3365	1/1	0.78	0.18	66,66,66,66	0
55	MG	2A	3080	1/1	0.78	0.21	67,67,67,67	0
55	MG	2A	3258	1/1	0.78	0.25	64,64,64,64	0
55	MG	1a	1750	1/1	0.78	0.15	77,77,77,77	0
55	MG	18	105	1/1	0.78	0.22	75,75,75,75	0
55	MG	2a	3145	1/1	0.78	0.39	67,67,67,67	0
55	MG	2B	214	1/1	0.78	0.37	82,82,82,82	0
55	MG	2A	3612	1/1	0.78	0.30	53,53,53,53	0
55	MG	1A	3988	1/1	0.78	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3689	1/1	0.78	0.12	71,71,71,71	0
55	MG	1A	3549	1/1	0.78	0.29	45,45,45,45	0
55	MG	2A	3707	1/1	0.78	0.13	56,56,56,56	0
55	MG	2A	3227	1/1	0.78	0.21	69,69,69,69	0
55	MG	2A	3725	1/1	0.78	0.29	68,68,68,68	0
55	MG	1a	1642	1/1	0.78	0.27	67,67,67,67	0
55	MG	2A	3740	1/1	0.78	0.20	68,68,68,68	0
55	MG	2a	3091	1/1	0.78	0.26	71,71,71,71	0
55	MG	2A	3230	1/1	0.78	0.10	78,78,78,78	0
55	MG	1A	3346	1/1	0.79	0.15	55,55,55,55	0
55	MG	2a	3110	1/1	0.79	0.18	61,61,61,61	0
55	MG	2B	206	1/1	0.79	0.21	57,57,57,57	0
55	MG	2A	3654	1/1	0.79	0.12	63,63,63,63	0
55	MG	2a	3129	1/1	0.79	0.40	64,64,64,64	0
55	MG	1a	1636	1/1	0.79	0.22	63,63,63,63	0
55	MG	1A	3464	1/1	0.79	0.08	40,40,40,40	0
55	MG	2F	306	1/1	0.79	0.14	62,62,62,62	0
55	MG	1A	3303	1/1	0.79	0.13	62,62,62,62	0
55	MG	2U	201	1/1	0.79	0.27	58,58,58,58	0
55	MG	1A	3683	1/1	0.79	0.09	53,53,53,53	0
55	MG	1a	1748	1/1	0.79	0.13	63,63,63,63	0
55	MG	2A	3094	1/1	0.79	0.14	67,67,67,67	0
55	MG	2A	3484	1/1	0.79	0.58	58,58,58,58	0
55	MG	1A	3527	1/1	0.79	0.29	53,53,53,53	0
55	MG	2a	3069	1/1	0.79	0.28	57,57,57,57	0
55	MG	2A	3551	1/1	0.79	0.15	42,42,42,42	0
55	MG	2A	3827	1/1	0.79	0.16	64,64,64,64	0
55	MG	2A	3570	1/1	0.79	0.19	65,65,65,65	0
55	MG	1a	1601	1/1	0.79	0.12	63,63,63,63	0
55	MG	2A	3158	1/1	0.80	0.21	51,51,51,51	0
55	MG	1a	1773	1/1	0.80	0.21	70,70,70,70	0
55	MG	2A	3170	1/1	0.80	0.31	65,65,65,65	0
55	MG	2B	210	1/1	0.80	0.19	59,59,59,59	0
55	MG	1A	3284	1/1	0.80	0.09	37,37,37,37	0
55	MG	1A	3742	1/1	0.80	0.18	51,51,51,51	0
55	MG	1a	1618	1/1	0.80	0.12	51,51,51,51	0
55	MG	1A	3305	1/1	0.80	0.25	51,51,51,51	0
55	MG	2A	3369	1/1	0.80	0.18	78,78,78,78	0
55	MG	2A	3090	1/1	0.80	0.23	57,57,57,57	0
55	MG	2a	3162	1/1	0.80	0.22	61,61,61,61	0
55	MG	2a	3021	1/1	0.80	0.12	55,55,55,55	0
55	MG	1A	3858	1/1	0.80	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	3175	1/1	0.80	0.15	70,70,70,70	0
55	MG	2A	3454	1/1	0.80	0.14	47,47,47,47	0
55	MG	2A	3461	1/1	0.80	0.19	60,60,60,60	0
55	MG	2A	3260	1/1	0.80	0.25	60,60,60,60	0
55	MG	2A	3475	1/1	0.80	0.19	67,67,67,67	0
55	MG	2a	3063	1/1	0.80	0.33	69,69,69,69	0
55	MG	2A	3778	1/1	0.80	0.11	63,63,63,63	0
55	MG	1B	223	1/1	0.80	0.15	56,56,56,56	0
55	MG	2A	3285	1/1	0.80	0.14	52,52,52,52	0
55	MG	2A	3852	1/1	0.80	0.20	61,61,61,61	0
55	MG	1a	1803	1/1	0.81	0.11	66,66,66,66	0
55	MG	1a	1834	1/1	0.81	0.37	68,68,68,68	0
55	MG	1t	201	1/1	0.81	0.28	59,59,59,59	0
55	MG	1v	102	1/1	0.81	0.18	74,74,74,74	0
55	MG	1x	109	1/1	0.81	0.22	73,73,73,73	0
55	MG	1A	3824	1/1	0.81	0.29	47,47,47,47	0
55	MG	2A	3049	1/1	0.81	0.15	68,68,68,68	0
55	MG	2A	3465	1/1	0.81	0.28	54,54,54,54	0
55	MG	1A	3212	1/1	0.81	0.19	53,53,53,53	0
55	MG	1Y	203	1/1	0.81	0.07	68,68,68,68	0
55	MG	1A	3120	1/1	0.81	0.13	49,49,49,49	0
55	MG	2a	3135	1/1	0.81	0.31	64,64,64,64	0
55	MG	2A	3516	1/1	0.81	0.28	60,60,60,60	0
55	MG	2A	3521	1/1	0.81	0.14	55,55,55,55	0
55	MG	2A	3527	1/1	0.81	0.15	54,54,54,54	0
55	MG	1B	207	1/1	0.81	0.16	49,49,49,49	0
55	MG	2A	3554	1/1	0.81	0.23	67,67,67,67	0
55	MG	2D	303	1/1	0.81	0.15	62,62,62,62	0
55	MG	2A	3290	1/1	0.81	0.36	68,68,68,68	0
55	MG	2a	3176	1/1	0.81	0.25	67,67,67,67	0
55	MG	2A	3596	1/1	0.81	0.11	48,48,48,48	0
55	MG	1A	3861	1/1	0.81	0.08	48,48,48,48	0
55	MG	2A	3645	1/1	0.81	0.22	54,54,54,54	0
55	MG	2A	3118	1/1	0.81	0.18	59,59,59,59	0
55	MG	2A	3323	1/1	0.81	0.21	67,67,67,67	0
55	MG	2A	3130	1/1	0.81	0.25	57,57,57,57	0
55	MG	2A	3348	1/1	0.81	0.30	64,64,64,64	0
55	MG	1A	3873	1/1	0.81	0.20	75,75,75,75	0
55	MG	1A	3131	1/1	0.81	0.09	73,73,73,73	0
55	MG	2a	3101	1/1	0.82	0.19	73,73,73,73	0
55	MG	2A	3068	1/1	0.82	0.34	69,69,69,69	0
55	MG	2A	3310	1/1	0.82	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	3116	1/1	0.82	0.21	54,54,54,54	0
55	MG	2A	3666	1/1	0.82	0.23	72,72,72,72	0
55	MG	2a	3125	1/1	0.82	0.29	61,61,61,61	0
55	MG	2A	3678	1/1	0.82	0.11	79,79,79,79	0
55	MG	1a	1671	1/1	0.82	0.29	63,63,63,63	0
55	MG	2A	3234	1/1	0.82	0.24	61,61,61,61	0
55	MG	2A	3704	1/1	0.82	0.12	53,53,53,53	0
55	MG	1a	1787	1/1	0.82	0.12	73,73,73,73	0
55	MG	2A	3710	1/1	0.82	0.15	50,50,50,50	0
55	MG	2a	3150	1/1	0.82	0.29	71,71,71,71	0
55	MG	2A	3253	1/1	0.82	0.08	64,64,64,64	0
55	MG	2a	3004	1/1	0.82	0.33	65,65,65,65	0
55	MG	2a	3164	1/1	0.82	0.15	66,66,66,66	0
55	MG	2A	3355	1/1	0.82	0.19	61,61,61,61	0
55	MG	2A	3730	1/1	0.82	0.10	60,60,60,60	0
55	MG	1A	3680	1/1	0.82	0.18	33,33,33,33	0
55	MG	2a	3037	1/1	0.82	0.22	80,80,80,80	0
55	MG	2A	3166	1/1	0.82	0.26	71,71,71,71	0
55	MG	2A	3266	1/1	0.82	0.15	59,59,59,59	0
55	MG	2a	3191	1/1	0.82	0.26	55,55,55,55	0
55	MG	1A	3879	1/1	0.82	0.14	64,64,64,64	0
55	MG	2A	3201	1/1	0.82	0.17	66,66,66,66	0
55	MG	2a	3208	1/1	0.82	0.20	58,58,58,58	0
55	MG	2a	3209	1/1	0.82	0.24	63,63,63,63	0
55	MG	2A	3582	1/1	0.82	0.13	56,56,56,56	0
55	MG	2A	3384	1/1	0.82	0.21	68,68,68,68	0
55	MG	2A	3836	1/1	0.82	0.15	49,49,49,49	0
55	MG	1A	3603	1/1	0.82	0.32	53,53,53,53	0
55	MG	2A	3111	1/1	0.82	0.17	65,65,65,65	0
55	MG	1a	1727	1/1	0.83	0.35	67,67,67,67	0
55	MG	1A	3302	1/1	0.83	0.17	45,45,45,45	0
55	MG	2A	3070	1/1	0.83	0.12	60,60,60,60	0
55	MG	1A	3488	1/1	0.83	0.11	58,58,58,58	0
55	MG	2A	3082	1/1	0.83	0.26	57,57,57,57	0
55	MG	1A	3895	1/1	0.83	0.13	41,41,41,41	0
55	MG	1A	3901	1/1	0.83	0.13	48,48,48,48	0
55	MG	2A	3486	1/1	0.83	0.30	50,50,50,50	0
55	MG	2a	3108	1/1	0.83	0.23	72,72,72,72	0
55	MG	2A	3773	1/1	0.83	0.19	62,62,62,62	0
55	MG	1a	1670	1/1	0.83	0.10	67,67,67,67	0
55	MG	2A	3817	1/1	0.83	0.16	40,40,40,40	0
55	MG	1A	3156	1/1	0.83	0.25	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	3127	1/1	0.83	0.23	60,60,60,60	0
55	MG	2A	3095	1/1	0.83	0.30	65,65,65,65	0
55	MG	1D	310	1/1	0.83	0.15	40,40,40,40	0
55	MG	2A	3536	1/1	0.83	0.32	58,58,58,58	0
55	MG	2A	3540	1/1	0.83	0.15	40,40,40,40	0
55	MG	2B	201	1/1	0.83	0.13	68,68,68,68	0
55	MG	1A	3940	1/1	0.83	0.15	52,52,52,52	0
55	MG	1a	1807	1/1	0.83	0.15	63,63,63,63	0
55	MG	2A	3151	1/1	0.83	0.17	68,68,68,68	0
55	MG	2a	3159	1/1	0.83	0.15	53,53,53,53	0
55	MG	1a	1815	1/1	0.83	0.23	63,63,63,63	0
55	MG	1a	1829	1/1	0.83	0.16	79,79,79,79	0
55	MG	2A	3165	1/1	0.83	0.11	60,60,60,60	0
55	MG	2A	3615	1/1	0.83	0.27	67,67,67,67	0
55	MG	1A	3509	1/1	0.83	0.20	32,32,32,32	0
55	MG	2G	201	1/1	0.83	0.16	68,68,68,68	0
55	MG	1A	3523	1/1	0.83	0.17	47,47,47,47	0
55	MG	2A	3177	1/1	0.83	0.35	56,56,56,56	0
55	MG	20	101	1/1	0.83	0.14	65,65,65,65	0
55	MG	2a	3197	1/1	0.83	0.20	57,57,57,57	0
55	MG	2A	3189	1/1	0.83	0.10	55,55,55,55	0
55	MG	2A	3669	1/1	0.83	0.26	52,52,52,52	0
55	MG	2A	3676	1/1	0.83	0.11	69,69,69,69	0
55	MG	2a	3028	1/1	0.83	0.22	70,70,70,70	0
55	MG	2A	3190	1/1	0.83	0.31	65,65,65,65	0
55	MG	1A	3223	1/1	0.83	0.24	55,55,55,55	0
55	MG	2j	201	1/1	0.83	0.08	71,71,71,71	0
55	MG	1A	4027	1/1	0.83	0.10	21,21,21,21	0
55	MG	2A	3378	1/1	0.83	0.10	67,67,67,67	0
55	MG	1A	4107	1/1	0.83	0.16	63,63,63,63	0
55	MG	2A	3320	1/1	0.84	0.11	64,64,64,64	0
55	MG	2A	3083	1/1	0.84	0.11	35,35,35,35	0
55	MG	1a	1714	1/1	0.84	0.15	51,51,51,51	0
55	MG	2A	3781	1/1	0.84	0.15	62,62,62,62	0
55	MG	1A	3620	1/1	0.84	0.24	38,38,38,38	0
55	MG	2A	3563	1/1	0.84	0.12	41,41,41,41	0
55	MG	1a	1639	1/1	0.84	0.29	73,73,73,73	0
55	MG	15	105	1/1	0.84	0.10	43,43,43,43	0
55	MG	1a	1831	1/1	0.84	0.29	70,70,70,70	0
55	MG	2A	3853	1/1	0.84	0.07	64,64,64,64	0
55	MG	2A	3605	1/1	0.84	0.14	34,34,34,34	0
55	MG	1A	3385	1/1	0.84	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3244	1/1	0.84	0.20	51,51,51,51	0
55	MG	2B	205	1/1	0.84	0.13	64,64,64,64	0
55	MG	2A	3374	1/1	0.84	0.13	65,65,65,65	0
55	MG	2A	3646	1/1	0.84	0.20	70,70,70,70	0
55	MG	1A	3654	1/1	0.84	0.13	36,36,36,36	0
55	MG	1a	1604	1/1	0.84	0.19	65,65,65,65	0
55	MG	2A	3141	1/1	0.84	0.30	69,69,69,69	0
55	MG	1A	3804	1/1	0.84	0.12	24,24,24,24	0
55	MG	2A	3674	1/1	0.84	0.15	57,57,57,57	0
55	MG	1a	1614	1/1	0.84	0.10	69,69,69,69	0
55	MG	2A	3161	1/1	0.84	0.30	50,50,50,50	0
55	MG	2A	3685	1/1	0.84	0.11	68,68,68,68	0
55	MG	2A	3462	1/1	0.84	0.24	60,60,60,60	0
55	MG	28	103	1/1	0.84	0.30	67,67,67,67	0
55	MG	2A	3274	1/1	0.84	0.09	54,54,54,54	0
55	MG	2a	3017	1/1	0.84	0.14	49,49,49,49	0
55	MG	2A	3280	1/1	0.84	0.17	70,70,70,70	0
55	MG	1A	4113	1/1	0.84	0.16	57,57,57,57	0
55	MG	1a	1775	1/1	0.84	0.18	59,59,59,59	0
55	MG	1a	1783	1/1	0.84	0.18	61,61,61,61	0
55	MG	2A	3716	1/1	0.84	0.10	64,64,64,64	0
55	MG	2A	3720	1/1	0.84	0.20	53,53,53,53	0
55	MG	2a	3041	1/1	0.84	0.10	55,55,55,55	0
55	MG	2A	3492	1/1	0.84	0.24	49,49,49,49	0
55	MG	2A	3077	1/1	0.84	0.13	64,64,64,64	0
55	MG	1a	1686	1/1	0.84	0.22	67,67,67,67	0
55	MG	2t	201	1/1	0.84	0.18	62,62,62,62	0
55	MG	1A	3465	1/1	0.84	0.24	57,57,57,57	0
55	MG	2A	3318	1/1	0.84	0.33	81,81,81,81	0
55	MG	2a	3030	1/1	0.85	0.17	60,60,60,60	0
55	MG	1a	1643	1/1	0.85	0.09	65,65,65,65	0
55	MG	1a	1753	1/1	0.85	0.20	67,67,67,67	0
55	MG	1a	1763	1/1	0.85	0.14	59,59,59,59	0
55	MG	2a	3044	1/1	0.85	0.12	78,78,78,78	0
55	MG	2a	3048	1/1	0.85	0.18	68,68,68,68	0
55	MG	1a	1644	1/1	0.85	0.14	72,72,72,72	0
55	MG	2a	3052	1/1	0.85	0.27	62,62,62,62	0
55	MG	1a	1656	1/1	0.85	0.18	59,59,59,59	0
55	MG	2A	3259	1/1	0.85	0.20	61,61,61,61	0
55	MG	1A	3912	1/1	0.85	0.13	27,27,27,27	0
55	MG	2A	3485	1/1	0.85	0.12	60,60,60,60	0
55	MG	1A	4038	1/1	0.85	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	3088	1/1	0.85	0.22	61,61,61,61	0
55	MG	2a	3090	1/1	0.85	0.12	72,72,72,72	0
55	MG	1A	4098	1/1	0.85	0.10	57,57,57,57	0
55	MG	1A	3239	1/1	0.85	0.18	35,35,35,35	0
55	MG	1A	3928	1/1	0.85	0.09	44,44,44,44	0
55	MG	2A	3115	1/1	0.85	0.16	42,42,42,42	0
55	MG	1a	1792	1/1	0.85	0.19	84,84,84,84	0
55	MG	2A	3806	1/1	0.85	0.22	37,37,37,37	0
55	MG	2a	3111	1/1	0.85	0.20	47,47,47,47	0
55	MG	1A	3930	1/1	0.85	0.20	53,53,53,53	0
55	MG	2A	3136	1/1	0.85	0.20	59,59,59,59	0
55	MG	2a	3124	1/1	0.85	0.24	49,49,49,49	0
55	MG	1A	3495	1/1	0.85	0.13	60,60,60,60	0
55	MG	2A	3315	1/1	0.85	0.10	69,69,69,69	0
55	MG	2A	3844	1/1	0.85	0.30	73,73,73,73	0
55	MG	2A	3847	1/1	0.85	0.18	72,72,72,72	0
55	MG	1A	3384	1/1	0.85	0.14	37,37,37,37	0
55	MG	1a	1703	1/1	0.85	0.19	66,66,66,66	0
55	MG	1a	1708	1/1	0.85	0.24	58,58,58,58	0
55	MG	2A	3861	1/1	0.85	0.12	50,50,50,50	0
55	MG	2a	3147	1/1	0.85	0.29	56,56,56,56	0
55	MG	1a	1832	1/1	0.85	0.14	61,61,61,61	0
55	MG	2B	202	1/1	0.85	0.15	43,43,43,43	0
55	MG	2A	3332	1/1	0.85	0.18	61,61,61,61	0
55	MG	2A	3342	1/1	0.85	0.07	47,47,47,47	0
55	MG	1A	3900	1/1	0.85	0.13	50,50,50,50	0
55	MG	2A	3618	1/1	0.85	0.23	28,28,28,28	0
55	MG	1f	201	1/1	0.85	0.24	64,64,64,64	0
55	MG	1n	102	1/1	0.85	0.13	66,66,66,66	0
55	MG	2A	3647	1/1	0.85	0.12	74,74,74,74	0
55	MG	1a	1621	1/1	0.85	0.22	72,72,72,72	0
55	MG	2A	3185	1/1	0.85	0.09	55,55,55,55	0
55	MG	1v	101	1/1	0.85	0.29	71,71,71,71	0
55	MG	1a	1717	1/1	0.85	0.13	62,62,62,62	0
55	MG	1A	3992	1/1	0.85	0.18	58,58,58,58	0
55	MG	2X	101	1/1	0.85	0.21	63,63,63,63	0
55	MG	2A	3675	1/1	0.85	0.28	58,58,58,58	0
55	MG	23	101	1/1	0.85	0.13	58,58,58,58	0
55	MG	2A	3375	1/1	0.85	0.20	65,65,65,65	0
55	MG	1A	3872	1/1	0.85	0.12	52,52,52,52	0
55	MG	1a	1726	1/1	0.85	0.22	54,54,54,54	0
55	MG	1P	202	1/1	0.85	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2r	101	1/1	0.85	0.24	66,66,66,66	0
55	MG	2A	3414	1/1	0.85	0.45	52,52,52,52	0
55	MG	2A	3698	1/1	0.85	0.23	64,64,64,64	0
55	MG	1U	202	1/1	0.85	0.52	49,49,49,49	0
55	MG	2A	3238	1/1	0.86	0.20	56,56,56,56	0
55	MG	1a	1668	1/1	0.86	0.09	62,62,62,62	0
55	MG	1A	3554	1/1	0.86	0.10	49,49,49,49	0
55	MG	1A	4104	1/1	0.86	0.12	46,46,46,46	0
55	MG	2A	3717	1/1	0.86	0.17	65,65,65,65	0
55	MG	1a	1673	1/1	0.86	0.28	59,59,59,59	0
55	MG	1a	1676	1/1	0.86	0.28	59,59,59,59	0
55	MG	2A	3472	1/1	0.86	0.29	60,60,60,60	0
55	MG	1A	3717	1/1	0.86	0.13	41,41,41,41	0
55	MG	1A	4109	1/1	0.86	0.12	50,50,50,50	0
55	MG	1a	1602	1/1	0.86	0.24	64,64,64,64	0
55	MG	1A	3938	1/1	0.86	0.23	28,28,28,28	0
55	MG	1a	1814	1/1	0.86	0.11	71,71,71,71	0
55	MG	2A	3776	1/1	0.86	0.14	59,59,59,59	0
55	MG	2A	3493	1/1	0.86	0.14	55,55,55,55	0
55	MG	1a	1608	1/1	0.86	0.14	57,57,57,57	0
55	MG	2A	3784	1/1	0.86	0.12	39,39,39,39	0
55	MG	2A	3499	1/1	0.86	0.22	59,59,59,59	0
55	MG	2A	3288	1/1	0.86	0.11	72,72,72,72	0
55	MG	2A	3133	1/1	0.86	0.12	62,62,62,62	0
55	MG	1A	3576	1/1	0.86	0.13	54,54,54,54	0
55	MG	1a	1704	1/1	0.86	0.41	59,59,59,59	0
55	MG	2A	3296	1/1	0.86	0.15	47,47,47,47	0
55	MG	2A	3299	1/1	0.86	0.20	53,53,53,53	0
55	MG	2A	3300	1/1	0.86	0.29	53,53,53,53	0
55	MG	2A	3142	1/1	0.86	0.28	54,54,54,54	0
55	MG	2A	3147	1/1	0.86	0.19	60,60,60,60	0
55	MG	1A	3512	1/1	0.86	0.10	56,56,56,56	0
55	MG	2A	3595	1/1	0.86	0.34	51,51,51,51	0
55	MG	1B	226	1/1	0.86	0.20	68,68,68,68	0
55	MG	2A	3598	1/1	0.86	0.15	59,59,59,59	0
55	MG	1b	301	1/1	0.86	0.15	74,74,74,74	0
55	MG	2a	3148	1/1	0.86	0.39	69,69,69,69	0
55	MG	1A	3982	1/1	0.86	0.11	26,26,26,26	0
55	MG	1A	3394	1/1	0.86	0.27	65,65,65,65	0
55	MG	2B	211	1/1	0.86	0.26	63,63,63,63	0
55	MG	2a	3160	1/1	0.86	0.09	81,81,81,81	0
55	MG	1A	3991	1/1	0.86	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3625	1/1	0.86	0.11	41,41,41,41	0
55	MG	2a	3165	1/1	0.86	0.12	77,77,77,77	0
55	MG	2A	3630	1/1	0.86	0.38	54,54,54,54	0
55	MG	1A	3264	1/1	0.86	0.08	41,41,41,41	0
55	MG	2E	304	1/1	0.86	0.25	60,60,60,60	0
55	MG	1A	3165	1/1	0.86	0.17	51,51,51,51	0
55	MG	2A	3350	1/1	0.86	0.16	55,55,55,55	0
55	MG	1x	101	1/1	0.86	0.26	59,59,59,59	0
55	MG	1T	203	1/1	0.86	0.14	56,56,56,56	0
55	MG	2A	3660	1/1	0.86	0.19	54,54,54,54	0
55	MG	2a	3198	1/1	0.86	0.17	66,66,66,66	0
55	MG	1a	1741	1/1	0.86	0.26	58,58,58,58	0
55	MG	2A	3364	1/1	0.86	0.23	56,56,56,56	0
55	MG	2A	3192	1/1	0.86	0.22	70,70,70,70	0
55	MG	2A	3043	1/1	0.86	0.12	49,49,49,49	0
55	MG	2a	3012	1/1	0.86	0.15	63,63,63,63	0
55	MG	1A	3857	1/1	0.86	0.14	42,42,42,42	0
55	MG	1a	1654	1/1	0.86	0.13	42,42,42,42	0
55	MG	1A	3231	1/1	0.86	0.13	55,55,55,55	0
55	MG	2p	101	1/1	0.86	0.14	51,51,51,51	0
55	MG	1V	204	1/1	0.86	0.14	65,65,65,65	0
55	MG	2A	3380	1/1	0.86	0.18	74,74,74,74	0
55	MG	2A	3232	1/1	0.86	0.15	58,58,58,58	0
55	MG	1a	1663	1/1	0.86	0.10	65,65,65,65	0
55	MG	1A	3788	1/1	0.87	0.17	51,51,51,51	0
55	MG	1a	1679	1/1	0.87	0.18	64,64,64,64	0
55	MG	1A	3539	1/1	0.87	0.20	48,48,48,48	0
55	MG	28	101	1/1	0.87	0.16	63,63,63,63	0
55	MG	2A	3322	1/1	0.87	0.24	57,57,57,57	0
55	MG	2A	3150	1/1	0.87	0.21	66,66,66,66	0
55	MG	2a	3005	1/1	0.87	0.21	53,53,53,53	0
55	MG	2A	3327	1/1	0.87	0.30	53,53,53,53	0
55	MG	2A	3330	1/1	0.87	0.12	63,63,63,63	0
55	MG	1A	3810	1/1	0.87	0.10	52,52,52,52	0
55	MG	2A	3341	1/1	0.87	0.14	56,56,56,56	0
55	MG	2A	3157	1/1	0.87	0.12	60,60,60,60	0
55	MG	1A	3819	1/1	0.87	0.14	52,52,52,52	0
55	MG	1A	4008	1/1	0.87	0.16	25,25,25,25	0
55	MG	2a	3032	1/1	0.87	0.24	58,58,58,58	0
55	MG	2a	3034	1/1	0.87	0.27	56,56,56,56	0
55	MG	1A	4018	1/1	0.87	0.38	57,57,57,57	0
55	MG	1A	3298	1/1	0.87	0.20	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	1n	101	1/1	0.87	0.49	78,78,78,78	0
55	MG	1A	3839	1/1	0.87	0.20	64,64,64,64	0
55	MG	2A	3362	1/1	0.87	0.13	57,57,57,57	0
55	MG	1A	3431	1/1	0.87	0.07	36,36,36,36	0
55	MG	2A	3183	1/1	0.87	0.21	53,53,53,53	0
55	MG	1A	3016	1/1	0.87	0.17	55,55,55,55	0
55	MG	1A	3241	1/1	0.87	0.12	42,42,42,42	0
55	MG	1A	3585	1/1	0.87	0.21	44,44,44,44	0
55	MG	2A	3376	1/1	0.87	0.20	60,60,60,60	0
55	MG	2A	3191	1/1	0.87	0.10	62,62,62,62	0
55	MG	2a	3087	1/1	0.87	0.25	61,61,61,61	0
55	MG	1x	107	1/1	0.87	0.18	66,66,66,66	0
55	MG	2A	3200	1/1	0.87	0.25	66,66,66,66	0
55	MG	2A	3382	1/1	0.87	0.14	66,66,66,66	0
55	MG	1a	1723	1/1	0.87	0.23	49,49,49,49	0
55	MG	2a	3098	1/1	0.87	0.25	62,62,62,62	0
55	MG	2A	3718	1/1	0.87	0.17	57,57,57,57	0
55	MG	2A	3202	1/1	0.87	0.13	55,55,55,55	0
55	MG	2A	3423	1/1	0.87	0.21	48,48,48,48	0
55	MG	1A	3592	1/1	0.87	0.17	50,50,50,50	0
55	MG	2A	3445	1/1	0.87	0.15	52,52,52,52	0
55	MG	2A	3036	1/1	0.87	0.10	49,49,49,49	0
55	MG	2A	3457	1/1	0.87	0.21	62,62,62,62	0
55	MG	2A	3039	1/1	0.87	0.13	49,49,49,49	0
55	MG	2A	3766	1/1	0.87	0.19	47,47,47,47	0
55	MG	2A	3768	1/1	0.87	0.15	58,58,58,58	0
55	MG	1A	3060	1/1	0.87	0.29	46,46,46,46	0
55	MG	1A	3329	1/1	0.87	0.24	58,58,58,58	0
55	MG	2A	3063	1/1	0.87	0.25	50,50,50,50	0
55	MG	1A	3256	1/1	0.87	0.16	37,37,37,37	0
55	MG	2A	3069	1/1	0.87	0.10	41,41,41,41	0
55	MG	2a	3143	1/1	0.87	0.27	56,56,56,56	0
55	MG	2A	3250	1/1	0.87	0.10	56,56,56,56	0
55	MG	1A	3081	1/1	0.87	0.11	57,57,57,57	0
55	MG	2A	3071	1/1	0.87	0.17	55,55,55,55	0
55	MG	1a	1650	1/1	0.87	0.24	69,69,69,69	0
55	MG	2a	3152	1/1	0.87	0.23	45,45,45,45	0
55	MG	1A	3655	1/1	0.87	0.09	30,30,30,30	0
55	MG	2A	3841	1/1	0.87	0.10	57,57,57,57	0
55	MG	1A	3904	1/1	0.87	0.14	20,20,20,20	0
55	MG	1B	231	1/1	0.87	0.13	30,30,30,30	0
55	MG	2A	3505	1/1	0.87	0.18	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	2A	3085	1/1	0.87	0.11	60,60,60,60	0
55	MG	2A	3520	1/1	0.87	0.12	44,44,44,44	0
55	MG	2A	3856	1/1	0.87	0.30	63,63,63,63	0
55	MG	1a	1770	1/1	0.87	0.13	65,65,65,65	0
55	MG	1A	3502	1/1	0.87	0.10	45,45,45,45	0
55	MG	2a	3177	1/1	0.87	0.10	64,64,64,64	0
55	MG	1a	1667	1/1	0.87	0.17	61,61,61,61	0
55	MG	2a	3185	1/1	0.87	0.12	58,58,58,58	0
55	MG	1A	3350	1/1	0.87	0.20	62,62,62,62	0
55	MG	2A	3550	1/1	0.87	0.20	37,37,37,37	0
55	MG	2a	3193	1/1	0.87	0.19	47,47,47,47	0
55	MG	1a	1786	1/1	0.87	0.18	74,74,74,74	0
55	MG	2A	3106	1/1	0.87	0.10	62,62,62,62	0
55	MG	1A	3376	1/1	0.87	0.10	39,39,39,39	0
55	MG	2A	3568	1/1	0.87	0.15	38,38,38,38	0
55	MG	1A	3737	1/1	0.87	0.11	23,23,23,23	0
55	MG	2A	3571	1/1	0.87	0.17	69,69,69,69	0
55	MG	1A	3282	1/1	0.87	0.24	58,58,58,58	0
55	MG	2A	3586	1/1	0.87	0.13	66,66,66,66	0
55	MG	2F	302	1/1	0.87	0.11	43,43,43,43	0
55	MG	1a	1795	1/1	0.87	0.13	79,79,79,79	0
55	MG	1A	3088	1/1	0.87	0.23	35,35,35,35	0
55	MG	1A	3776	1/1	0.87	0.10	60,60,60,60	0
55	MG	2A	3599	1/1	0.87	0.19	60,60,60,60	0
55	MG	2W	201	1/1	0.87	0.09	36,36,36,36	0
55	MG	2W	202	1/1	0.87	0.21	52,52,52,52	0
57	V7A	1a	1835	35/35	0.87	0.16	65,73,81,85	0
57	V7A	2a	3210	35/35	0.87	0.17	68,82,90,91	0
55	MG	1A	4084	1/1	0.88	0.13	43,43,43,43	0
55	MG	1A	4088	1/1	0.88	0.12	28,28,28,28	0
55	MG	2A	3333	1/1	0.88	0.20	58,58,58,58	0
55	MG	2A	3627	1/1	0.88	0.19	39,39,39,39	0
55	MG	1A	3170	1/1	0.88	0.16	47,47,47,47	0
55	MG	1A	3505	1/1	0.88	0.22	65,65,65,65	0
55	MG	1a	1657	1/1	0.88	0.26	56,56,56,56	0
55	MG	2a	3018	1/1	0.88	0.10	60,60,60,60	0
55	MG	2A	3152	1/1	0.88	0.18	59,59,59,59	0
55	MG	2a	3023	1/1	0.88	0.27	60,60,60,60	0
55	MG	1A	3877	1/1	0.88	0.18	40,40,40,40	0
55	MG	2A	3353	1/1	0.88	0.12	61,61,61,61	0
55	MG	1A	3262	1/1	0.88	0.09	54,54,54,54	0
55	MG	1a	1666	1/1	0.88	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3162	1/1	0.88	0.29	66,66,66,66	0
55	MG	2A	3671	1/1	0.88	0.32	60,60,60,60	0
55	MG	1a	1825	1/1	0.88	0.19	58,58,58,58	0
55	MG	1A	3028	1/1	0.88	0.13	65,65,65,65	0
55	MG	1A	3708	1/1	0.88	0.16	25,25,25,25	0
55	MG	1A	3413	1/1	0.88	0.11	55,55,55,55	0
55	MG	2a	3047	1/1	0.88	0.37	67,67,67,67	0
55	MG	2A	3681	1/1	0.88	0.10	37,37,37,37	0
55	MG	2a	3049	1/1	0.88	0.21	67,67,67,67	0
55	MG	2A	3174	1/1	0.88	0.34	58,58,58,58	0
55	MG	1B	224	1/1	0.88	0.11	53,53,53,53	0
55	MG	2a	3056	1/1	0.88	0.21	47,47,47,47	0
55	MG	2a	3058	1/1	0.88	0.14	52,52,52,52	0
55	MG	1A	3735	1/1	0.88	0.12	58,58,58,58	0
55	MG	1A	3268	1/1	0.88	0.11	46,46,46,46	0
55	MG	1A	3915	1/1	0.88	0.11	25,25,25,25	0
55	MG	2a	3076	1/1	0.88	0.20	50,50,50,50	0
55	MG	1A	3434	1/1	0.88	0.21	51,51,51,51	0
55	MG	1A	3436	1/1	0.88	0.17	45,45,45,45	0
55	MG	1A	3445	1/1	0.88	0.24	51,51,51,51	0
55	MG	2A	3403	1/1	0.88	0.17	55,55,55,55	0
55	MG	1a	1684	1/1	0.88	0.22	49,49,49,49	0
55	MG	2A	3422	1/1	0.88	0.13	51,51,51,51	0
55	MG	1G	203	1/1	0.88	0.14	50,50,50,50	0
55	MG	2a	3093	1/1	0.88	0.14	51,51,51,51	0
55	MG	2A	3432	1/1	0.88	0.22	50,50,50,50	0
55	MG	2A	3729	1/1	0.88	0.27	51,51,51,51	0
55	MG	2a	3102	1/1	0.88	0.20	67,67,67,67	0
55	MG	2a	3103	1/1	0.88	0.22	54,54,54,54	0
55	MG	1O	202	1/1	0.88	0.13	56,56,56,56	0
55	MG	2A	3205	1/1	0.88	0.19	51,51,51,51	0
55	MG	2A	3738	1/1	0.88	0.10	50,50,50,50	0
55	MG	2A	3447	1/1	0.88	0.29	71,71,71,71	0
55	MG	2A	3448	1/1	0.88	0.14	49,49,49,49	0
55	MG	2A	3219	1/1	0.88	0.07	50,50,50,50	0
55	MG	1A	3096	1/1	0.88	0.18	60,60,60,60	0
55	MG	1A	3567	1/1	0.88	0.15	31,31,31,31	0
55	MG	2A	3771	1/1	0.88	0.14	56,56,56,56	0
55	MG	2A	3003	1/1	0.88	0.20	50,50,50,50	0
55	MG	1A	3946	1/1	0.88	0.10	50,50,50,50	0
55	MG	2A	3231	1/1	0.88	0.17	65,65,65,65	0
55	MG	2a	3134	1/1	0.88	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3467	1/1	0.88	0.35	64,64,64,64	0
55	MG	1A	3569	1/1	0.88	0.29	40,40,40,40	0
55	MG	2a	3140	1/1	0.88	0.41	59,59,59,59	0
55	MG	2a	3141	1/1	0.88	0.22	66,66,66,66	0
55	MG	2A	3793	1/1	0.88	0.13	49,49,49,49	0
55	MG	1V	203	1/1	0.88	0.14	47,47,47,47	0
55	MG	2A	3813	1/1	0.88	0.13	52,52,52,52	0
55	MG	2A	3044	1/1	0.88	0.26	66,66,66,66	0
55	MG	1A	3039	1/1	0.88	0.12	57,57,57,57	0
55	MG	1A	3984	1/1	0.88	0.19	53,53,53,53	0
55	MG	2a	3157	1/1	0.88	0.12	61,61,61,61	0
55	MG	1l	104	1/1	0.88	0.16	62,62,62,62	0
55	MG	1A	3288	1/1	0.88	0.13	40,40,40,40	0
55	MG	1A	3989	1/1	0.88	0.15	36,36,36,36	0
55	MG	1A	3589	1/1	0.88	0.15	28,28,28,28	0
55	MG	1a	1730	1/1	0.88	0.37	60,60,60,60	0
55	MG	1a	1731	1/1	0.88	0.25	63,63,63,63	0
55	MG	1A	3847	1/1	0.88	0.10	35,35,35,35	0
55	MG	2A	3855	1/1	0.88	0.15	52,52,52,52	0
55	MG	1a	1744	1/1	0.88	0.15	50,50,50,50	0
55	MG	2A	3860	1/1	0.88	0.10	43,43,43,43	0
55	MG	1a	1745	1/1	0.88	0.21	62,62,62,62	0
55	MG	2A	3086	1/1	0.88	0.25	66,66,66,66	0
55	MG	1A	3850	1/1	0.88	0.09	56,56,56,56	0
55	MG	1a	1749	1/1	0.88	0.14	56,56,56,56	0
55	MG	1A	3361	1/1	0.88	0.12	56,56,56,56	0
55	MG	2A	3552	1/1	0.88	0.17	38,38,38,38	0
55	MG	2A	3293	1/1	0.88	0.19	68,68,68,68	0
55	MG	2A	3558	1/1	0.88	0.12	36,36,36,36	0
55	MG	2a	3202	1/1	0.88	0.37	76,76,76,76	0
55	MG	1A	3489	1/1	0.88	0.31	40,40,40,40	0
55	MG	1A	3369	1/1	0.88	0.12	49,49,49,49	0
55	MG	2a	3207	1/1	0.88	0.21	53,53,53,53	0
55	MG	1A	3255	1/1	0.88	0.14	53,53,53,53	0
55	MG	2A	3107	1/1	0.88	0.11	74,74,74,74	0
55	MG	2A	3108	1/1	0.88	0.09	61,61,61,61	0
55	MG	1A	4041	1/1	0.88	0.09	74,74,74,74	0
55	MG	1A	4045	1/1	0.88	0.09	49,49,49,49	0
55	MG	1A	4050	1/1	0.88	0.31	70,70,70,70	0
55	MG	2N	201	1/1	0.88	0.29	62,62,62,62	0
55	MG	2q	201	1/1	0.88	0.21	67,67,67,67	0
55	MG	1A	4061	1/1	0.88	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3131	1/1	0.88	0.07	64,64,64,64	0
55	MG	1A	4076	1/1	0.88	0.10	61,61,61,61	0
55	MG	2A	3606	1/1	0.88	0.23	39,39,39,39	0
55	MG	2A	3607	1/1	0.88	0.22	49,49,49,49	0
55	MG	1A	4081	1/1	0.88	0.15	43,43,43,43	0
55	MG	2A	3617	1/1	0.89	0.10	23,23,23,23	0
55	MG	1x	105	1/1	0.89	0.24	65,65,65,65	0
55	MG	2A	3347	1/1	0.89	0.10	46,46,46,46	0
55	MG	1A	3897	1/1	0.89	0.25	28,28,28,28	0
55	MG	1A	4062	1/1	0.89	0.08	37,37,37,37	0
55	MG	1x	111	1/1	0.89	0.17	65,65,65,65	0
55	MG	2A	3172	1/1	0.89	0.23	41,41,41,41	0
55	MG	2a	3019	1/1	0.89	0.25	60,60,60,60	0
55	MG	1A	3419	1/1	0.89	0.10	46,46,46,46	0
55	MG	2A	3648	1/1	0.89	0.16	55,55,55,55	0
55	MG	1A	3785	1/1	0.89	0.15	46,46,46,46	0
55	MG	2A	3005	1/1	0.89	0.11	38,38,38,38	0
55	MG	2A	3659	1/1	0.89	0.36	44,44,44,44	0
55	MG	2A	3020	1/1	0.89	0.15	54,54,54,54	0
55	MG	2A	3021	1/1	0.89	0.13	40,40,40,40	0
55	MG	2A	3025	1/1	0.89	0.15	56,56,56,56	0
55	MG	2a	3035	1/1	0.89	0.13	63,63,63,63	0
55	MG	2A	3372	1/1	0.89	0.25	59,59,59,59	0
55	MG	1A	3601	1/1	0.89	0.13	56,56,56,56	0
55	MG	1A	3481	1/1	0.89	0.14	56,56,56,56	0
55	MG	2a	3043	1/1	0.89	0.13	60,60,60,60	0
55	MG	2A	3199	1/1	0.89	0.09	52,52,52,52	0
55	MG	2a	3046	1/1	0.89	0.08	56,56,56,56	0
55	MG	1a	1624	1/1	0.89	0.10	59,59,59,59	0
55	MG	1A	3808	1/1	0.89	0.15	40,40,40,40	0
55	MG	1A	3919	1/1	0.89	0.09	33,33,33,33	0
55	MG	1A	4105	1/1	0.89	0.11	53,53,53,53	0
55	MG	2A	3215	1/1	0.89	0.16	69,69,69,69	0
55	MG	2A	3218	1/1	0.89	0.24	49,49,49,49	0
55	MG	2A	3405	1/1	0.89	0.24	57,57,57,57	0
55	MG	2A	3406	1/1	0.89	0.24	45,45,45,45	0
55	MG	2A	3066	1/1	0.89	0.15	43,43,43,43	0
55	MG	2A	3418	1/1	0.89	0.16	56,56,56,56	0
55	MG	1A	3922	1/1	0.89	0.11	38,38,38,38	0
55	MG	2a	3079	1/1	0.89	0.40	61,61,61,61	0
55	MG	1A	3609	1/1	0.89	0.15	27,27,27,27	0
55	MG	2A	3425	1/1	0.89	0.19	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	3427	1/1	0.89	0.36	54,54,54,54	0
55	MG	2A	3721	1/1	0.89	0.16	48,48,48,48	0
55	MG	1A	3818	1/1	0.89	0.14	40,40,40,40	0
55	MG	1A	3486	1/1	0.89	0.15	56,56,56,56	0
55	MG	2A	3076	1/1	0.89	0.11	75,75,75,75	0
55	MG	2A	3732	1/1	0.89	0.14	44,44,44,44	0
55	MG	2A	3734	1/1	0.89	0.17	42,42,42,42	0
55	MG	1B	209	1/1	0.89	0.25	53,53,53,53	0
55	MG	1B	214	1/1	0.89	0.22	51,51,51,51	0
55	MG	2A	3081	1/1	0.89	0.22	69,69,69,69	0
55	MG	1A	3932	1/1	0.89	0.35	38,38,38,38	0
55	MG	2a	3107	1/1	0.89	0.24	65,65,65,65	0
55	MG	2A	3743	1/1	0.89	0.17	69,69,69,69	0
55	MG	2A	3754	1/1	0.89	0.27	48,48,48,48	0
55	MG	2A	3758	1/1	0.89	0.12	53,53,53,53	0
55	MG	2A	3459	1/1	0.89	0.43	52,52,52,52	0
55	MG	1A	3524	1/1	0.89	0.26	59,59,59,59	0
55	MG	1A	3644	1/1	0.89	0.14	21,21,21,21	0
55	MG	1A	3842	1/1	0.89	0.43	35,35,35,35	0
55	MG	2A	3254	1/1	0.89	0.16	49,49,49,49	0
55	MG	2A	3255	1/1	0.89	0.17	61,61,61,61	0
55	MG	1A	3371	1/1	0.89	0.14	40,40,40,40	0
55	MG	1A	3185	1/1	0.89	0.22	50,50,50,50	0
55	MG	1A	3492	1/1	0.89	0.10	47,47,47,47	0
55	MG	2A	3265	1/1	0.89	0.19	56,56,56,56	0
55	MG	1A	3852	1/1	0.89	0.08	39,39,39,39	0
55	MG	2A	3807	1/1	0.89	0.12	36,36,36,36	0
55	MG	2A	3268	1/1	0.89	0.12	68,68,68,68	0
55	MG	2a	3142	1/1	0.89	0.19	54,54,54,54	0
55	MG	2A	3816	1/1	0.89	0.26	54,54,54,54	0
55	MG	2A	3269	1/1	0.89	0.11	55,55,55,55	0
55	MG	2A	3494	1/1	0.89	0.15	64,64,64,64	0
55	MG	2A	3496	1/1	0.89	0.10	53,53,53,53	0
55	MG	2a	3149	1/1	0.89	0.10	59,59,59,59	0
55	MG	1F	310	1/1	0.89	0.21	46,46,46,46	0
55	MG	1A	3493	1/1	0.89	0.15	45,45,45,45	0
55	MG	2A	3275	1/1	0.89	0.10	64,64,64,64	0
55	MG	2A	3513	1/1	0.89	0.12	43,43,43,43	0
55	MG	2A	3276	1/1	0.89	0.26	60,60,60,60	0
55	MG	1a	1804	1/1	0.89	0.14	49,49,49,49	0
55	MG	1a	1806	1/1	0.89	0.14	43,43,43,43	0
55	MG	1A	3027	1/1	0.89	0.26	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3496	1/1	0.89	0.16	59,59,59,59	0
55	MG	2A	3858	1/1	0.89	0.13	68,68,68,68	0
55	MG	2A	3859	1/1	0.89	0.20	53,53,53,53	0
55	MG	1A	3862	1/1	0.89	0.11	52,52,52,52	0
55	MG	2A	3548	1/1	0.89	0.12	39,39,39,39	0
55	MG	2A	3291	1/1	0.89	0.21	47,47,47,47	0
55	MG	2a	3179	1/1	0.89	0.19	54,54,54,54	0
55	MG	1A	4012	1/1	0.89	0.18	47,47,47,47	0
55	MG	2a	3183	1/1	0.89	0.15	53,53,53,53	0
55	MG	1A	3497	1/1	0.89	0.11	31,31,31,31	0
55	MG	1A	4019	1/1	0.89	0.11	28,28,28,28	0
55	MG	1a	1692	1/1	0.89	0.16	55,55,55,55	0
55	MG	1a	1698	1/1	0.89	0.20	51,51,51,51	0
55	MG	1A	3002	1/1	0.89	0.11	49,49,49,49	0
55	MG	2A	3145	1/1	0.89	0.31	51,51,51,51	0
55	MG	2A	3146	1/1	0.89	0.18	42,42,42,42	0
55	MG	1Y	201	1/1	0.89	0.08	48,48,48,48	0
55	MG	2A	3148	1/1	0.89	0.07	48,48,48,48	0
55	MG	2E	301	1/1	0.89	0.20	55,55,55,55	0
55	MG	2A	3321	1/1	0.89	0.06	70,70,70,70	0
55	MG	2F	301	1/1	0.89	0.12	49,49,49,49	0
55	MG	2A	3149	1/1	0.89	0.12	61,61,61,61	0
55	MG	2e	201	1/1	0.89	0.07	80,80,80,80	0
55	MG	1l	202	1/1	0.89	0.18	61,61,61,61	0
55	MG	1A	3180	1/1	0.89	0.15	49,49,49,49	0
55	MG	1A	3290	1/1	0.89	0.25	48,48,48,48	0
55	MG	1A	3883	1/1	0.89	0.21	30,30,30,30	0
55	MG	2T	202	1/1	0.89	0.18	59,59,59,59	0
55	MG	1A	3892	1/1	0.89	0.14	36,36,36,36	0
55	MG	2A	3609	1/1	0.89	0.22	33,33,33,33	0
55	MG	2A	3610	1/1	0.89	0.17	59,59,59,59	0
55	MG	1A	3764	1/1	0.89	0.09	45,45,45,45	0
55	MG	2x	105	1/1	0.89	0.24	67,67,67,67	0
55	MG	2A	3613	1/1	0.89	0.11	40,40,40,40	0
55	MG	1A	4058	1/1	0.89	0.13	38,38,38,38	0
55	MG	1A	3466	1/1	0.90	0.09	50,50,50,50	0
55	MG	1a	1820	1/1	0.90	0.20	66,66,66,66	0
55	MG	2A	3611	1/1	0.90	0.10	47,47,47,47	0
55	MG	2A	3334	1/1	0.90	0.19	64,64,64,64	0
55	MG	2A	3338	1/1	0.90	0.07	52,52,52,52	0
55	MG	28	102	1/1	0.90	0.41	59,59,59,59	0
55	MG	2A	3614	1/1	0.90	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	1824	1/1	0.90	0.15	64,64,64,64	0
55	MG	1A	3476	1/1	0.90	0.10	45,45,45,45	0
55	MG	2a	3006	1/1	0.90	0.21	57,57,57,57	0
55	MG	2A	3344	1/1	0.90	0.24	45,45,45,45	0
55	MG	2a	3013	1/1	0.90	0.17	56,56,56,56	0
55	MG	2a	3015	1/1	0.90	0.19	55,55,55,55	0
55	MG	1a	1826	1/1	0.90	0.23	45,45,45,45	0
55	MG	2A	3156	1/1	0.90	0.12	58,58,58,58	0
55	MG	2A	3628	1/1	0.90	0.16	33,33,33,33	0
55	MG	1a	1827	1/1	0.90	0.20	48,48,48,48	0
55	MG	1a	1828	1/1	0.90	0.09	50,50,50,50	0
55	MG	1A	3740	1/1	0.90	0.10	34,34,34,34	0
55	MG	2a	3025	1/1	0.90	0.21	55,55,55,55	0
55	MG	2a	3027	1/1	0.90	0.29	50,50,50,50	0
55	MG	1A	3326	1/1	0.90	0.16	40,40,40,40	0
55	MG	1A	3516	1/1	0.90	0.17	69,69,69,69	0
55	MG	2A	3650	1/1	0.90	0.10	56,56,56,56	0
55	MG	2A	3360	1/1	0.90	0.20	56,56,56,56	0
55	MG	1a	1833	1/1	0.90	0.16	61,61,61,61	0
55	MG	1E	306	1/1	0.90	0.14	22,22,22,22	0
55	MG	1a	1675	1/1	0.90	0.25	57,57,57,57	0
55	MG	1A	4011	1/1	0.90	0.12	57,57,57,57	0
55	MG	2A	3173	1/1	0.90	0.13	44,44,44,44	0
55	MG	2A	3670	1/1	0.90	0.20	49,49,49,49	0
55	MG	1A	3748	1/1	0.90	0.18	45,45,45,45	0
55	MG	1G	204	1/1	0.90	0.11	50,50,50,50	0
55	MG	1O	201	1/1	0.90	0.31	45,45,45,45	0
55	MG	1A	4015	1/1	0.90	0.13	39,39,39,39	0
55	MG	1a	1683	1/1	0.90	0.22	46,46,46,46	0
55	MG	1A	3762	1/1	0.90	0.10	54,54,54,54	0
55	MG	2A	3682	1/1	0.90	0.14	59,59,59,59	0
55	MG	2A	3683	1/1	0.90	0.08	79,79,79,79	0
55	MG	1Q	203	1/1	0.90	0.09	55,55,55,55	0
55	MG	2a	3060	1/1	0.90	0.31	63,63,63,63	0
55	MG	1T	202	1/1	0.90	0.07	44,44,44,44	0
55	MG	1A	3878	1/1	0.90	0.16	57,57,57,57	0
55	MG	2a	3064	1/1	0.90	0.16	46,46,46,46	0
55	MG	2a	3066	1/1	0.90	0.14	61,61,61,61	0
55	MG	2A	3392	1/1	0.90	0.21	31,31,31,31	0
55	MG	2a	3075	1/1	0.90	0.12	59,59,59,59	0
55	MG	2A	3402	1/1	0.90	0.24	47,47,47,47	0
55	MG	1a	1701	1/1	0.90	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3602	1/1	0.90	0.14	39,39,39,39	0
55	MG	1A	3775	1/1	0.90	0.09	19,19,19,19	0
55	MG	2A	3412	1/1	0.90	0.22	55,55,55,55	0
55	MG	2A	3002	1/1	0.90	0.17	53,53,53,53	0
55	MG	2a	3089	1/1	0.90	0.14	59,59,59,59	0
55	MG	1A	4029	1/1	0.90	0.07	42,42,42,42	0
55	MG	2A	3719	1/1	0.90	0.16	70,70,70,70	0
55	MG	1A	3890	1/1	0.90	0.11	52,52,52,52	0
55	MG	2A	3013	1/1	0.90	0.13	51,51,51,51	0
55	MG	2a	3096	1/1	0.90	0.07	44,44,44,44	0
55	MG	1a	1710	1/1	0.90	0.06	53,53,53,53	0
55	MG	2a	3099	1/1	0.90	0.19	66,66,66,66	0
55	MG	1A	3519	1/1	0.90	0.09	48,48,48,48	0
55	MG	2A	3228	1/1	0.90	0.09	58,58,58,58	0
55	MG	2A	3023	1/1	0.90	0.10	49,49,49,49	0
55	MG	1A	3182	1/1	0.90	0.07	38,38,38,38	0
55	MG	1a	1716	1/1	0.90	0.28	56,56,56,56	0
55	MG	2A	3737	1/1	0.90	0.19	50,50,50,50	0
55	MG	1A	3095	1/1	0.90	0.20	51,51,51,51	0
55	MG	1A	3796	1/1	0.90	0.10	34,34,34,34	0
55	MG	17	101	1/1	0.90	0.21	54,54,54,54	0
55	MG	2A	3045	1/1	0.90	0.17	57,57,57,57	0
55	MG	1A	3800	1/1	0.90	0.10	22,22,22,22	0
55	MG	1a	1724	1/1	0.90	0.18	49,49,49,49	0
55	MG	2A	3463	1/1	0.90	0.22	25,25,25,25	0
55	MG	1A	3084	1/1	0.90	0.21	33,33,33,33	0
55	MG	2A	3067	1/1	0.90	0.13	53,53,53,53	0
55	MG	1A	3109	1/1	0.90	0.22	50,50,50,50	0
55	MG	2A	3468	1/1	0.90	0.35	51,51,51,51	0
55	MG	2A	3775	1/1	0.90	0.16	74,74,74,74	0
55	MG	2a	3137	1/1	0.90	0.17	58,58,58,58	0
55	MG	1A	4079	1/1	0.90	0.20	61,61,61,61	0
55	MG	1A	3914	1/1	0.90	0.12	35,35,35,35	0
55	MG	1a	1740	1/1	0.90	0.32	42,42,42,42	0
55	MG	2A	3783	1/1	0.90	0.09	72,72,72,72	0
55	MG	2A	3264	1/1	0.90	0.31	55,55,55,55	0
55	MG	1A	3292	1/1	0.90	0.24	29,29,29,29	0
55	MG	2A	3801	1/1	0.90	0.14	51,51,51,51	0
55	MG	2A	3488	1/1	0.90	0.20	73,73,73,73	0
55	MG	1A	3367	1/1	0.90	0.13	34,34,34,34	0
55	MG	1A	4089	1/1	0.90	0.26	39,39,39,39	0
55	MG	1a	1619	1/1	0.90	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	3154	1/1	0.90	0.19	47,47,47,47	0
55	MG	1A	3662	1/1	0.90	0.10	42,42,42,42	0
55	MG	2A	3826	1/1	0.90	0.14	72,72,72,72	0
55	MG	1A	4102	1/1	0.90	0.09	38,38,38,38	0
55	MG	1a	1625	1/1	0.90	0.13	58,58,58,58	0
55	MG	2A	3834	1/1	0.90	0.10	29,29,29,29	0
55	MG	1a	1758	1/1	0.90	0.12	51,51,51,51	0
55	MG	1A	3668	1/1	0.90	0.11	49,49,49,49	0
55	MG	2a	3167	1/1	0.90	0.11	50,50,50,50	0
55	MG	2A	3282	1/1	0.90	0.12	72,72,72,72	0
55	MG	2A	3283	1/1	0.90	0.39	54,54,54,54	0
55	MG	1A	3833	1/1	0.90	0.14	52,52,52,52	0
55	MG	1a	1766	1/1	0.90	0.19	49,49,49,49	0
55	MG	1A	3221	1/1	0.90	0.18	54,54,54,54	0
55	MG	2A	3537	1/1	0.90	0.28	54,54,54,54	0
55	MG	1a	1641	1/1	0.90	0.21	60,60,60,60	0
55	MG	2A	3541	1/1	0.90	0.13	40,40,40,40	0
55	MG	2A	3543	1/1	0.90	0.11	35,35,35,35	0
55	MG	2a	3188	1/1	0.90	0.26	60,60,60,60	0
55	MG	2A	3545	1/1	0.90	0.16	45,45,45,45	0
55	MG	2A	3099	1/1	0.90	0.13	54,54,54,54	0
55	MG	2A	3292	1/1	0.90	0.12	45,45,45,45	0
55	MG	1A	3117	1/1	0.90	0.17	31,31,31,31	0
55	MG	1A	3844	1/1	0.90	0.07	45,45,45,45	0
55	MG	2a	3199	1/1	0.90	0.30	69,69,69,69	0
55	MG	1A	3703	1/1	0.90	0.11	41,41,41,41	0
55	MG	1a	1645	1/1	0.90	0.18	70,70,70,70	0
55	MG	1a	1649	1/1	0.90	0.30	61,61,61,61	0
55	MG	2A	3567	1/1	0.90	0.18	38,38,38,38	0
55	MG	1A	3229	1/1	0.90	0.09	51,51,51,51	0
55	MG	2A	3312	1/1	0.90	0.09	51,51,51,51	0
55	MG	1B	210	1/1	0.90	0.18	50,50,50,50	0
55	MG	2A	3581	1/1	0.90	0.13	55,55,55,55	0
55	MG	2g	201	1/1	0.90	0.08	73,73,73,73	0
55	MG	1A	3715	1/1	0.90	0.11	40,40,40,40	0
55	MG	1A	3949	1/1	0.90	0.14	56,56,56,56	0
55	MG	1a	1658	1/1	0.90	0.23	76,76,76,76	0
55	MG	1A	3024	1/1	0.90	0.12	23,23,23,23	0
55	MG	1A	3854	1/1	0.90	0.11	33,33,33,33	0
55	MG	1a	1808	1/1	0.90	0.11	67,67,67,67	0
55	MG	2A	3601	1/1	0.90	0.09	57,57,57,57	0
55	MG	2O	201	1/1	0.90	0.22	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2x	102	1/1	0.90	0.16	73,73,73,73	0
55	MG	2A	3602	1/1	0.90	0.10	65,65,65,65	0
55	MG	1a	1812	1/1	0.90	0.15	71,71,71,71	0
55	MG	1a	1664	1/1	0.90	0.18	68,68,68,68	0
55	MG	2A	3331	1/1	0.90	0.26	64,64,64,64	0
55	MG	1A	3579	1/1	0.91	0.17	45,45,45,45	0
55	MG	1A	3583	1/1	0.91	0.17	36,36,36,36	0
55	MG	2V	201	1/1	0.91	0.38	62,62,62,62	0
55	MG	1a	1606	1/1	0.91	0.11	49,49,49,49	0
55	MG	1a	1607	1/1	0.91	0.08	75,75,75,75	0
55	MG	1a	1784	1/1	0.91	0.19	58,58,58,58	0
55	MG	1A	3234	1/1	0.91	0.14	29,29,29,29	0
55	MG	2A	3339	1/1	0.91	0.27	60,60,60,60	0
55	MG	1a	1611	1/1	0.91	0.07	43,43,43,43	0
55	MG	1A	4016	1/1	0.91	0.13	22,22,22,22	0
55	MG	1A	3286	1/1	0.91	0.18	40,40,40,40	0
55	MG	1a	1794	1/1	0.91	0.08	50,50,50,50	0
55	MG	1A	3590	1/1	0.91	0.07	31,31,31,31	0
55	MG	1A	3834	1/1	0.91	0.16	33,33,33,33	0
55	MG	2a	3007	1/1	0.91	0.26	59,59,59,59	0
55	MG	2a	3008	1/1	0.91	0.13	62,62,62,62	0
55	MG	2A	3349	1/1	0.91	0.08	45,45,45,45	0
55	MG	1A	3482	1/1	0.91	0.11	50,50,50,50	0
55	MG	2A	3632	1/1	0.91	0.11	53,53,53,53	0
55	MG	2A	3638	1/1	0.91	0.19	53,53,53,53	0
55	MG	2A	3639	1/1	0.91	0.15	67,67,67,67	0
55	MG	2A	3352	1/1	0.91	0.23	43,43,43,43	0
55	MG	1A	3596	1/1	0.91	0.18	43,43,43,43	0
55	MG	1A	4034	1/1	0.91	0.20	57,57,57,57	0
55	MG	2A	3357	1/1	0.91	0.07	44,44,44,44	0
55	MG	1a	1626	1/1	0.91	0.10	48,48,48,48	0
55	MG	1A	3103	1/1	0.91	0.29	58,58,58,58	0
55	MG	1A	4040	1/1	0.91	0.09	57,57,57,57	0
55	MG	1A	3487	1/1	0.91	0.11	44,44,44,44	0
55	MG	1A	3190	1/1	0.91	0.73	34,34,34,34	0
55	MG	2a	3031	1/1	0.91	0.17	51,51,51,51	0
55	MG	2A	3662	1/1	0.91	0.12	63,63,63,63	0
55	MG	1a	1821	1/1	0.91	0.11	53,53,53,53	0
55	MG	1A	3208	1/1	0.91	0.14	64,64,64,64	0
55	MG	2A	3371	1/1	0.91	0.16	68,68,68,68	0
55	MG	1A	3610	1/1	0.91	0.15	44,44,44,44	0
55	MG	1A	3853	1/1	0.91	0.12	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	1A	3380	1/1	0.91	0.21	38,38,38,38	0
55	MG	1A	4072	1/1	0.91	0.09	47,47,47,47	0
55	MG	1A	3250	1/1	0.91	0.10	40,40,40,40	0
55	MG	1a	1830	1/1	0.91	0.14	59,59,59,59	0
55	MG	2A	3179	1/1	0.91	0.14	56,56,56,56	0
55	MG	2A	3182	1/1	0.91	0.11	63,63,63,63	0
55	MG	1A	3627	1/1	0.91	0.16	41,41,41,41	0
55	MG	2a	3051	1/1	0.91	0.16	45,45,45,45	0
55	MG	2A	3391	1/1	0.91	0.21	45,45,45,45	0
55	MG	1A	3634	1/1	0.91	0.36	55,55,55,55	0
55	MG	2a	3057	1/1	0.91	0.23	45,45,45,45	0
55	MG	2A	3697	1/1	0.91	0.14	57,57,57,57	0
55	MG	1A	3641	1/1	0.91	0.11	23,23,23,23	0
55	MG	1A	3870	1/1	0.91	0.14	46,46,46,46	0
55	MG	2A	3706	1/1	0.91	0.10	39,39,39,39	0
55	MG	1A	3253	1/1	0.91	0.19	55,55,55,55	0
55	MG	1e	201	1/1	0.91	0.09	71,71,71,71	0
55	MG	2a	3067	1/1	0.91	0.27	58,58,58,58	0
55	MG	2a	3068	1/1	0.91	0.22	50,50,50,50	0
55	MG	2A	3711	1/1	0.91	0.14	39,39,39,39	0
55	MG	2a	3070	1/1	0.91	0.13	63,63,63,63	0
55	MG	2A	3193	1/1	0.91	0.45	54,54,54,54	0
55	MG	2A	3197	1/1	0.91	0.20	54,54,54,54	0
55	MG	1A	3388	1/1	0.91	0.16	28,28,28,28	0
55	MG	2a	3081	1/1	0.91	0.13	75,75,75,75	0
55	MG	1A	4101	1/1	0.91	0.15	61,61,61,61	0
55	MG	1A	3154	1/1	0.91	0.05	34,34,34,34	0
55	MG	2a	3086	1/1	0.91	0.13	56,56,56,56	0
55	MG	1A	3657	1/1	0.91	0.16	36,36,36,36	0
55	MG	2A	3426	1/1	0.91	0.21	56,56,56,56	0
55	MG	2A	3722	1/1	0.91	0.12	72,72,72,72	0
55	MG	1A	3408	1/1	0.91	0.25	45,45,45,45	0
55	MG	1A	3411	1/1	0.91	0.15	43,43,43,43	0
55	MG	1A	4108	1/1	0.91	0.19	53,53,53,53	0
55	MG	2A	3442	1/1	0.91	0.12	51,51,51,51	0
55	MG	2a	3094	1/1	0.91	0.19	63,63,63,63	0
55	MG	1A	3679	1/1	0.91	0.12	24,24,24,24	0
55	MG	1A	3062	1/1	0.91	0.11	43,43,43,43	0
55	MG	1A	3310	1/1	0.91	0.23	60,60,60,60	0
55	MG	2A	3453	1/1	0.91	0.21	66,66,66,66	0
55	MG	1A	3511	1/1	0.91	0.10	48,48,48,48	0
55	MG	1A	3428	1/1	0.91	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3742	1/1	0.91	0.17	59,59,59,59	0
55	MG	1A	3323	1/1	0.91	0.14	52,52,52,52	0
55	MG	2A	3748	1/1	0.91	0.10	50,50,50,50	0
55	MG	2A	3751	1/1	0.91	0.07	50,50,50,50	0
55	MG	2A	3001	1/1	0.91	0.20	48,48,48,48	0
55	MG	1B	220	1/1	0.91	0.09	40,40,40,40	0
55	MG	1A	3903	1/1	0.91	0.19	54,54,54,54	0
55	MG	2A	3761	1/1	0.91	0.12	49,49,49,49	0
55	MG	2A	3765	1/1	0.91	0.12	72,72,72,72	0
55	MG	2A	3236	1/1	0.91	0.12	51,51,51,51	0
55	MG	2A	3237	1/1	0.91	0.26	50,50,50,50	0
55	MG	1A	3517	1/1	0.91	0.08	50,50,50,50	0
55	MG	2A	3012	1/1	0.91	0.14	36,36,36,36	0
55	MG	2A	3248	1/1	0.91	0.27	58,58,58,58	0
55	MG	1A	3907	1/1	0.91	0.12	28,28,28,28	0
55	MG	2a	3136	1/1	0.91	0.41	59,59,59,59	0
55	MG	2A	3478	1/1	0.91	0.22	30,30,30,30	0
55	MG	2A	3779	1/1	0.91	0.19	73,73,73,73	0
55	MG	1A	3723	1/1	0.91	0.12	14,14,14,14	0
55	MG	1A	3518	1/1	0.91	0.09	50,50,50,50	0
55	MG	1A	3110	1/1	0.91	0.53	35,35,35,35	0
55	MG	1A	3435	1/1	0.91	0.09	47,47,47,47	0
55	MG	2a	3144	1/1	0.91	0.20	57,57,57,57	0
55	MG	2A	3489	1/1	0.91	0.12	49,49,49,49	0
55	MG	1A	3055	1/1	0.91	0.28	47,47,47,47	0
55	MG	1E	301	1/1	0.91	0.18	45,45,45,45	0
55	MG	2A	3041	1/1	0.91	0.25	55,55,55,55	0
55	MG	1E	302	1/1	0.91	0.19	26,26,26,26	0
55	MG	1A	3338	1/1	0.91	0.20	46,46,46,46	0
55	MG	2A	3824	1/1	0.91	0.13	54,54,54,54	0
55	MG	1A	3745	1/1	0.91	0.14	48,48,48,48	0
55	MG	1G	201	1/1	0.91	0.22	39,39,39,39	0
55	MG	2A	3058	1/1	0.91	0.16	41,41,41,41	0
55	MG	2A	3831	1/1	0.91	0.09	51,51,51,51	0
55	MG	2A	3832	1/1	0.91	0.17	65,65,65,65	0
55	MG	2A	3833	1/1	0.91	0.12	57,57,57,57	0
55	MG	1A	3747	1/1	0.91	0.07	34,34,34,34	0
55	MG	2A	3517	1/1	0.91	0.12	65,65,65,65	0
55	MG	1A	3529	1/1	0.91	0.21	42,42,42,42	0
55	MG	1A	3937	1/1	0.91	0.15	33,33,33,33	0
55	MG	1A	3532	1/1	0.91	0.17	33,33,33,33	0
55	MG	1a	1722	1/1	0.91	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3537	1/1	0.91	0.17	44,44,44,44	0
55	MG	1A	3767	1/1	0.91	0.07	43,43,43,43	0
55	MG	1A	3768	1/1	0.91	0.13	36,36,36,36	0
55	MG	1A	3448	1/1	0.91	0.14	40,40,40,40	0
55	MG	1A	3950	1/1	0.91	0.07	51,51,51,51	0
55	MG	2A	3547	1/1	0.91	0.15	59,59,59,59	0
55	MG	1A	3449	1/1	0.91	0.14	58,58,58,58	0
55	MG	1A	3047	1/1	0.91	0.19	43,43,43,43	0
55	MG	2a	3192	1/1	0.91	0.23	55,55,55,55	0
55	MG	1A	3270	1/1	0.91	0.17	43,43,43,43	0
55	MG	1a	1742	1/1	0.91	0.28	35,35,35,35	0
55	MG	2A	3553	1/1	0.91	0.16	42,42,42,42	0
55	MG	1A	3564	1/1	0.91	0.12	31,31,31,31	0
55	MG	2A	3087	1/1	0.91	0.10	45,45,45,45	0
55	MG	2a	3204	1/1	0.91	0.16	55,55,55,55	0
55	MG	1A	3349	1/1	0.91	0.12	42,42,42,42	0
55	MG	1A	3129	1/1	0.91	0.13	39,39,39,39	0
55	MG	2A	3301	1/1	0.91	0.12	62,62,62,62	0
55	MG	2A	3303	1/1	0.91	0.10	60,60,60,60	0
55	MG	2B	215	1/1	0.91	0.15	47,47,47,47	0
55	MG	13	102	1/1	0.91	0.17	41,41,41,41	0
55	MG	2B	219	1/1	0.91	0.27	60,60,60,60	0
55	MG	2f	201	1/1	0.91	0.15	55,55,55,55	0
55	MG	15	101	1/1	0.91	0.15	34,34,34,34	0
55	MG	1A	3999	1/1	0.91	0.14	64,64,64,64	0
55	MG	2E	303	1/1	0.91	0.15	50,50,50,50	0
55	MG	1A	4005	1/1	0.91	0.10	34,34,34,34	0
55	MG	2l	201	1/1	0.91	0.28	76,76,76,76	0
55	MG	17	104	1/1	0.91	0.11	45,45,45,45	0
55	MG	1a	1764	1/1	0.91	0.19	39,39,39,39	0
55	MG	1A	3470	1/1	0.91	0.10	46,46,46,46	0
55	MG	19	101	1/1	0.91	0.15	43,43,43,43	0
55	MG	2A	3114	1/1	0.91	0.08	46,46,46,46	0
55	MG	2A	3325	1/1	0.91	0.09	44,44,44,44	0
55	MG	2Q	201	1/1	0.91	0.16	57,57,57,57	0
55	MG	2Q	202	1/1	0.91	0.28	56,56,56,56	0
55	MG	2R	201	1/1	0.91	0.12	48,48,48,48	0
55	MG	1A	4009	1/1	0.91	0.19	30,30,30,30	0
55	MG	2A	3006	1/1	0.92	0.07	56,56,56,56	0
55	MG	2D	302	1/1	0.92	0.24	42,42,42,42	0
55	MG	2A	3267	1/1	0.92	0.11	66,66,66,66	0
55	MG	2A	3008	1/1	0.92	0.12	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	1B	201	1/1	0.92	0.14	50,50,50,50	0
55	MG	1A	3418	1/1	0.92	0.17	58,58,58,58	0
55	MG	2E	307	1/1	0.92	0.11	56,56,56,56	0
55	MG	2E	309	1/1	0.92	0.07	38,38,38,38	0
55	MG	2A	3272	1/1	0.92	0.21	57,57,57,57	0
55	MG	2A	3273	1/1	0.92	0.07	50,50,50,50	0
55	MG	1A	3736	1/1	0.92	0.10	17,17,17,17	0
55	MG	1A	3520	1/1	0.92	0.23	58,58,58,58	0
55	MG	1A	3917	1/1	0.92	0.08	43,43,43,43	0
55	MG	2A	3562	1/1	0.92	0.17	57,57,57,57	0
55	MG	2A	3277	1/1	0.92	0.21	50,50,50,50	0
55	MG	1A	3522	1/1	0.92	0.37	43,43,43,43	0
55	MG	1A	3127	1/1	0.92	0.20	34,34,34,34	0
55	MG	1A	3423	1/1	0.92	0.17	43,43,43,43	0
55	MG	1A	3525	1/1	0.92	0.23	35,35,35,35	0
55	MG	1a	1693	1/1	0.92	0.25	59,59,59,59	0
55	MG	2U	202	1/1	0.92	0.22	30,30,30,30	0
55	MG	1A	3426	1/1	0.92	0.09	50,50,50,50	0
55	MG	2V	202	1/1	0.92	0.42	53,53,53,53	0
55	MG	2A	3585	1/1	0.92	0.17	34,34,34,34	0
55	MG	1a	1699	1/1	0.92	0.28	48,48,48,48	0
55	MG	2A	3589	1/1	0.92	0.10	44,44,44,44	0
55	MG	2Z	301	1/1	0.92	0.19	67,67,67,67	0
55	MG	2A	3594	1/1	0.92	0.16	49,49,49,49	0
55	MG	1A	3427	1/1	0.92	0.10	55,55,55,55	0
55	MG	25	102	1/1	0.92	0.08	43,43,43,43	0
55	MG	2A	3050	1/1	0.92	0.15	56,56,56,56	0
55	MG	1A	3936	1/1	0.92	0.09	39,39,39,39	0
55	MG	1A	3240	1/1	0.92	0.10	61,61,61,61	0
55	MG	2A	3295	1/1	0.92	0.08	52,52,52,52	0
55	MG	1B	234	1/1	0.92	0.10	44,44,44,44	0
55	MG	2A	3297	1/1	0.92	0.14	47,47,47,47	0
55	MG	1a	1707	1/1	0.92	0.06	62,62,62,62	0
55	MG	1D	309	1/1	0.92	0.11	53,53,53,53	0
55	MG	2a	3010	1/1	0.92	0.09	55,55,55,55	0
55	MG	1a	1709	1/1	0.92	0.27	59,59,59,59	0
55	MG	1A	3171	1/1	0.92	0.11	31,31,31,31	0
55	MG	2a	3014	1/1	0.92	0.11	71,71,71,71	0
55	MG	2A	3308	1/1	0.92	0.10	54,54,54,54	0
55	MG	1D	312	1/1	0.92	0.22	41,41,41,41	0
55	MG	1A	3433	1/1	0.92	0.19	44,44,44,44	0
55	MG	2A	3313	1/1	0.92	0.07	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	3020	1/1	0.92	0.40	67,67,67,67	0
55	MG	1A	3944	1/1	0.92	0.13	56,56,56,56	0
55	MG	2a	3022	1/1	0.92	0.09	47,47,47,47	0
55	MG	1A	3308	1/1	0.92	0.14	36,36,36,36	0
55	MG	1E	310	1/1	0.92	0.26	43,43,43,43	0
55	MG	2A	3621	1/1	0.92	0.12	46,46,46,46	0
55	MG	2a	3026	1/1	0.92	0.23	49,49,49,49	0
55	MG	1F	305	1/1	0.92	0.15	41,41,41,41	0
55	MG	1A	3244	1/1	0.92	0.24	38,38,38,38	0
55	MG	1A	3319	1/1	0.92	0.15	54,54,54,54	0
55	MG	1A	3438	1/1	0.92	0.13	41,41,41,41	0
55	MG	1A	3965	1/1	0.92	0.08	27,27,27,27	0
55	MG	2A	3633	1/1	0.92	0.19	50,50,50,50	0
55	MG	1N	201	1/1	0.92	0.23	43,43,43,43	0
55	MG	1N	204	1/1	0.92	0.20	47,47,47,47	0
55	MG	1A	3967	1/1	0.92	0.14	49,49,49,49	0
55	MG	1a	1738	1/1	0.92	0.27	52,52,52,52	0
55	MG	1A	3972	1/1	0.92	0.14	43,43,43,43	0
55	MG	2A	3098	1/1	0.92	0.13	44,44,44,44	0
55	MG	2A	3335	1/1	0.92	0.10	57,57,57,57	0
55	MG	2a	3045	1/1	0.92	0.12	92,92,92,92	0
55	MG	2A	3652	1/1	0.92	0.14	50,50,50,50	0
55	MG	1A	3973	1/1	0.92	0.10	67,67,67,67	0
55	MG	1A	3975	1/1	0.92	0.08	53,53,53,53	0
55	MG	1Q	204	1/1	0.92	0.07	51,51,51,51	0
55	MG	1A	3115	1/1	0.92	0.08	47,47,47,47	0
55	MG	2A	3343	1/1	0.92	0.06	50,50,50,50	0
55	MG	2A	3665	1/1	0.92	0.12	55,55,55,55	0
55	MG	1A	3794	1/1	0.92	0.10	29,29,29,29	0
55	MG	1A	3031	1/1	0.92	0.24	32,32,32,32	0
55	MG	1A	3184	1/1	0.92	0.12	40,40,40,40	0
55	MG	2A	3116	1/1	0.92	0.18	43,43,43,43	0
55	MG	2A	3673	1/1	0.92	0.13	52,52,52,52	0
55	MG	1a	1752	1/1	0.92	0.10	58,58,58,58	0
55	MG	2A	3129	1/1	0.92	0.13	57,57,57,57	0
55	MG	1V	202	1/1	0.92	0.18	45,45,45,45	0
55	MG	1a	1755	1/1	0.92	0.08	60,60,60,60	0
55	MG	1A	3333	1/1	0.92	0.07	41,41,41,41	0
55	MG	1A	3805	1/1	0.92	0.18	33,33,33,33	0
55	MG	1A	3995	1/1	0.92	0.16	53,53,53,53	0
55	MG	2a	3074	1/1	0.92	0.20	47,47,47,47	0
55	MG	1A	3998	1/1	0.92	0.14	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	10	103	1/1	0.92	0.18	55,55,55,55	0
55	MG	1A	3452	1/1	0.92	0.10	45,45,45,45	0
55	MG	1A	3458	1/1	0.92	0.18	47,47,47,47	0
55	MG	1A	3463	1/1	0.92	0.19	48,48,48,48	0
55	MG	2A	3368	1/1	0.92	0.18	54,54,54,54	0
55	MG	1A	3336	1/1	0.92	0.18	53,53,53,53	0
55	MG	1a	1782	1/1	0.92	0.08	57,57,57,57	0
55	MG	1A	3134	1/1	0.92	0.08	45,45,45,45	0
55	MG	1A	3137	1/1	0.92	0.29	35,35,35,35	0
55	MG	1A	3598	1/1	0.92	0.27	47,47,47,47	0
55	MG	1A	3599	1/1	0.92	0.15	39,39,39,39	0
55	MG	1A	3260	1/1	0.92	0.10	38,38,38,38	0
55	MG	1A	3471	1/1	0.92	0.07	27,27,27,27	0
55	MG	1a	1793	1/1	0.92	0.10	63,63,63,63	0
55	MG	1A	4021	1/1	0.92	0.12	64,64,64,64	0
55	MG	1A	4022	1/1	0.92	0.11	57,57,57,57	0
55	MG	2A	3385	1/1	0.92	0.17	37,37,37,37	0
55	MG	2A	3724	1/1	0.92	0.13	61,61,61,61	0
55	MG	1a	1796	1/1	0.92	0.17	69,69,69,69	0
55	MG	2A	3168	1/1	0.92	0.09	51,51,51,51	0
55	MG	1a	1798	1/1	0.92	0.15	73,73,73,73	0
55	MG	1a	1800	1/1	0.92	0.08	72,72,72,72	0
55	MG	1a	1802	1/1	0.92	0.08	66,66,66,66	0
55	MG	1A	3348	1/1	0.92	0.19	55,55,55,55	0
55	MG	2A	3175	1/1	0.92	0.19	52,52,52,52	0
55	MG	2a	3112	1/1	0.92	0.16	58,58,58,58	0
55	MG	1A	4026	1/1	0.92	0.10	29,29,29,29	0
55	MG	1A	3607	1/1	0.92	0.24	33,33,33,33	0
55	MG	2a	3119	1/1	0.92	0.36	62,62,62,62	0
55	MG	2a	3120	1/1	0.92	0.16	57,57,57,57	0
55	MG	2A	3419	1/1	0.92	0.16	53,53,53,53	0
55	MG	2A	3420	1/1	0.92	0.21	38,38,38,38	0
55	MG	1A	3261	1/1	0.92	0.11	33,33,33,33	0
55	MG	2A	3745	1/1	0.92	0.18	27,27,27,27	0
55	MG	1A	3196	1/1	0.92	0.07	41,41,41,41	0
55	MG	2A	3424	1/1	0.92	0.26	48,48,48,48	0
55	MG	2A	3753	1/1	0.92	0.18	58,58,58,58	0
55	MG	1a	1810	1/1	0.92	0.07	58,58,58,58	0
55	MG	2A	3188	1/1	0.92	0.17	48,48,48,48	0
55	MG	1a	1615	1/1	0.92	0.05	73,73,73,73	0
55	MG	2a	3138	1/1	0.92	0.32	67,67,67,67	0
55	MG	2A	3429	1/1	0.92	0.27	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	3431	1/1	0.92	0.19	46,46,46,46	0
55	MG	1A	4037	1/1	0.92	0.11	58,58,58,58	0
55	MG	1A	3617	1/1	0.92	0.08	29,29,29,29	0
55	MG	2A	3770	1/1	0.92	0.08	69,69,69,69	0
55	MG	1a	1818	1/1	0.92	0.08	73,73,73,73	0
55	MG	2A	3772	1/1	0.92	0.13	80,80,80,80	0
55	MG	2a	3146	1/1	0.92	0.23	38,38,38,38	0
55	MG	1A	3619	1/1	0.92	0.10	32,32,32,32	0
55	MG	2A	3774	1/1	0.92	0.15	42,42,42,42	0
55	MG	2A	3196	1/1	0.92	0.11	50,50,50,50	0
55	MG	1A	3356	1/1	0.92	0.13	62,62,62,62	0
55	MG	2A	3449	1/1	0.92	0.07	66,66,66,66	0
55	MG	1A	3138	1/1	0.92	0.09	20,20,20,20	0
55	MG	1A	3859	1/1	0.92	0.19	59,59,59,59	0
55	MG	1a	1628	1/1	0.92	0.17	61,61,61,61	0
55	MG	1a	1630	1/1	0.92	0.09	44,44,44,44	0
55	MG	2A	3785	1/1	0.92	0.09	60,60,60,60	0
55	MG	2A	3789	1/1	0.92	0.10	47,47,47,47	0
55	MG	1A	4057	1/1	0.92	0.10	47,47,47,47	0
55	MG	2A	3798	1/1	0.92	0.07	57,57,57,57	0
55	MG	2A	3208	1/1	0.92	0.39	57,57,57,57	0
55	MG	1A	3266	1/1	0.92	0.08	50,50,50,50	0
55	MG	1A	3210	1/1	0.92	0.11	43,43,43,43	0
55	MG	1a	1640	1/1	0.92	0.09	48,48,48,48	0
55	MG	2A	3221	1/1	0.92	0.15	47,47,47,47	0
55	MG	1A	3144	1/1	0.92	0.13	39,39,39,39	0
55	MG	2A	3226	1/1	0.92	0.09	61,61,61,61	0
55	MG	1A	4064	1/1	0.92	0.09	39,39,39,39	0
55	MG	2a	3181	1/1	0.92	0.20	56,56,56,56	0
55	MG	2A	3477	1/1	0.92	0.20	34,34,34,34	0
55	MG	2A	3828	1/1	0.92	0.12	48,48,48,48	0
55	MG	2a	3187	1/1	0.92	0.23	75,75,75,75	0
55	MG	1A	3279	1/1	0.92	0.10	47,47,47,47	0
55	MG	2A	3480	1/1	0.92	0.26	37,37,37,37	0
55	MG	1A	3377	1/1	0.92	0.14	37,37,37,37	0
55	MG	1A	3215	1/1	0.92	0.14	36,36,36,36	0
55	MG	1A	3382	1/1	0.92	0.13	43,43,43,43	0
55	MG	1A	4082	1/1	0.92	0.06	42,42,42,42	0
55	MG	1l	204	1/1	0.92	0.07	64,64,64,64	0
55	MG	1A	3145	1/1	0.92	0.14	25,25,25,25	0
55	MG	2A	3846	1/1	0.92	0.10	51,51,51,51	0
55	MG	2a	3203	1/1	0.92	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3881	1/1	0.92	0.09	34,34,34,34	0
55	MG	2A	3848	1/1	0.92	0.21	55,55,55,55	0
55	MG	1A	3069	1/1	0.92	0.14	36,36,36,36	0
55	MG	2A	3241	1/1	0.92	0.30	58,58,58,58	0
55	MG	1A	3678	1/1	0.92	0.12	20,20,20,20	0
55	MG	1a	1659	1/1	0.92	0.07	67,67,67,67	0
55	MG	1A	3124	1/1	0.92	0.13	47,47,47,47	0
55	MG	2A	3506	1/1	0.92	0.16	60,60,60,60	0
55	MG	2A	3509	1/1	0.92	0.16	57,57,57,57	0
55	MG	1A	3508	1/1	0.92	0.17	35,35,35,35	0
55	MG	1A	3161	1/1	0.92	0.11	37,37,37,37	0
55	MG	1A	3395	1/1	0.92	0.06	58,58,58,58	0
55	MG	2A	3519	1/1	0.92	0.12	39,39,39,39	0
55	MG	1A	3291	1/1	0.92	0.23	43,43,43,43	0
55	MG	2A	3257	1/1	0.92	0.12	52,52,52,52	0
55	MG	1A	3410	1/1	0.92	0.10	40,40,40,40	0
55	MG	2B	207	1/1	0.92	0.18	57,57,57,57	0
55	MG	2A	3528	1/1	0.92	0.08	32,32,32,32	0
55	MG	2A	3529	1/1	0.92	0.11	49,49,49,49	0
55	MG	1A	3162	1/1	0.92	0.14	43,43,43,43	0
55	MG	2x	103	1/1	0.92	0.18	63,63,63,63	0
55	MG	1A	4110	1/1	0.92	0.16	53,53,53,53	0
55	MG	1A	3125	1/1	0.92	0.58	30,30,30,30	0
55	MG	1A	4117	1/1	0.92	0.22	49,49,49,49	0
55	MG	2B	218	1/1	0.92	0.08	59,59,59,59	0
55	MG	2A	3518	1/1	0.93	0.21	68,68,68,68	0
55	MG	1a	1637	1/1	0.93	0.25	59,59,59,59	0
55	MG	1A	3421	1/1	0.93	0.27	52,52,52,52	0
55	MG	1A	3875	1/1	0.93	0.12	32,32,32,32	0
55	MG	2A	3240	1/1	0.93	0.17	54,54,54,54	0
55	MG	1A	3017	1/1	0.93	0.07	25,25,25,25	0
55	MG	1A	3646	1/1	0.93	0.13	30,30,30,30	0
55	MG	2A	3531	1/1	0.93	0.20	31,31,31,31	0
55	MG	1A	3052	1/1	0.93	0.20	21,21,21,21	0
55	MG	1A	3098	1/1	0.93	0.06	36,36,36,36	0
55	MG	2E	302	1/1	0.93	0.10	47,47,47,47	0
55	MG	1l	201	1/1	0.93	0.11	38,38,38,38	0
55	MG	1A	3337	1/1	0.93	0.11	45,45,45,45	0
55	MG	1A	3889	1/1	0.93	0.15	43,43,43,43	0
55	MG	1A	3659	1/1	0.93	0.18	52,52,52,52	0
55	MG	1A	3430	1/1	0.93	0.35	41,41,41,41	0
55	MG	1a	1653	1/1	0.93	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3549	1/1	0.93	0.13	35,35,35,35	0
55	MG	1A	3274	1/1	0.93	0.09	37,37,37,37	0
55	MG	1A	3896	1/1	0.93	0.38	32,32,32,32	0
55	MG	1A	3669	1/1	0.93	0.08	21,21,21,21	0
55	MG	1A	4106	1/1	0.93	0.08	52,52,52,52	0
55	MG	1x	106	1/1	0.93	0.13	55,55,55,55	0
55	MG	2Q	203	1/1	0.93	0.09	43,43,43,43	0
55	MG	1A	3675	1/1	0.93	0.10	14,14,14,14	0
55	MG	2R	202	1/1	0.93	0.22	52,52,52,52	0
55	MG	1a	1660	1/1	0.93	0.15	77,77,77,77	0
55	MG	1a	1661	1/1	0.93	0.15	62,62,62,62	0
55	MG	1x	112	1/1	0.93	0.13	64,64,64,64	0
55	MG	1A	3054	1/1	0.93	0.11	37,37,37,37	0
55	MG	1A	3186	1/1	0.93	0.13	37,37,37,37	0
55	MG	1A	3128	1/1	0.93	0.41	37,37,37,37	0
55	MG	2A	3573	1/1	0.93	0.13	34,34,34,34	0
55	MG	2A	3576	1/1	0.93	0.10	50,50,50,50	0
55	MG	1a	1665	1/1	0.93	0.15	49,49,49,49	0
55	MG	1A	4112	1/1	0.93	0.10	56,56,56,56	0
55	MG	1A	3159	1/1	0.93	0.21	47,47,47,47	0
55	MG	1A	4114	1/1	0.93	0.17	53,53,53,53	0
55	MG	1A	4116	1/1	0.93	0.13	61,61,61,61	0
55	MG	26	101	1/1	0.93	0.25	52,52,52,52	0
55	MG	2A	3591	1/1	0.93	0.14	56,56,56,56	0
55	MG	2A	3593	1/1	0.93	0.12	68,68,68,68	0
55	MG	1A	3910	1/1	0.93	0.09	41,41,41,41	0
55	MG	2a	3001	1/1	0.93	0.10	57,57,57,57	0
55	MG	2A	3015	1/1	0.93	0.24	63,63,63,63	0
55	MG	2A	3017	1/1	0.93	0.12	46,46,46,46	0
55	MG	2A	3597	1/1	0.93	0.10	49,49,49,49	0
55	MG	1a	1672	1/1	0.93	0.12	47,47,47,47	0
55	MG	1A	3688	1/1	0.93	0.11	52,52,52,52	0
55	MG	1a	1674	1/1	0.93	0.32	56,56,56,56	0
55	MG	1A	3695	1/1	0.93	0.09	20,20,20,20	0
55	MG	2A	3029	1/1	0.93	0.12	27,27,27,27	0
55	MG	2A	3030	1/1	0.93	0.34	56,56,56,56	0
55	MG	2A	3033	1/1	0.93	0.28	59,59,59,59	0
55	MG	2a	3016	1/1	0.93	0.05	46,46,46,46	0
55	MG	1A	3247	1/1	0.93	0.19	57,57,57,57	0
55	MG	1A	3444	1/1	0.93	0.16	43,43,43,43	0
55	MG	2A	3040	1/1	0.93	0.15	59,59,59,59	0
55	MG	1A	3206	1/1	0.93	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3042	1/1	0.93	0.08	54,54,54,54	0
55	MG	1A	3035	1/1	0.93	0.35	36,36,36,36	0
55	MG	1A	3362	1/1	0.93	0.27	52,52,52,52	0
55	MG	2A	3616	1/1	0.93	0.17	45,45,45,45	0
55	MG	1a	1682	1/1	0.93	0.09	45,45,45,45	0
55	MG	1A	3528	1/1	0.93	0.13	29,29,29,29	0
55	MG	1B	225	1/1	0.93	0.11	46,46,46,46	0
55	MG	2A	3624	1/1	0.93	0.13	47,47,47,47	0
55	MG	1A	3251	1/1	0.93	0.08	28,28,28,28	0
55	MG	2A	3060	1/1	0.93	0.21	38,38,38,38	0
55	MG	2A	3061	1/1	0.93	0.17	51,51,51,51	0
55	MG	1a	1688	1/1	0.93	0.09	53,53,53,53	0
55	MG	1a	1689	1/1	0.93	0.18	42,42,42,42	0
55	MG	1A	3451	1/1	0.93	0.09	36,36,36,36	0
55	MG	1A	3296	1/1	0.93	0.13	27,27,27,27	0
55	MG	1A	3455	1/1	0.93	0.09	48,48,48,48	0
55	MG	2A	3641	1/1	0.93	0.15	55,55,55,55	0
55	MG	2A	3643	1/1	0.93	0.08	64,64,64,64	0
55	MG	1A	3004	1/1	0.93	0.07	23,23,23,23	0
55	MG	1B	233	1/1	0.93	0.15	53,53,53,53	0
55	MG	1A	3939	1/1	0.93	0.06	49,49,49,49	0
55	MG	1D	301	1/1	0.93	0.46	36,36,36,36	0
55	MG	2A	3079	1/1	0.93	0.11	35,35,35,35	0
55	MG	1A	3546	1/1	0.93	0.09	31,31,31,31	0
55	MG	1A	3460	1/1	0.93	0.14	38,38,38,38	0
55	MG	1A	3551	1/1	0.93	0.16	31,31,31,31	0
55	MG	1A	3750	1/1	0.93	0.08	41,41,41,41	0
55	MG	2a	3055	1/1	0.93	0.15	59,59,59,59	0
55	MG	1A	3752	1/1	0.93	0.13	23,23,23,23	0
55	MG	2A	3661	1/1	0.93	0.18	52,52,52,52	0
55	MG	1a	1713	1/1	0.93	0.17	49,49,49,49	0
55	MG	1E	304	1/1	0.93	0.16	37,37,37,37	0
55	MG	1A	3461	1/1	0.93	0.21	48,48,48,48	0
55	MG	2a	3062	1/1	0.93	0.07	50,50,50,50	0
55	MG	1A	3962	1/1	0.93	0.15	51,51,51,51	0
55	MG	1A	3963	1/1	0.93	0.24	42,42,42,42	0
55	MG	1A	3462	1/1	0.93	0.12	57,57,57,57	0
55	MG	1A	3765	1/1	0.93	0.08	34,34,34,34	0
55	MG	1A	3766	1/1	0.93	0.24	64,64,64,64	0
55	MG	1A	3254	1/1	0.93	0.30	58,58,58,58	0
55	MG	2A	3103	1/1	0.93	0.06	30,30,30,30	0
55	MG	2a	3072	1/1	0.93	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2a	3073	1/1	0.93	0.24	61,61,61,61	0
55	MG	1A	3132	1/1	0.93	0.17	40,40,40,40	0
55	MG	2A	3356	1/1	0.93	0.08	37,37,37,37	0
55	MG	1a	1725	1/1	0.93	0.20	48,48,48,48	0
55	MG	2a	3077	1/1	0.93	0.22	39,39,39,39	0
55	MG	1A	3981	1/1	0.93	0.08	59,59,59,59	0
55	MG	1A	3213	1/1	0.93	0.21	50,50,50,50	0
55	MG	2A	3112	1/1	0.93	0.10	89,89,89,89	0
55	MG	1a	1729	1/1	0.93	0.18	54,54,54,54	0
55	MG	2a	3085	1/1	0.93	0.24	64,64,64,64	0
55	MG	2A	3691	1/1	0.93	0.14	57,57,57,57	0
55	MG	1A	3307	1/1	0.93	0.22	43,43,43,43	0
55	MG	1O	204	1/1	0.93	0.17	60,60,60,60	0
55	MG	2A	3701	1/1	0.93	0.14	49,49,49,49	0
55	MG	2A	3366	1/1	0.93	0.19	49,49,49,49	0
55	MG	1A	3987	1/1	0.93	0.13	32,32,32,32	0
55	MG	2A	3123	1/1	0.93	0.15	39,39,39,39	0
55	MG	2A	3127	1/1	0.93	0.18	44,44,44,44	0
55	MG	1Q	202	1/1	0.93	0.07	35,35,35,35	0
55	MG	2a	3095	1/1	0.93	0.20	46,46,46,46	0
55	MG	2A	3373	1/1	0.93	0.22	64,64,64,64	0
55	MG	1A	3777	1/1	0.93	0.07	51,51,51,51	0
55	MG	1A	3469	1/1	0.93	0.29	49,49,49,49	0
55	MG	2A	3132	1/1	0.93	0.18	52,52,52,52	0
55	MG	1a	1743	1/1	0.93	0.25	62,62,62,62	0
55	MG	1R	201	1/1	0.93	0.35	44,44,44,44	0
55	MG	2A	3379	1/1	0.93	0.06	45,45,45,45	0
55	MG	1A	3089	1/1	0.93	0.11	42,42,42,42	0
55	MG	1a	1746	1/1	0.93	0.28	52,52,52,52	0
55	MG	2a	3109	1/1	0.93	0.07	75,75,75,75	0
55	MG	1a	1747	1/1	0.93	0.30	50,50,50,50	0
55	MG	2A	3726	1/1	0.93	0.12	51,51,51,51	0
55	MG	1A	3586	1/1	0.93	0.11	44,44,44,44	0
55	MG	2a	3113	1/1	0.93	0.13	50,50,50,50	0
55	MG	2A	3386	1/1	0.93	0.15	53,53,53,53	0
55	MG	2A	3389	1/1	0.93	0.23	47,47,47,47	0
55	MG	1A	3309	1/1	0.93	0.16	40,40,40,40	0
55	MG	1A	3997	1/1	0.93	0.08	56,56,56,56	0
55	MG	2A	3396	1/1	0.93	0.25	47,47,47,47	0
55	MG	2A	3398	1/1	0.93	0.22	33,33,33,33	0
55	MG	2a	3126	1/1	0.93	0.27	62,62,62,62	0
55	MG	2A	3739	1/1	0.93	0.18	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	3472	1/1	0.93	0.26	54,54,54,54	0
55	MG	1A	3092	1/1	0.93	0.20	32,32,32,32	0
55	MG	1A	4000	1/1	0.93	0.13	60,60,60,60	0
55	MG	1W	202	1/1	0.93	0.10	44,44,44,44	0
55	MG	2A	3410	1/1	0.93	0.18	35,35,35,35	0
55	MG	2A	3747	1/1	0.93	0.10	56,56,56,56	0
55	MG	2A	3411	1/1	0.93	0.25	51,51,51,51	0
55	MG	2A	3154	1/1	0.93	0.11	38,38,38,38	0
55	MG	2A	3413	1/1	0.93	0.36	42,42,42,42	0
55	MG	2A	3155	1/1	0.93	0.10	47,47,47,47	0
55	MG	2A	3417	1/1	0.93	0.10	50,50,50,50	0
55	MG	1a	1762	1/1	0.93	0.20	54,54,54,54	0
55	MG	1X	103	1/1	0.93	0.13	37,37,37,37	0
55	MG	1A	3479	1/1	0.93	0.12	33,33,33,33	0
55	MG	2A	3160	1/1	0.93	0.13	30,30,30,30	0
55	MG	1A	4007	1/1	0.93	0.12	25,25,25,25	0
55	MG	1Y	204	1/1	0.93	0.24	49,49,49,49	0
55	MG	1A	3480	1/1	0.93	0.12	42,42,42,42	0
55	MG	1l	103	1/1	0.93	0.08	35,35,35,35	0
55	MG	1a	1772	1/1	0.93	0.08	64,64,64,64	0
55	MG	2a	3151	1/1	0.93	0.13	69,69,69,69	0
55	MG	1A	3313	1/1	0.93	0.14	44,44,44,44	0
55	MG	1a	1774	1/1	0.93	0.16	34,34,34,34	0
55	MG	12	102	1/1	0.93	0.15	43,43,43,43	0
55	MG	1A	3814	1/1	0.93	0.09	41,41,41,41	0
55	MG	1A	3600	1/1	0.93	0.15	40,40,40,40	0
55	MG	1A	3314	1/1	0.93	0.06	27,27,27,27	0
55	MG	2A	3782	1/1	0.93	0.20	77,77,77,77	0
55	MG	1A	3399	1/1	0.93	0.17	32,32,32,32	0
55	MG	17	102	1/1	0.93	0.14	39,39,39,39	0
55	MG	1a	1788	1/1	0.93	0.20	66,66,66,66	0
55	MG	2a	3172	1/1	0.93	0.16	56,56,56,56	0
55	MG	2A	3452	1/1	0.93	0.50	46,46,46,46	0
55	MG	2A	3791	1/1	0.93	0.20	46,46,46,46	0
55	MG	1A	3827	1/1	0.93	0.13	42,42,42,42	0
55	MG	2A	3795	1/1	0.93	0.08	42,42,42,42	0
55	MG	2A	3796	1/1	0.93	0.13	61,61,61,61	0
55	MG	18	104	1/1	0.93	0.11	40,40,40,40	0
55	MG	2A	3800	1/1	0.93	0.10	52,52,52,52	0
55	MG	2A	3456	1/1	0.93	0.07	54,54,54,54	0
55	MG	1A	3400	1/1	0.93	0.09	40,40,40,40	0
55	MG	1A	3318	1/1	0.93	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3409	1/1	0.93	0.08	54,54,54,54	0
55	MG	1A	3177	1/1	0.93	0.13	41,41,41,41	0
55	MG	2a	3189	1/1	0.93	0.21	62,62,62,62	0
55	MG	1A	3612	1/1	0.93	0.28	61,61,61,61	0
55	MG	2A	3819	1/1	0.93	0.15	33,33,33,33	0
55	MG	1a	1605	1/1	0.93	0.19	60,60,60,60	0
55	MG	1A	3320	1/1	0.93	0.21	45,45,45,45	0
55	MG	2a	3194	1/1	0.93	0.18	61,61,61,61	0
55	MG	1A	3321	1/1	0.93	0.17	47,47,47,47	0
55	MG	1A	3416	1/1	0.93	0.30	49,49,49,49	0
55	MG	2A	3469	1/1	0.93	0.16	48,48,48,48	0
55	MG	1A	3621	1/1	0.93	0.12	26,26,26,26	0
55	MG	2A	3473	1/1	0.93	0.23	23,23,23,23	0
55	MG	1A	3263	1/1	0.93	0.16	38,38,38,38	0
55	MG	1A	3625	1/1	0.93	0.23	50,50,50,50	0
55	MG	2A	3203	1/1	0.93	0.34	45,45,45,45	0
55	MG	2A	3204	1/1	0.93	0.21	49,49,49,49	0
55	MG	2A	3483	1/1	0.93	0.18	34,34,34,34	0
55	MG	1A	3626	1/1	0.93	0.12	53,53,53,53	0
55	MG	1a	1616	1/1	0.93	0.13	51,51,51,51	0
55	MG	1A	3179	1/1	0.93	0.17	42,42,42,42	0
55	MG	1A	3630	1/1	0.93	0.22	30,30,30,30	0
55	MG	1a	1816	1/1	0.93	0.16	48,48,48,48	0
55	MG	1a	1620	1/1	0.93	0.13	46,46,46,46	0
55	MG	1A	3631	1/1	0.93	0.21	16,16,16,16	0
55	MG	2A	3223	1/1	0.93	0.10	52,52,52,52	0
55	MG	2A	3224	1/1	0.93	0.13	45,45,45,45	0
55	MG	1A	3632	1/1	0.93	0.14	35,35,35,35	0
55	MG	1A	3869	1/1	0.93	0.10	60,60,60,60	0
55	MG	2A	3501	1/1	0.93	0.17	58,58,58,58	0
55	MG	1A	3633	1/1	0.93	0.09	54,54,54,54	0
55	MG	1A	3501	1/1	0.93	0.11	46,46,46,46	0
55	MG	2B	203	1/1	0.93	0.10	40,40,40,40	0
55	MG	1A	4069	1/1	0.93	0.10	34,34,34,34	0
55	MG	2A	3512	1/1	0.93	0.19	53,53,53,53	0
55	MG	1a	1632	1/1	0.93	0.17	50,50,50,50	0
55	MG	1a	1633	1/1	0.93	0.26	48,48,48,48	0
55	MG	1A	4071	1/1	0.93	0.08	20,20,20,20	0
55	MG	2A	3842	1/1	0.94	0.13	48,48,48,48	0
55	MG	1A	3608	1/1	0.94	0.19	23,23,23,23	0
55	MG	1A	3823	1/1	0.94	0.12	17,17,17,17	0
55	MG	1a	1811	1/1	0.94	0.14	73,73,73,73	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	0.94	0.10	17,17,17,17	0
55	MG	2A	3850	1/1	0.94	0.09	51,51,51,51	0
55	MG	2A	3851	1/1	0.94	0.17	49,49,49,49	0
55	MG	1A	3390	1/1	0.94	0.29	34,34,34,34	0
55	MG	1A	4030	1/1	0.94	0.05	21,21,21,21	0
55	MG	1A	4032	1/1	0.94	0.07	39,39,39,39	0
55	MG	2A	3482	1/1	0.94	0.25	51,51,51,51	0
55	MG	1A	3831	1/1	0.94	0.12	31,31,31,31	0
55	MG	1A	3832	1/1	0.94	0.30	32,32,32,32	0
55	MG	2A	3209	1/1	0.94	0.09	45,45,45,45	0
55	MG	2A	3212	1/1	0.94	0.08	42,42,42,42	0
55	MG	2A	3487	1/1	0.94	0.36	49,49,49,49	0
55	MG	1a	1622	1/1	0.94	0.15	44,44,44,44	0
55	MG	2A	3217	1/1	0.94	0.07	35,35,35,35	0
55	MG	1a	1623	1/1	0.94	0.08	50,50,50,50	0
55	MG	1A	3393	1/1	0.94	0.06	43,43,43,43	0
55	MG	1A	3613	1/1	0.94	0.08	32,32,32,32	0
55	MG	2A	3495	1/1	0.94	0.16	43,43,43,43	0
55	MG	1A	3838	1/1	0.94	0.12	40,40,40,40	0
55	MG	1A	3104	1/1	0.94	0.12	31,31,31,31	0
55	MG	1a	1629	1/1	0.94	0.17	51,51,51,51	0
55	MG	1A	4047	1/1	0.94	0.10	56,56,56,56	0
55	MG	2A	3503	1/1	0.94	0.12	39,39,39,39	0
55	MG	1A	3136	1/1	0.94	0.08	44,44,44,44	0
55	MG	1A	3843	1/1	0.94	0.07	44,44,44,44	0
55	MG	1A	3077	1/1	0.94	0.09	30,30,30,30	0
55	MG	1A	3845	1/1	0.94	0.11	29,29,29,29	0
55	MG	1A	3311	1/1	0.94	0.07	28,28,28,28	0
55	MG	2A	3515	1/1	0.94	0.15	57,57,57,57	0
55	MG	1A	3848	1/1	0.94	0.09	37,37,37,37	0
55	MG	2A	3233	1/1	0.94	0.08	54,54,54,54	0
55	MG	1A	4065	1/1	0.94	0.14	26,26,26,26	0
55	MG	1f	202	1/1	0.94	0.07	48,48,48,48	0
55	MG	1A	4066	1/1	0.94	0.11	29,29,29,29	0
55	MG	1A	3622	1/1	0.94	0.13	37,37,37,37	0
55	MG	2A	3525	1/1	0.94	0.10	42,42,42,42	0
55	MG	2A	3526	1/1	0.94	0.12	60,60,60,60	0
55	MG	2A	3239	1/1	0.94	0.13	49,49,49,49	0
55	MG	1A	3623	1/1	0.94	0.11	38,38,38,38	0
55	MG	1A	3312	1/1	0.94	0.12	38,38,38,38	0
55	MG	1A	3188	1/1	0.94	0.17	46,46,46,46	0
55	MG	2A	3245	1/1	0.94	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1a	1646	1/1	0.94	0.12	37,37,37,37	0
55	MG	1A	3011	1/1	0.94	0.15	39,39,39,39	0
55	MG	1A	4080	1/1	0.94	0.17	40,40,40,40	0
55	MG	2A	3542	1/1	0.94	0.23	45,45,45,45	0
55	MG	1a	1652	1/1	0.94	0.19	51,51,51,51	0
55	MG	2A	3544	1/1	0.94	0.10	41,41,41,41	0
55	MG	1x	103	1/1	0.94	0.25	67,67,67,67	0
55	MG	1A	3316	1/1	0.94	0.18	42,42,42,42	0
55	MG	1A	3140	1/1	0.94	0.16	36,36,36,36	0
55	MG	1A	4083	1/1	0.94	0.06	26,26,26,26	0
55	MG	1x	108	1/1	0.94	0.06	55,55,55,55	0
55	MG	1A	3198	1/1	0.94	0.09	38,38,38,38	0
55	MG	2A	3262	1/1	0.94	0.21	41,41,41,41	0
55	MG	1A	3202	1/1	0.94	0.08	38,38,38,38	0
55	MG	1A	3112	1/1	0.94	0.10	38,38,38,38	0
55	MG	1A	3865	1/1	0.94	0.05	45,45,45,45	0
55	MG	1A	3083	1/1	0.94	0.14	41,41,41,41	0
55	MG	1A	3422	1/1	0.94	0.16	41,41,41,41	0
55	MG	2A	3565	1/1	0.94	0.13	44,44,44,44	0
55	MG	2A	3566	1/1	0.94	0.17	48,48,48,48	0
55	MG	1A	3871	1/1	0.94	0.06	32,32,32,32	0
55	MG	1A	3515	1/1	0.94	0.13	55,55,55,55	0
55	MG	2a	3002	1/1	0.94	0.14	60,60,60,60	0
55	MG	1A	3645	1/1	0.94	0.08	50,50,50,50	0
55	MG	1A	3874	1/1	0.94	0.10	50,50,50,50	0
55	MG	2A	3011	1/1	0.94	0.10	50,50,50,50	0
55	MG	2A	3574	1/1	0.94	0.17	48,48,48,48	0
55	MG	1A	3324	1/1	0.94	0.24	43,43,43,43	0
55	MG	1A	3650	1/1	0.94	0.11	12,12,12,12	0
55	MG	1a	1669	1/1	0.94	0.12	54,54,54,54	0
55	MG	2A	3278	1/1	0.94	0.16	76,76,76,76	0
55	MG	1A	3147	1/1	0.94	0.07	32,32,32,32	0
55	MG	2A	3587	1/1	0.94	0.10	39,39,39,39	0
55	MG	2A	3281	1/1	0.94	0.05	42,42,42,42	0
55	MG	2A	3590	1/1	0.94	0.08	53,53,53,53	0
55	MG	2A	3019	1/1	0.94	0.13	53,53,53,53	0
55	MG	1A	3053	1/1	0.94	0.24	33,33,33,33	0
55	MG	2A	3284	1/1	0.94	0.23	50,50,50,50	0
55	MG	1A	3331	1/1	0.94	0.08	41,41,41,41	0
55	MG	2A	3286	1/1	0.94	0.19	60,60,60,60	0
55	MG	2A	3022	1/1	0.94	0.10	54,54,54,54	0
55	MG	1A	3040	1/1	0.94	0.24	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	4115	1/1	0.94	0.13	59,59,59,59	0
55	MG	2A	3600	1/1	0.94	0.12	50,50,50,50	0
55	MG	1A	3521	1/1	0.94	0.11	40,40,40,40	0
55	MG	1A	3267	1/1	0.94	0.09	33,33,33,33	0
55	MG	2A	3604	1/1	0.94	0.09	31,31,31,31	0
55	MG	2A	3031	1/1	0.94	0.25	45,45,45,45	0
55	MG	1A	3157	1/1	0.94	0.14	26,26,26,26	0
55	MG	1A	3672	1/1	0.94	0.11	37,37,37,37	0
55	MG	2a	3033	1/1	0.94	0.31	60,60,60,60	0
55	MG	2A	3037	1/1	0.94	0.15	35,35,35,35	0
55	MG	2A	3038	1/1	0.94	0.18	44,44,44,44	0
55	MG	1A	3674	1/1	0.94	0.11	14,14,14,14	0
55	MG	2a	3038	1/1	0.94	0.12	45,45,45,45	0
55	MG	1A	3216	1/1	0.94	0.08	37,37,37,37	0
55	MG	1A	3676	1/1	0.94	0.12	55,55,55,55	0
55	MG	2a	3042	1/1	0.94	0.20	54,54,54,54	0
55	MG	1A	3677	1/1	0.94	0.11	57,57,57,57	0
55	MG	2A	3304	1/1	0.94	0.21	51,51,51,51	0
55	MG	2A	3305	1/1	0.94	0.12	53,53,53,53	0
55	MG	2A	3307	1/1	0.94	0.08	47,47,47,47	0
55	MG	1A	3340	1/1	0.94	0.10	35,35,35,35	0
55	MG	1A	3526	1/1	0.94	0.12	43,43,43,43	0
55	MG	2A	3622	1/1	0.94	0.15	61,61,61,61	0
55	MG	1A	3341	1/1	0.94	0.10	33,33,33,33	0
55	MG	1A	3908	1/1	0.94	0.12	40,40,40,40	0
55	MG	2A	3314	1/1	0.94	0.08	50,50,50,50	0
55	MG	1a	1691	1/1	0.94	0.17	46,46,46,46	0
55	MG	2A	3629	1/1	0.94	0.18	36,36,36,36	0
55	MG	2A	3316	1/1	0.94	0.26	48,48,48,48	0
55	MG	1B	228	1/1	0.94	0.14	37,37,37,37	0
55	MG	1A	3681	1/1	0.94	0.07	34,34,34,34	0
55	MG	2A	3635	1/1	0.94	0.08	42,42,42,42	0
55	MG	1a	1694	1/1	0.94	0.05	53,53,53,53	0
55	MG	1a	1695	1/1	0.94	0.13	39,39,39,39	0
55	MG	1A	3911	1/1	0.94	0.11	17,17,17,17	0
55	MG	2a	3065	1/1	0.94	0.22	60,60,60,60	0
55	MG	1A	3217	1/1	0.94	0.13	40,40,40,40	0
55	MG	2A	3644	1/1	0.94	0.17	68,68,68,68	0
55	MG	1A	3686	1/1	0.94	0.07	33,33,33,33	0
55	MG	1A	3687	1/1	0.94	0.07	35,35,35,35	0
55	MG	1A	3439	1/1	0.94	0.09	37,37,37,37	0
55	MG	1A	3918	1/1	0.94	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3074	1/1	0.94	0.19	43,43,43,43	0
55	MG	1a	1705	1/1	0.94	0.11	57,57,57,57	0
55	MG	1a	1706	1/1	0.94	0.24	54,54,54,54	0
55	MG	1A	3531	1/1	0.94	0.24	49,49,49,49	0
55	MG	1A	3920	1/1	0.94	0.07	56,56,56,56	0
55	MG	2a	3078	1/1	0.94	0.28	53,53,53,53	0
55	MG	1D	311	1/1	0.94	0.28	30,30,30,30	0
55	MG	2a	3080	1/1	0.94	0.18	51,51,51,51	0
55	MG	2A	3340	1/1	0.94	0.10	61,61,61,61	0
55	MG	1A	3921	1/1	0.94	0.07	45,45,45,45	0
55	MG	1A	3121	1/1	0.94	0.15	29,29,29,29	0
55	MG	1A	3925	1/1	0.94	0.18	49,49,49,49	0
55	MG	1A	3122	1/1	0.94	0.19	34,34,34,34	0
55	MG	2A	3345	1/1	0.94	0.12	49,49,49,49	0
55	MG	1A	3714	1/1	0.94	0.08	30,30,30,30	0
55	MG	1A	3538	1/1	0.94	0.07	44,44,44,44	0
55	MG	1A	3716	1/1	0.94	0.13	30,30,30,30	0
55	MG	1A	3123	1/1	0.94	0.09	35,35,35,35	0
55	MG	1F	311	1/1	0.94	0.15	27,27,27,27	0
55	MG	1A	3041	1/1	0.94	0.14	45,45,45,45	0
55	MG	2A	3096	1/1	0.94	0.20	47,47,47,47	0
55	MG	1A	3725	1/1	0.94	0.07	25,25,25,25	0
55	MG	1A	3731	1/1	0.94	0.08	31,31,31,31	0
55	MG	1A	3733	1/1	0.94	0.16	20,20,20,20	0
55	MG	2A	3358	1/1	0.94	0.15	37,37,37,37	0
55	MG	1A	3542	1/1	0.94	0.36	35,35,35,35	0
55	MG	1a	1728	1/1	0.94	0.13	50,50,50,50	0
55	MG	2A	3693	1/1	0.94	0.08	44,44,44,44	0
55	MG	2A	3696	1/1	0.94	0.10	36,36,36,36	0
55	MG	1A	3354	1/1	0.94	0.12	48,48,48,48	0
55	MG	1A	3548	1/1	0.94	0.28	42,42,42,42	0
55	MG	1A	3355	1/1	0.94	0.10	45,45,45,45	0
55	MG	2A	3703	1/1	0.94	0.11	55,55,55,55	0
55	MG	1a	1734	1/1	0.94	0.22	43,43,43,43	0
55	MG	1A	3550	1/1	0.94	0.21	41,41,41,41	0
55	MG	2A	3367	1/1	0.94	0.20	41,41,41,41	0
55	MG	2a	3114	1/1	0.94	0.26	56,56,56,56	0
55	MG	2a	3115	1/1	0.94	0.38	57,57,57,57	0
55	MG	1A	3952	1/1	0.94	0.10	45,45,45,45	0
55	MG	2A	3117	1/1	0.94	0.19	38,38,38,38	0
55	MG	2a	3118	1/1	0.94	0.17	45,45,45,45	0
55	MG	2A	3712	1/1	0.94	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3287	1/1	0.94	0.13	51,51,51,51	0
55	MG	2A	3120	1/1	0.94	0.16	55,55,55,55	0
55	MG	1A	3360	1/1	0.94	0.11	41,41,41,41	0
55	MG	2A	3124	1/1	0.94	0.20	55,55,55,55	0
55	MG	1A	3560	1/1	0.94	0.07	41,41,41,41	0
55	MG	1A	3456	1/1	0.94	0.15	32,32,32,32	0
55	MG	1A	3969	1/1	0.94	0.10	45,45,45,45	0
55	MG	1A	3042	1/1	0.94	0.10	25,25,25,25	0
55	MG	1A	3232	1/1	0.94	0.15	23,23,23,23	0
55	MG	1A	3755	1/1	0.94	0.15	55,55,55,55	0
55	MG	1A	3979	1/1	0.94	0.07	52,52,52,52	0
55	MG	2A	3727	1/1	0.94	0.07	66,66,66,66	0
55	MG	2A	3138	1/1	0.94	0.21	52,52,52,52	0
55	MG	2A	3139	1/1	0.94	0.16	59,59,59,59	0
55	MG	1A	3756	1/1	0.94	0.07	49,49,49,49	0
55	MG	2A	3388	1/1	0.94	0.14	42,42,42,42	0
55	MG	1A	3364	1/1	0.94	0.07	29,29,29,29	0
55	MG	2A	3143	1/1	0.94	0.20	44,44,44,44	0
55	MG	1X	101	1/1	0.94	0.12	35,35,35,35	0
55	MG	2A	3394	1/1	0.94	0.27	37,37,37,37	0
55	MG	2A	3395	1/1	0.94	0.23	35,35,35,35	0
55	MG	1a	1754	1/1	0.94	0.24	61,61,61,61	0
55	MG	1A	3983	1/1	0.94	0.10	56,56,56,56	0
55	MG	2A	3399	1/1	0.94	0.06	47,47,47,47	0
55	MG	2A	3744	1/1	0.94	0.17	61,61,61,61	0
55	MG	2A	3400	1/1	0.94	0.36	48,48,48,48	0
55	MG	1A	3763	1/1	0.94	0.07	46,46,46,46	0
55	MG	1A	3046	1/1	0.94	0.07	33,33,33,33	0
55	MG	2A	3749	1/1	0.94	0.18	45,45,45,45	0
55	MG	2A	3750	1/1	0.94	0.11	40,40,40,40	0
55	MG	1A	3368	1/1	0.94	0.10	40,40,40,40	0
55	MG	1Z	301	1/1	0.94	0.09	36,36,36,36	0
55	MG	2A	3407	1/1	0.94	0.21	53,53,53,53	0
55	MG	2a	3163	1/1	0.94	0.09	60,60,60,60	0
55	MG	2A	3755	1/1	0.94	0.06	52,52,52,52	0
55	MG	2A	3757	1/1	0.94	0.12	50,50,50,50	0
55	MG	2a	3166	1/1	0.94	0.21	54,54,54,54	0
55	MG	10	102	1/1	0.94	0.07	37,37,37,37	0
55	MG	2a	3168	1/1	0.94	0.17	40,40,40,40	0
55	MG	1A	3237	1/1	0.94	0.20	33,33,33,33	0
55	MG	1A	3370	1/1	0.94	0.13	42,42,42,42	0
55	MG	1A	3588	1/1	0.94	0.33	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3993	1/1	0.94	0.07	54,54,54,54	0
55	MG	2A	3415	1/1	0.94	0.10	57,57,57,57	0
55	MG	2A	3416	1/1	0.94	0.23	44,44,44,44	0
55	MG	13	101	1/1	0.94	0.11	50,50,50,50	0
55	MG	2A	3159	1/1	0.94	0.16	48,48,48,48	0
55	MG	1A	3770	1/1	0.94	0.08	37,37,37,37	0
55	MG	1A	3293	1/1	0.94	0.23	31,31,31,31	0
55	MG	2A	3421	1/1	0.94	0.27	48,48,48,48	0
55	MG	15	102	1/1	0.94	0.07	47,47,47,47	0
55	MG	2A	3777	1/1	0.94	0.08	52,52,52,52	0
55	MG	15	103	1/1	0.94	0.11	41,41,41,41	0
55	MG	1A	3372	1/1	0.94	0.22	38,38,38,38	0
55	MG	1A	3591	1/1	0.94	0.14	48,48,48,48	0
55	MG	2A	3167	1/1	0.94	0.18	68,68,68,68	0
55	MG	1A	3172	1/1	0.94	0.23	28,28,28,28	0
55	MG	1A	3063	1/1	0.94	0.14	44,44,44,44	0
55	MG	18	101	1/1	0.94	0.12	44,44,44,44	0
55	MG	2A	3787	1/1	0.94	0.26	66,66,66,66	0
55	MG	1a	1790	1/1	0.94	0.09	48,48,48,48	0
55	MG	2A	3436	1/1	0.94	0.07	55,55,55,55	0
55	MG	2A	3437	1/1	0.94	0.18	36,36,36,36	0
55	MG	1a	1791	1/1	0.94	0.09	54,54,54,54	0
55	MG	18	102	1/1	0.94	0.39	46,46,46,46	0
55	MG	2A	3443	1/1	0.94	0.13	41,41,41,41	0
55	MG	2A	3176	1/1	0.94	0.24	56,56,56,56	0
55	MG	1A	3025	1/1	0.94	0.09	44,44,44,44	0
55	MG	2A	3178	1/1	0.94	0.09	37,37,37,37	0
55	MG	2d	301	1/1	0.94	0.18	50,50,50,50	0
55	MG	1A	3381	1/1	0.94	0.05	38,38,38,38	0
55	MG	2A	3450	1/1	0.94	0.28	61,61,61,61	0
55	MG	2A	3451	1/1	0.94	0.48	51,51,51,51	0
55	MG	2A	3181	1/1	0.94	0.08	59,59,59,59	0
55	MG	1A	3243	1/1	0.94	0.06	41,41,41,41	0
55	MG	2A	3821	1/1	0.94	0.21	54,54,54,54	0
55	MG	2A	3823	1/1	0.94	0.23	60,60,60,60	0
55	MG	1A	3803	1/1	0.94	0.06	45,45,45,45	0
55	MG	2l	203	1/1	0.94	0.07	47,47,47,47	0
55	MG	2A	3184	1/1	0.94	0.06	39,39,39,39	0
55	MG	1A	3102	1/1	0.94	0.09	47,47,47,47	0
55	MG	1A	3306	1/1	0.94	0.08	47,47,47,47	0
55	MG	1A	3806	1/1	0.94	0.09	28,28,28,28	0
55	MG	1A	3387	1/1	0.94	0.27	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3605	1/1	0.94	0.12	33,33,33,33	0
55	MG	1a	1805	1/1	0.94	0.12	74,74,74,74	0
55	MG	1A	3606	1/1	0.94	0.18	37,37,37,37	0
55	MG	2A	3194	1/1	0.94	0.09	28,28,28,28	0
55	MG	2A	3837	1/1	0.94	0.11	48,48,48,48	0
55	MG	1A	3485	1/1	0.94	0.09	50,50,50,50	0
55	MG	2A	3474	1/1	0.95	0.17	38,38,38,38	0
55	MG	1A	3322	1/1	0.95	0.18	43,43,43,43	0
55	MG	2A	3476	1/1	0.95	0.26	37,37,37,37	0
55	MG	1A	3797	1/1	0.95	0.13	26,26,26,26	0
55	MG	2A	3829	1/1	0.95	0.10	40,40,40,40	0
55	MG	1A	3798	1/1	0.95	0.15	29,29,29,29	0
55	MG	2A	3479	1/1	0.95	0.41	51,51,51,51	0
55	MG	2A	3207	1/1	0.95	0.10	50,50,50,50	0
55	MG	1A	3038	1/1	0.95	0.14	18,18,18,18	0
55	MG	15	104	1/1	0.95	0.09	36,36,36,36	0
55	MG	2A	3835	1/1	0.95	0.05	59,59,59,59	0
55	MG	2A	3211	1/1	0.95	0.07	38,38,38,38	0
55	MG	1A	3126	1/1	0.95	0.27	37,37,37,37	0
55	MG	2A	3839	1/1	0.95	0.13	40,40,40,40	0
55	MG	2A	3840	1/1	0.95	0.17	43,43,43,43	0
55	MG	1A	4001	1/1	0.95	0.07	43,43,43,43	0
55	MG	1A	3325	1/1	0.95	0.18	48,48,48,48	0
55	MG	1A	3500	1/1	0.95	0.07	37,37,37,37	0
55	MG	1A	3265	1/1	0.95	0.06	37,37,37,37	0
55	MG	2A	3491	1/1	0.95	0.26	49,49,49,49	0
55	MG	1A	3414	1/1	0.95	0.04	47,47,47,47	0
55	MG	2A	3849	1/1	0.95	0.07	48,48,48,48	0
55	MG	1a	1819	1/1	0.95	0.05	71,71,71,71	0
55	MG	1A	4010	1/1	0.95	0.09	54,54,54,54	0
55	MG	1A	3503	1/1	0.95	0.27	49,49,49,49	0
55	MG	1A	3812	1/1	0.95	0.09	24,24,24,24	0
55	MG	1A	4013	1/1	0.95	0.24	35,35,35,35	0
55	MG	1A	3415	1/1	0.95	0.08	44,44,44,44	0
55	MG	2A	3500	1/1	0.95	0.17	38,38,38,38	0
55	MG	1A	3506	1/1	0.95	0.18	21,21,21,21	0
55	MG	1A	3327	1/1	0.95	0.11	41,41,41,41	0
55	MG	1A	3417	1/1	0.95	0.08	44,44,44,44	0
55	MG	1A	3510	1/1	0.95	0.14	33,33,33,33	0
55	MG	2A	3507	1/1	0.95	0.13	30,30,30,30	0
55	MG	1A	3826	1/1	0.95	0.08	35,35,35,35	0
55	MG	1a	1610	1/1	0.95	0.08	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	1A	3628	1/1	0.95	0.11	54,54,54,54	0
55	MG	1A	4024	1/1	0.95	0.15	39,39,39,39	0
55	MG	1A	3100	1/1	0.95	0.17	40,40,40,40	0
55	MG	1A	3330	1/1	0.95	0.09	34,34,34,34	0
55	MG	2B	209	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3513	1/1	0.95	0.15	39,39,39,39	0
55	MG	1A	3073	1/1	0.95	0.16	37,37,37,37	0
55	MG	1A	3835	1/1	0.95	0.09	39,39,39,39	0
55	MG	1A	3836	1/1	0.95	0.11	40,40,40,40	0
55	MG	2A	3522	1/1	0.95	0.15	31,31,31,31	0
55	MG	2A	3523	1/1	0.95	0.12	42,42,42,42	0
55	MG	2A	3524	1/1	0.95	0.10	37,37,37,37	0
55	MG	2A	3247	1/1	0.95	0.08	54,54,54,54	0
55	MG	1l	203	1/1	0.95	0.07	54,54,54,54	0
55	MG	1A	4035	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3837	1/1	0.95	0.10	51,51,51,51	0
55	MG	1A	3163	1/1	0.95	0.21	23,23,23,23	0
55	MG	1A	3334	1/1	0.95	0.14	33,33,33,33	0
55	MG	2A	3533	1/1	0.95	0.25	50,50,50,50	0
55	MG	1A	3642	1/1	0.95	0.14	26,26,26,26	0
55	MG	2A	3256	1/1	0.95	0.17	47,47,47,47	0
55	MG	1A	3425	1/1	0.95	0.07	53,53,53,53	0
55	MG	1a	1627	1/1	0.95	0.13	52,52,52,52	0
55	MG	2F	304	1/1	0.95	0.19	51,51,51,51	0
55	MG	1A	3335	1/1	0.95	0.14	36,36,36,36	0
55	MG	1A	3164	1/1	0.95	0.17	42,42,42,42	0
55	MG	1A	4054	1/1	0.95	0.09	37,37,37,37	0
55	MG	2N	202	1/1	0.95	0.06	48,48,48,48	0
55	MG	1a	1631	1/1	0.95	0.13	57,57,57,57	0
55	MG	2P	201	1/1	0.95	0.07	40,40,40,40	0
55	MG	2A	3546	1/1	0.95	0.21	33,33,33,33	0
55	MG	1A	4056	1/1	0.95	0.14	56,56,56,56	0
55	MG	1A	3074	1/1	0.95	0.14	24,24,24,24	0
55	MG	1x	110	1/1	0.95	0.14	63,63,63,63	0
55	MG	1A	3277	1/1	0.95	0.07	38,38,38,38	0
55	MG	1A	4059	1/1	0.95	0.06	34,34,34,34	0
55	MG	1A	3849	1/1	0.95	0.07	39,39,39,39	0
55	MG	2T	203	1/1	0.95	0.09	35,35,35,35	0
55	MG	2A	3271	1/1	0.95	0.23	61,61,61,61	0
55	MG	1A	3278	1/1	0.95	0.07	40,40,40,40	0
55	MG	2A	3555	1/1	0.95	0.17	44,44,44,44	0
55	MG	2A	3556	1/1	0.95	0.08	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	2V	203	1/1	0.95	0.08	47,47,47,47	0
55	MG	1A	4063	1/1	0.95	0.12	36,36,36,36	0
55	MG	1A	3166	1/1	0.95	0.15	28,28,28,28	0
55	MG	1A	3658	1/1	0.95	0.10	43,43,43,43	0
55	MG	1A	3167	1/1	0.95	0.11	37,37,37,37	0
55	MG	1A	3168	1/1	0.95	0.08	38,38,38,38	0
55	MG	2A	3009	1/1	0.95	0.11	40,40,40,40	0
55	MG	2A	3010	1/1	0.95	0.06	30,30,30,30	0
55	MG	2A	3569	1/1	0.95	0.14	38,38,38,38	0
55	MG	1A	3667	1/1	0.95	0.20	49,49,49,49	0
55	MG	1A	3225	1/1	0.95	0.12	26,26,26,26	0
55	MG	1a	1647	1/1	0.95	0.13	53,53,53,53	0
55	MG	1A	4074	1/1	0.95	0.09	14,14,14,14	0
55	MG	1A	3169	1/1	0.95	0.10	26,26,26,26	0
55	MG	2A	3577	1/1	0.95	0.09	44,44,44,44	0
55	MG	2A	3578	1/1	0.95	0.21	28,28,28,28	0
55	MG	2A	3579	1/1	0.95	0.08	55,55,55,55	0
55	MG	1A	4077	1/1	0.95	0.10	34,34,34,34	0
55	MG	1A	3670	1/1	0.95	0.08	46,46,46,46	0
55	MG	2A	3583	1/1	0.95	0.16	53,53,53,53	0
55	MG	2a	3011	1/1	0.95	0.32	55,55,55,55	0
55	MG	2A	3584	1/1	0.95	0.10	35,35,35,35	0
55	MG	1A	3671	1/1	0.95	0.05	36,36,36,36	0
55	MG	1a	1655	1/1	0.95	0.20	39,39,39,39	0
55	MG	1A	3130	1/1	0.95	0.11	27,27,27,27	0
55	MG	2A	3588	1/1	0.95	0.12	49,49,49,49	0
55	MG	2A	3024	1/1	0.95	0.16	40,40,40,40	0
55	MG	1A	3057	1/1	0.95	0.07	21,21,21,21	0
55	MG	2A	3026	1/1	0.95	0.13	42,42,42,42	0
55	MG	1A	3233	1/1	0.95	0.21	38,38,38,38	0
55	MG	1A	3446	1/1	0.95	0.07	31,31,31,31	0
55	MG	1A	3447	1/1	0.95	0.09	42,42,42,42	0
55	MG	1A	3079	1/1	0.95	0.15	34,34,34,34	0
55	MG	1A	4090	1/1	0.95	0.06	42,42,42,42	0
55	MG	1A	4094	1/1	0.95	0.10	14,14,14,14	0
55	MG	1A	4096	1/1	0.95	0.08	47,47,47,47	0
55	MG	1A	4097	1/1	0.95	0.12	35,35,35,35	0
55	MG	1A	3359	1/1	0.95	0.07	44,44,44,44	0
55	MG	2A	3306	1/1	0.95	0.14	55,55,55,55	0
55	MG	1A	4100	1/1	0.95	0.09	37,37,37,37	0
55	MG	1A	3235	1/1	0.95	0.18	35,35,35,35	0
55	MG	1A	3876	1/1	0.95	0.11	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3311	1/1	0.95	0.12	41,41,41,41	0
55	MG	1A	4103	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3295	1/1	0.95	0.08	31,31,31,31	0
55	MG	2A	3046	1/1	0.95	0.17	55,55,55,55	0
55	MG	2A	3047	1/1	0.95	0.12	53,53,53,53	0
55	MG	1A	3058	1/1	0.95	0.17	35,35,35,35	0
55	MG	1A	3685	1/1	0.95	0.08	34,34,34,34	0
55	MG	2A	3053	1/1	0.95	0.06	41,41,41,41	0
55	MG	2A	3319	1/1	0.95	0.22	62,62,62,62	0
55	MG	2A	3056	1/1	0.95	0.06	42,42,42,42	0
55	MG	1A	3297	1/1	0.95	0.12	36,36,36,36	0
55	MG	2A	3620	1/1	0.95	0.15	38,38,38,38	0
55	MG	1A	3365	1/1	0.95	0.10	48,48,48,48	0
55	MG	1A	3885	1/1	0.95	0.10	50,50,50,50	0
55	MG	2A	3623	1/1	0.95	0.15	26,26,26,26	0
55	MG	2A	3062	1/1	0.95	0.20	45,45,45,45	0
55	MG	1A	3238	1/1	0.95	0.10	31,31,31,31	0
55	MG	2A	3626	1/1	0.95	0.19	44,44,44,44	0
55	MG	2a	3053	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3328	1/1	0.95	0.06	43,43,43,43	0
55	MG	1A	3553	1/1	0.95	0.06	33,33,33,33	0
55	MG	1A	3699	1/1	0.95	0.09	21,21,21,21	0
55	MG	1A	3299	1/1	0.95	0.15	42,42,42,42	0
55	MG	1A	3704	1/1	0.95	0.11	42,42,42,42	0
55	MG	1A	3705	1/1	0.95	0.09	23,23,23,23	0
55	MG	1A	3556	1/1	0.95	0.20	31,31,31,31	0
55	MG	2A	3636	1/1	0.95	0.13	57,57,57,57	0
55	MG	2A	3637	1/1	0.95	0.28	38,38,38,38	0
55	MG	2A	3337	1/1	0.95	0.12	51,51,51,51	0
55	MG	1A	3710	1/1	0.95	0.07	21,21,21,21	0
55	MG	2A	3640	1/1	0.95	0.10	55,55,55,55	0
55	MG	1B	203	1/1	0.95	0.13	39,39,39,39	0
55	MG	2A	3642	1/1	0.95	0.07	69,69,69,69	0
55	MG	1B	204	1/1	0.95	0.13	52,52,52,52	0
55	MG	2A	3078	1/1	0.95	0.09	43,43,43,43	0
55	MG	1B	205	1/1	0.95	0.07	39,39,39,39	0
55	MG	1A	3902	1/1	0.95	0.07	58,58,58,58	0
55	MG	1A	3712	1/1	0.95	0.10	41,41,41,41	0
55	MG	1A	3713	1/1	0.95	0.14	42,42,42,42	0
55	MG	2A	3649	1/1	0.95	0.07	40,40,40,40	0
55	MG	1B	211	1/1	0.95	0.05	33,33,33,33	0
55	MG	1a	1696	1/1	0.95	0.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3558	1/1	0.95	0.36	30,30,30,30	0
55	MG	1B	217	1/1	0.95	0.06	38,38,38,38	0
55	MG	2A	3656	1/1	0.95	0.09	53,53,53,53	0
55	MG	1A	3300	1/1	0.95	0.05	28,28,28,28	0
55	MG	2a	3084	1/1	0.95	0.06	69,69,69,69	0
55	MG	1A	3111	1/1	0.95	0.18	30,30,30,30	0
55	MG	1A	3565	1/1	0.95	0.12	40,40,40,40	0
55	MG	2A	3093	1/1	0.95	0.21	48,48,48,48	0
55	MG	2A	3663	1/1	0.95	0.10	52,52,52,52	0
55	MG	1A	3719	1/1	0.95	0.06	60,60,60,60	0
55	MG	1A	3913	1/1	0.95	0.08	22,22,22,22	0
55	MG	1B	227	1/1	0.95	0.11	57,57,57,57	0
55	MG	1A	3721	1/1	0.95	0.09	27,27,27,27	0
55	MG	1A	3566	1/1	0.95	0.09	32,32,32,32	0
55	MG	2A	3672	1/1	0.95	0.14	59,59,59,59	0
55	MG	2A	3102	1/1	0.95	0.07	63,63,63,63	0
55	MG	1A	3916	1/1	0.95	0.18	68,68,68,68	0
55	MG	1A	3051	1/1	0.95	0.15	23,23,23,23	0
55	MG	1a	1711	1/1	0.95	0.06	57,57,57,57	0
55	MG	2A	3677	1/1	0.95	0.08	37,37,37,37	0
55	MG	1a	1712	1/1	0.95	0.16	65,65,65,65	0
55	MG	2A	3680	1/1	0.95	0.12	47,47,47,47	0
55	MG	2a	3104	1/1	0.95	0.10	64,64,64,64	0
55	MG	2A	3109	1/1	0.95	0.15	52,52,52,52	0
55	MG	2a	3106	1/1	0.95	0.10	46,46,46,46	0
55	MG	1A	3726	1/1	0.95	0.08	64,64,64,64	0
55	MG	1A	3304	1/1	0.95	0.22	34,34,34,34	0
55	MG	2A	3370	1/1	0.95	0.08	63,63,63,63	0
55	MG	2A	3688	1/1	0.95	0.16	32,32,32,32	0
55	MG	2A	3113	1/1	0.95	0.08	40,40,40,40	0
55	MG	1A	3572	1/1	0.95	0.06	32,32,32,32	0
55	MG	1A	3574	1/1	0.95	0.12	41,41,41,41	0
55	MG	1D	304	1/1	0.95	0.13	32,32,32,32	0
55	MG	1D	307	1/1	0.95	0.29	38,38,38,38	0
55	MG	1D	308	1/1	0.95	0.37	35,35,35,35	0
55	MG	1a	1720	1/1	0.95	0.10	41,41,41,41	0
55	MG	1A	3373	1/1	0.95	0.20	47,47,47,47	0
55	MG	1A	3181	1/1	0.95	0.17	58,58,58,58	0
55	MG	2A	3125	1/1	0.95	0.23	58,58,58,58	0
55	MG	2A	3705	1/1	0.95	0.06	55,55,55,55	0
55	MG	1A	3242	1/1	0.95	0.17	36,36,36,36	0
55	MG	2A	3128	1/1	0.95	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3018	1/1	0.95	0.20	43,43,43,43	0
55	MG	1A	3929	1/1	0.95	0.08	37,37,37,37	0
55	MG	1A	3086	1/1	0.95	0.12	39,39,39,39	0
55	MG	1A	3744	1/1	0.95	0.05	53,53,53,53	0
55	MG	2A	3390	1/1	0.95	0.12	53,53,53,53	0
55	MG	1E	305	1/1	0.95	0.21	30,30,30,30	0
55	MG	2A	3134	1/1	0.95	0.08	45,45,45,45	0
55	MG	1A	3935	1/1	0.95	0.09	21,21,21,21	0
55	MG	1E	307	1/1	0.95	0.11	44,44,44,44	0
55	MG	1a	1732	1/1	0.95	0.12	42,42,42,42	0
55	MG	2A	3140	1/1	0.95	0.08	40,40,40,40	0
55	MG	1a	1733	1/1	0.95	0.20	50,50,50,50	0
55	MG	1A	3587	1/1	0.95	0.07	57,57,57,57	0
55	MG	2A	3401	1/1	0.95	0.24	43,43,43,43	0
55	MG	1a	1737	1/1	0.95	0.14	42,42,42,42	0
55	MG	2A	3728	1/1	0.95	0.07	53,53,53,53	0
55	MG	1F	304	1/1	0.95	0.19	46,46,46,46	0
55	MG	2A	3404	1/1	0.95	0.12	61,61,61,61	0
55	MG	1A	3746	1/1	0.95	0.24	39,39,39,39	0
55	MG	2A	3733	1/1	0.95	0.13	49,49,49,49	0
55	MG	1F	308	1/1	0.95	0.11	34,34,34,34	0
55	MG	1A	3044	1/1	0.95	0.17	27,27,27,27	0
55	MG	2A	3408	1/1	0.95	0.30	60,60,60,60	0
55	MG	2A	3409	1/1	0.95	0.22	45,45,45,45	0
55	MG	1A	3474	1/1	0.95	0.19	39,39,39,39	0
55	MG	1A	3067	1/1	0.95	0.10	49,49,49,49	0
55	MG	1A	3751	1/1	0.95	0.17	50,50,50,50	0
55	MG	1A	3477	1/1	0.95	0.08	49,49,49,49	0
55	MG	2a	3161	1/1	0.95	0.13	51,51,51,51	0
55	MG	2A	3153	1/1	0.95	0.19	47,47,47,47	0
55	MG	1A	3478	1/1	0.95	0.08	44,44,44,44	0
55	MG	1N	203	1/1	0.95	0.06	47,47,47,47	0
55	MG	1A	3594	1/1	0.95	0.15	23,23,23,23	0
55	MG	1A	3757	1/1	0.95	0.10	55,55,55,55	0
55	MG	1A	3951	1/1	0.95	0.09	34,34,34,34	0
55	MG	1A	3036	1/1	0.95	0.07	34,34,34,34	0
55	MG	2a	3171	1/1	0.95	0.15	53,53,53,53	0
55	MG	1P	201	1/1	0.95	0.20	27,27,27,27	0
55	MG	2A	3752	1/1	0.95	0.18	51,51,51,51	0
55	MG	1A	3958	1/1	0.95	0.11	31,31,31,31	0
55	MG	1A	3961	1/1	0.95	0.08	41,41,41,41	0
55	MG	1A	3597	1/1	0.95	0.21	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	1A	3149	1/1	0.95	0.31	30,30,30,30	0
55	MG	1A	3964	1/1	0.95	0.13	18,18,18,18	0
55	MG	1R	202	1/1	0.95	0.11	35,35,35,35	0
55	MG	1S	201	1/1	0.95	0.09	47,47,47,47	0
55	MG	2A	3430	1/1	0.95	0.22	31,31,31,31	0
55	MG	1A	3195	1/1	0.95	0.06	40,40,40,40	0
55	MG	2A	3767	1/1	0.95	0.19	51,51,51,51	0
55	MG	1A	3152	1/1	0.95	0.10	26,26,26,26	0
55	MG	2A	3769	1/1	0.95	0.11	48,48,48,48	0
55	MG	2A	3435	1/1	0.95	0.16	41,41,41,41	0
55	MG	1A	3483	1/1	0.95	0.31	53,53,53,53	0
55	MG	1U	206	1/1	0.95	0.18	28,28,28,28	0
55	MG	2A	3438	1/1	0.95	0.17	51,51,51,51	0
55	MG	2A	3440	1/1	0.95	0.19	50,50,50,50	0
55	MG	2a	3195	1/1	0.95	0.04	62,62,62,62	0
55	MG	1A	3971	1/1	0.95	0.14	42,42,42,42	0
55	MG	1A	3391	1/1	0.95	0.18	52,52,52,52	0
55	MG	1a	1778	1/1	0.95	0.12	43,43,43,43	0
55	MG	2a	3200	1/1	0.95	0.13	47,47,47,47	0
55	MG	1a	1780	1/1	0.95	0.17	42,42,42,42	0
55	MG	1A	3070	1/1	0.95	0.16	49,49,49,49	0
55	MG	1A	3772	1/1	0.95	0.09	16,16,16,16	0
55	MG	1A	3976	1/1	0.95	0.07	46,46,46,46	0
55	MG	1W	205	1/1	0.95	0.10	35,35,35,35	0
55	MG	1A	3977	1/1	0.95	0.05	40,40,40,40	0
55	MG	1A	3604	1/1	0.95	0.15	31,31,31,31	0
55	MG	1A	3155	1/1	0.95	0.10	32,32,32,32	0
55	MG	1A	3205	1/1	0.95	0.07	39,39,39,39	0
55	MG	1A	3778	1/1	0.95	0.09	29,29,29,29	0
55	MG	1A	3784	1/1	0.95	0.09	49,49,49,49	0
55	MG	2A	3794	1/1	0.95	0.06	57,57,57,57	0
55	MG	10	101	1/1	0.95	0.06	31,31,31,31	0
55	MG	1A	3071	1/1	0.95	0.09	28,28,28,28	0
55	MG	2A	3797	1/1	0.95	0.07	35,35,35,35	0
55	MG	1A	3207	1/1	0.95	0.12	41,41,41,41	0
55	MG	2A	3799	1/1	0.95	0.15	56,56,56,56	0
55	MG	2A	3195	1/1	0.95	0.09	39,39,39,39	0
55	MG	10	105	1/1	0.95	0.05	44,44,44,44	0
55	MG	2A	3802	1/1	0.95	0.08	40,40,40,40	0
55	MG	11	102	1/1	0.95	0.08	28,28,28,28	0
55	MG	2A	3198	1/1	0.95	0.26	47,47,47,47	0
55	MG	2A	3812	1/1	0.95	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3789	1/1	0.95	0.12	37,37,37,37	0
55	MG	1A	3790	1/1	0.95	0.12	16,16,16,16	0
55	MG	2A	3470	1/1	0.95	0.13	49,49,49,49	0
55	MG	2A	3471	1/1	0.95	0.12	21,21,21,21	0
56	ZN	24	501	1/1	0.95	0.09	132,132,132,132	0
55	MG	1A	3791	1/1	0.95	0.09	24,24,24,24	0
55	MG	1A	3404	1/1	0.95	0.13	55,55,55,55	0
55	MG	1A	3825	1/1	0.96	0.04	27,27,27,27	0
55	MG	2A	3336	1/1	0.96	0.20	48,48,48,48	0
55	MG	1P	203	1/1	0.96	0.15	49,49,49,49	0
55	MG	2A	3104	1/1	0.96	0.18	51,51,51,51	0
55	MG	2B	217	1/1	0.96	0.07	57,57,57,57	0
55	MG	1Q	201	1/1	0.96	0.17	28,28,28,28	0
55	MG	2A	3592	1/1	0.96	0.12	36,36,36,36	0
55	MG	1A	3994	1/1	0.96	0.12	36,36,36,36	0
55	MG	1a	1735	1/1	0.96	0.20	50,50,50,50	0
55	MG	1A	3091	1/1	0.96	0.11	49,49,49,49	0
55	MG	1A	3996	1/1	0.96	0.06	50,50,50,50	0
55	MG	1a	1739	1/1	0.96	0.18	47,47,47,47	0
55	MG	1A	3150	1/1	0.96	0.08	25,25,25,25	0
55	MG	1A	3828	1/1	0.96	0.10	25,25,25,25	0
55	MG	2E	308	1/1	0.96	0.06	26,26,26,26	0
55	MG	1A	3829	1/1	0.96	0.08	24,24,24,24	0
55	MG	1A	3543	1/1	0.96	0.10	48,48,48,48	0
55	MG	1A	3545	1/1	0.96	0.17	31,31,31,31	0
55	MG	2F	303	1/1	0.96	0.15	45,45,45,45	0
55	MG	2A	3603	1/1	0.96	0.12	34,34,34,34	0
55	MG	2F	305	1/1	0.96	0.14	49,49,49,49	0
55	MG	1A	4002	1/1	0.96	0.07	60,60,60,60	0
55	MG	2A	3351	1/1	0.96	0.19	38,38,38,38	0
55	MG	2A	3119	1/1	0.96	0.20	32,32,32,32	0
55	MG	1A	4004	1/1	0.96	0.11	14,14,14,14	0
55	MG	2A	3608	1/1	0.96	0.22	38,38,38,38	0
55	MG	2O	202	1/1	0.96	0.16	46,46,46,46	0
55	MG	2A	3122	1/1	0.96	0.13	32,32,32,32	0
55	MG	1A	3383	1/1	0.96	0.12	35,35,35,35	0
55	MG	1A	4006	1/1	0.96	0.08	30,30,30,30	0
55	MG	1A	3547	1/1	0.96	0.23	30,30,30,30	0
55	MG	1A	3007	1/1	0.96	0.08	39,39,39,39	0
55	MG	1a	1751	1/1	0.96	0.10	54,54,54,54	0
55	MG	1A	3226	1/1	0.96	0.18	32,32,32,32	0
55	MG	1A	3227	1/1	0.96	0.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3228	1/1	0.96	0.17	44,44,44,44	0
55	MG	1A	3673	1/1	0.96	0.17	40,40,40,40	0
55	MG	2A	3619	1/1	0.96	0.18	48,48,48,48	0
55	MG	1X	104	1/1	0.96	0.07	40,40,40,40	0
55	MG	1X	105	1/1	0.96	0.05	34,34,34,34	0
55	MG	2A	3135	1/1	0.96	0.05	36,36,36,36	0
55	MG	1A	3840	1/1	0.96	0.10	28,28,28,28	0
55	MG	2A	3137	1/1	0.96	0.20	51,51,51,51	0
55	MG	1A	4014	1/1	0.96	0.09	39,39,39,39	0
55	MG	1A	3841	1/1	0.96	0.13	38,38,38,38	0
55	MG	1A	3552	1/1	0.96	0.04	33,33,33,33	0
55	MG	1Z	302	1/1	0.96	0.12	43,43,43,43	0
55	MG	25	101	1/1	0.96	0.11	44,44,44,44	0
55	MG	1A	4017	1/1	0.96	0.10	20,20,20,20	0
55	MG	1A	3389	1/1	0.96	0.14	48,48,48,48	0
55	MG	27	101	1/1	0.96	0.08	44,44,44,44	0
55	MG	2A	3631	1/1	0.96	0.11	35,35,35,35	0
55	MG	2A	3144	1/1	0.96	0.22	45,45,45,45	0
55	MG	1A	3093	1/1	0.96	0.10	41,41,41,41	0
55	MG	10	104	1/1	0.96	0.09	51,51,51,51	0
55	MG	1A	3555	1/1	0.96	0.21	32,32,32,32	0
55	MG	2A	3381	1/1	0.96	0.04	49,49,49,49	0
55	MG	1A	3001	1/1	0.96	0.05	33,33,33,33	0
55	MG	2A	3383	1/1	0.96	0.14	52,52,52,52	0
55	MG	1A	3557	1/1	0.96	0.12	21,21,21,21	0
55	MG	1a	1781	1/1	0.96	0.15	56,56,56,56	0
55	MG	2a	3009	1/1	0.96	0.12	59,59,59,59	0
55	MG	1A	3392	1/1	0.96	0.07	53,53,53,53	0
55	MG	12	101	1/1	0.96	0.08	42,42,42,42	0
55	MG	1A	3020	1/1	0.96	0.07	22,22,22,22	0
55	MG	1A	3561	1/1	0.96	0.19	38,38,38,38	0
55	MG	1A	3473	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3283	1/1	0.96	0.18	26,26,26,26	0
55	MG	2A	3393	1/1	0.96	0.10	40,40,40,40	0
55	MG	1A	4031	1/1	0.96	0.09	33,33,33,33	0
55	MG	1A	3475	1/1	0.96	0.15	40,40,40,40	0
55	MG	2A	3651	1/1	0.96	0.06	50,50,50,50	0
55	MG	1A	3855	1/1	0.96	0.18	50,50,50,50	0
55	MG	1A	3032	1/1	0.96	0.08	20,20,20,20	0
55	MG	1A	3692	1/1	0.96	0.08	36,36,36,36	0
55	MG	2A	3655	1/1	0.96	0.05	39,39,39,39	0
55	MG	1A	3397	1/1	0.96	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	17	103	1/1	0.96	0.09	32,32,32,32	0
55	MG	2A	3164	1/1	0.96	0.09	57,57,57,57	0
55	MG	1A	3860	1/1	0.96	0.07	38,38,38,38	0
55	MG	1A	3697	1/1	0.96	0.08	48,48,48,48	0
55	MG	1A	4042	1/1	0.96	0.06	57,57,57,57	0
55	MG	2A	3664	1/1	0.96	0.10	58,58,58,58	0
55	MG	1a	1801	1/1	0.96	0.15	62,62,62,62	0
55	MG	2A	3169	1/1	0.96	0.24	48,48,48,48	0
55	MG	18	103	1/1	0.96	0.16	38,38,38,38	0
55	MG	1A	4043	1/1	0.96	0.05	49,49,49,49	0
55	MG	1A	3570	1/1	0.96	0.17	31,31,31,31	0
55	MG	2a	3036	1/1	0.96	0.06	43,43,43,43	0
55	MG	1A	3863	1/1	0.96	0.07	45,45,45,45	0
55	MG	1A	3398	1/1	0.96	0.22	29,29,29,29	0
55	MG	2a	3039	1/1	0.96	0.11	43,43,43,43	0
55	MG	1A	3868	1/1	0.96	0.05	57,57,57,57	0
55	MG	1a	1603	1/1	0.96	0.08	55,55,55,55	0
55	MG	1A	3332	1/1	0.96	0.12	44,44,44,44	0
55	MG	1A	3285	1/1	0.96	0.13	38,38,38,38	0
55	MG	2A	3180	1/1	0.96	0.11	44,44,44,44	0
55	MG	2A	3679	1/1	0.96	0.05	43,43,43,43	0
55	MG	1A	3577	1/1	0.96	0.24	37,37,37,37	0
55	MG	1a	1813	1/1	0.96	0.13	40,40,40,40	0
55	MG	1A	3709	1/1	0.96	0.08	23,23,23,23	0
55	MG	1A	4060	1/1	0.96	0.08	37,37,37,37	0
55	MG	2A	3684	1/1	0.96	0.04	54,54,54,54	0
55	MG	1a	1609	1/1	0.96	0.29	62,62,62,62	0
55	MG	1A	3578	1/1	0.96	0.08	33,33,33,33	0
55	MG	1A	3401	1/1	0.96	0.07	37,37,37,37	0
55	MG	2a	3054	1/1	0.96	0.21	46,46,46,46	0
55	MG	1A	3580	1/1	0.96	0.08	35,35,35,35	0
55	MG	1a	1613	1/1	0.96	0.11	37,37,37,37	0
55	MG	1a	1822	1/1	0.96	0.16	54,54,54,54	0
55	MG	2A	3695	1/1	0.96	0.17	29,29,29,29	0
55	MG	2a	3059	1/1	0.96	0.10	50,50,50,50	0
55	MG	1a	1823	1/1	0.96	0.25	51,51,51,51	0
55	MG	1A	3581	1/1	0.96	0.14	41,41,41,41	0
55	MG	1A	3187	1/1	0.96	0.08	29,29,29,29	0
55	MG	2A	3699	1/1	0.96	0.06	43,43,43,43	0
55	MG	1A	3584	1/1	0.96	0.28	33,33,33,33	0
55	MG	2A	3434	1/1	0.96	0.05	69,69,69,69	0
55	MG	1A	3406	1/1	0.96	0.14	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	3880	1/1	0.96	0.10	21,21,21,21	0
55	MG	1A	3407	1/1	0.96	0.10	49,49,49,49	0
55	MG	1A	3158	1/1	0.96	0.11	34,34,34,34	0
55	MG	1A	4075	1/1	0.96	0.10	58,58,58,58	0
55	MG	1A	3884	1/1	0.96	0.12	28,28,28,28	0
55	MG	1A	3722	1/1	0.96	0.07	33,33,33,33	0
55	MG	2A	3713	1/1	0.96	0.06	52,52,52,52	0
55	MG	2A	3714	1/1	0.96	0.11	55,55,55,55	0
55	MG	1A	4078	1/1	0.96	0.08	61,61,61,61	0
55	MG	1A	3888	1/1	0.96	0.04	29,29,29,29	0
55	MG	2A	3446	1/1	0.96	0.08	48,48,48,48	0
55	MG	1A	3236	1/1	0.96	0.16	23,23,23,23	0
55	MG	1A	3056	1/1	0.96	0.10	39,39,39,39	0
55	MG	1A	3891	1/1	0.96	0.08	39,39,39,39	0
55	MG	1A	3191	1/1	0.96	0.17	29,29,29,29	0
55	MG	1A	3893	1/1	0.96	0.08	35,35,35,35	0
55	MG	2A	3723	1/1	0.96	0.07	29,29,29,29	0
55	MG	2A	3213	1/1	0.96	0.13	57,57,57,57	0
55	MG	2A	3214	1/1	0.96	0.28	43,43,43,43	0
55	MG	1A	3727	1/1	0.96	0.12	31,31,31,31	0
55	MG	1A	3730	1/1	0.96	0.07	16,16,16,16	0
55	MG	1A	3339	1/1	0.96	0.25	42,42,42,42	0
55	MG	2A	3458	1/1	0.96	0.13	52,52,52,52	0
55	MG	1A	3898	1/1	0.96	0.16	22,22,22,22	0
55	MG	2A	3220	1/1	0.96	0.14	62,62,62,62	0
55	MG	1A	3899	1/1	0.96	0.11	41,41,41,41	0
55	MG	1A	3193	1/1	0.96	0.47	33,33,33,33	0
55	MG	1A	3494	1/1	0.96	0.15	35,35,35,35	0
55	MG	2A	3736	1/1	0.96	0.05	58,58,58,58	0
55	MG	2a	3097	1/1	0.96	0.07	75,75,75,75	0
55	MG	1A	4099	1/1	0.96	0.08	37,37,37,37	0
55	MG	1x	102	1/1	0.96	0.06	59,59,59,59	0
55	MG	1A	3595	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3160	1/1	0.96	0.11	29,29,29,29	0
55	MG	1A	3739	1/1	0.96	0.15	27,27,27,27	0
55	MG	1A	3905	1/1	0.96	0.07	23,23,23,23	0
55	MG	1A	3342	1/1	0.96	0.21	28,28,28,28	0
55	MG	1A	3345	1/1	0.96	0.26	25,25,25,25	0
55	MG	1A	3498	1/1	0.96	0.09	24,24,24,24	0
55	MG	1A	3743	1/1	0.96	0.18	49,49,49,49	0
55	MG	2A	3235	1/1	0.96	0.07	53,53,53,53	0
55	MG	1A	3101	1/1	0.96	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3197	1/1	0.96	0.14	42,42,42,42	0
55	MG	1A	3420	1/1	0.96	0.06	45,45,45,45	0
55	MG	1A	3033	1/1	0.96	0.07	24,24,24,24	0
55	MG	2A	3481	1/1	0.96	0.17	38,38,38,38	0
55	MG	1A	3199	1/1	0.96	0.16	18,18,18,18	0
55	MG	1A	3245	1/1	0.96	0.13	57,57,57,57	0
55	MG	2A	3242	1/1	0.96	0.20	49,49,49,49	0
55	MG	1A	3352	1/1	0.96	0.07	40,40,40,40	0
55	MG	2A	3759	1/1	0.96	0.09	46,46,46,46	0
55	MG	1A	3353	1/1	0.96	0.07	50,50,50,50	0
55	MG	2a	3121	1/1	0.96	0.38	51,51,51,51	0
55	MG	2a	3122	1/1	0.96	0.25	34,34,34,34	0
55	MG	1A	3246	1/1	0.96	0.15	43,43,43,43	0
55	MG	1A	3021	1/1	0.96	0.06	24,24,24,24	0
55	MG	1A	3429	1/1	0.96	0.09	48,48,48,48	0
55	MG	2A	3490	1/1	0.96	0.19	46,46,46,46	0
55	MG	1A	3759	1/1	0.96	0.06	39,39,39,39	0
55	MG	1A	3203	1/1	0.96	0.17	29,29,29,29	0
55	MG	1A	3357	1/1	0.96	0.05	36,36,36,36	0
55	MG	2a	3131	1/1	0.96	0.21	37,37,37,37	0
55	MG	2a	3133	1/1	0.96	0.41	46,46,46,46	0
55	MG	1A	3614	1/1	0.96	0.14	15,15,15,15	0
55	MG	1A	3615	1/1	0.96	0.20	48,48,48,48	0
55	MG	1A	3931	1/1	0.96	0.17	35,35,35,35	0
55	MG	1B	212	1/1	0.96	0.14	52,52,52,52	0
55	MG	1A	3616	1/1	0.96	0.21	38,38,38,38	0
55	MG	1B	215	1/1	0.96	0.06	43,43,43,43	0
55	MG	1B	216	1/1	0.96	0.11	48,48,48,48	0
55	MG	1A	3934	1/1	0.96	0.06	28,28,28,28	0
55	MG	1A	3514	1/1	0.96	0.09	59,59,59,59	0
55	MG	1B	221	1/1	0.96	0.06	34,34,34,34	0
55	MG	1A	3358	1/1	0.96	0.10	56,56,56,56	0
55	MG	2A	3508	1/1	0.96	0.14	50,50,50,50	0
55	MG	1A	3249	1/1	0.96	0.15	37,37,37,37	0
55	MG	1A	3771	1/1	0.96	0.13	33,33,33,33	0
55	MG	2A	3035	1/1	0.96	0.17	58,58,58,58	0
55	MG	1A	3204	1/1	0.96	0.06	24,24,24,24	0
55	MG	1a	1680	1/1	0.96	0.08	61,61,61,61	0
55	MG	2A	3792	1/1	0.96	0.08	60,60,60,60	0
55	MG	1A	3013	1/1	0.96	0.18	27,27,27,27	0
55	MG	1A	3252	1/1	0.96	0.15	33,33,33,33	0
55	MG	2a	3156	1/1	0.96	0.15	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	3945	1/1	0.96	0.10	56,56,56,56	0
55	MG	1A	3108	1/1	0.96	0.04	29,29,29,29	0
55	MG	1a	1685	1/1	0.96	0.13	58,58,58,58	0
55	MG	1A	3440	1/1	0.96	0.17	39,39,39,39	0
55	MG	1A	3948	1/1	0.96	0.07	30,30,30,30	0
55	MG	1A	3780	1/1	0.96	0.08	57,57,57,57	0
55	MG	1A	3443	1/1	0.96	0.09	33,33,33,33	0
55	MG	1A	3049	1/1	0.96	0.11	27,27,27,27	0
55	MG	1A	3050	1/1	0.96	0.18	36,36,36,36	0
55	MG	1A	3954	1/1	0.96	0.06	52,52,52,52	0
55	MG	2A	3051	1/1	0.96	0.22	53,53,53,53	0
55	MG	2A	3287	1/1	0.96	0.10	46,46,46,46	0
55	MG	2a	3169	1/1	0.96	0.14	59,59,59,59	0
55	MG	2A	3815	1/1	0.96	0.10	40,40,40,40	0
55	MG	1A	3957	1/1	0.96	0.13	28,28,28,28	0
55	MG	2A	3535	1/1	0.96	0.11	39,39,39,39	0
55	MG	2A	3054	1/1	0.96	0.23	47,47,47,47	0
55	MG	2A	3820	1/1	0.96	0.12	33,33,33,33	0
55	MG	1A	3064	1/1	0.96	0.17	40,40,40,40	0
55	MG	2A	3538	1/1	0.96	0.16	32,32,32,32	0
55	MG	2A	3539	1/1	0.96	0.09	57,57,57,57	0
55	MG	1A	3065	1/1	0.96	0.20	50,50,50,50	0
55	MG	2A	3059	1/1	0.96	0.05	42,42,42,42	0
55	MG	2a	3182	1/1	0.96	0.09	51,51,51,51	0
55	MG	1A	3114	1/1	0.96	0.15	38,38,38,38	0
55	MG	2a	3184	1/1	0.96	0.10	72,72,72,72	0
55	MG	1A	3793	1/1	0.96	0.06	42,42,42,42	0
55	MG	1A	3087	1/1	0.96	0.17	29,29,29,29	0
55	MG	1A	3315	1/1	0.96	0.16	51,51,51,51	0
55	MG	1A	3966	1/1	0.96	0.11	57,57,57,57	0
55	MG	1A	3635	1/1	0.96	0.12	49,49,49,49	0
55	MG	1A	3637	1/1	0.96	0.07	39,39,39,39	0
55	MG	1A	3638	1/1	0.96	0.13	43,43,43,43	0
55	MG	2A	3302	1/1	0.96	0.06	42,42,42,42	0
55	MG	1E	309	1/1	0.96	0.07	43,43,43,43	0
55	MG	2A	3838	1/1	0.96	0.10	46,46,46,46	0
55	MG	2a	3196	1/1	0.96	0.11	52,52,52,52	0
55	MG	1A	3005	1/1	0.96	0.04	34,34,34,34	0
55	MG	2A	3072	1/1	0.96	0.18	29,29,29,29	0
55	MG	1F	301	1/1	0.96	0.08	49,49,49,49	0
55	MG	1A	3317	1/1	0.96	0.21	36,36,36,36	0
55	MG	1A	3533	1/1	0.96	0.09	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	3845	1/1	0.96	0.17	42,42,42,42	0
55	MG	2A	3557	1/1	0.96	0.11	40,40,40,40	0
55	MG	1A	3534	1/1	0.96	0.19	31,31,31,31	0
55	MG	2A	3559	1/1	0.96	0.11	50,50,50,50	0
55	MG	1F	309	1/1	0.96	0.11	41,41,41,41	0
55	MG	1A	3454	1/1	0.96	0.26	46,46,46,46	0
55	MG	1A	3809	1/1	0.96	0.10	28,28,28,28	0
55	MG	1A	3980	1/1	0.96	0.06	34,34,34,34	0
55	MG	1G	202	1/1	0.96	0.11	57,57,57,57	0
55	MG	2A	3084	1/1	0.96	0.25	48,48,48,48	0
55	MG	1A	3647	1/1	0.96	0.06	42,42,42,42	0
55	MG	2f	202	1/1	0.96	0.15	56,56,56,56	0
55	MG	1A	3648	1/1	0.96	0.15	41,41,41,41	0
55	MG	1a	1721	1/1	0.96	0.14	28,28,28,28	0
55	MG	2A	3088	1/1	0.96	0.07	32,32,32,32	0
55	MG	1A	3649	1/1	0.96	0.10	21,21,21,21	0
55	MG	2A	3575	1/1	0.96	0.18	49,49,49,49	0
55	MG	2l	202	1/1	0.96	0.07	67,67,67,67	0
55	MG	2A	3862	1/1	0.96	0.08	56,56,56,56	0
55	MG	1N	202	1/1	0.96	0.10	33,33,33,33	0
55	MG	1A	3174	1/1	0.96	0.16	25,25,25,25	0
55	MG	1A	3652	1/1	0.96	0.16	26,26,26,26	0
55	MG	1A	3820	1/1	0.96	0.09	22,22,22,22	0
55	MG	1A	3822	1/1	0.96	0.14	21,21,21,21	0
55	MG	1O	203	1/1	0.96	0.05	35,35,35,35	0
55	MG	1A	3068	1/1	0.96	0.12	34,34,34,34	0
55	MG	2B	208	1/1	0.96	0.27	57,57,57,57	0
55	MG	1A	3540	1/1	0.96	0.20	41,41,41,41	0
55	MG	2A	3100	1/1	0.96	0.12	27,27,27,27	0
55	MG	2A	3101	1/1	0.96	0.08	44,44,44,44	0
55	MG	2B	212	1/1	0.96	0.26	52,52,52,52	0
55	MG	1A	3432	1/1	0.97	0.12	32,32,32,32	0
55	MG	2A	3324	1/1	0.97	0.14	45,45,45,45	0
55	MG	1A	3294	1/1	0.97	0.14	40,40,40,40	0
55	MG	2A	3326	1/1	0.97	0.13	46,46,46,46	0
55	MG	1A	3618	1/1	0.97	0.12	23,23,23,23	0
55	MG	1A	3008	1/1	0.97	0.05	25,25,25,25	0
55	MG	2A	3329	1/1	0.97	0.23	45,45,45,45	0
55	MG	1A	3218	1/1	0.97	0.18	39,39,39,39	0
55	MG	1A	3094	1/1	0.97	0.09	16,16,16,16	0
55	MG	2A	3731	1/1	0.97	0.04	59,59,59,59	0
55	MG	1A	3220	1/1	0.97	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3133	1/1	0.97	0.23	31,31,31,31	0
55	MG	1A	3043	1/1	0.97	0.12	25,25,25,25	0
55	MG	1A	3441	1/1	0.97	0.14	32,32,32,32	0
55	MG	1Q	205	1/1	0.97	0.15	36,36,36,36	0
55	MG	1A	4067	1/1	0.97	0.07	26,26,26,26	0
55	MG	1A	3442	1/1	0.97	0.10	51,51,51,51	0
55	MG	1A	3559	1/1	0.97	0.20	31,31,31,31	0
55	MG	2A	3534	1/1	0.97	0.09	40,40,40,40	0
55	MG	1T	201	1/1	0.97	0.05	50,50,50,50	0
55	MG	1A	3942	1/1	0.97	0.08	34,34,34,34	0
55	MG	1A	4073	1/1	0.97	0.06	61,61,61,61	0
55	MG	1A	3257	1/1	0.97	0.06	40,40,40,40	0
55	MG	1U	204	1/1	0.97	0.09	25,25,25,25	0
55	MG	2A	3746	1/1	0.97	0.22	37,37,37,37	0
55	MG	1a	1690	1/1	0.97	0.11	28,28,28,28	0
55	MG	1x	104	1/1	0.97	0.16	41,41,41,41	0
55	MG	1U	205	1/1	0.97	0.21	32,32,32,32	0
55	MG	1A	3258	1/1	0.97	0.08	47,47,47,47	0
55	MG	1A	3729	1/1	0.97	0.06	23,23,23,23	0
55	MG	1V	201	1/1	0.97	0.23	26,26,26,26	0
55	MG	1A	3563	1/1	0.97	0.10	36,36,36,36	0
55	MG	1A	3343	1/1	0.97	0.11	33,33,33,33	0
55	MG	2A	3171	1/1	0.97	0.09	45,45,45,45	0
55	MG	2A	3354	1/1	0.97	0.10	28,28,28,28	0
55	MG	1a	1697	1/1	0.97	0.19	35,35,35,35	0
55	MG	1A	3732	1/1	0.97	0.15	27,27,27,27	0
55	MG	1W	201	1/1	0.97	0.17	34,34,34,34	0
55	MG	1A	3344	1/1	0.97	0.07	37,37,37,37	0
55	MG	2A	3762	1/1	0.97	0.10	74,74,74,74	0
55	MG	2A	3764	1/1	0.97	0.06	65,65,65,65	0
55	MG	1W	203	1/1	0.97	0.09	29,29,29,29	0
55	MG	1W	204	1/1	0.97	0.08	38,38,38,38	0
55	MG	1A	3734	1/1	0.97	0.10	16,16,16,16	0
55	MG	1A	3504	1/1	0.97	0.07	41,41,41,41	0
55	MG	2A	3363	1/1	0.97	0.06	44,44,44,44	0
55	MG	2A	3007	1/1	0.97	0.07	43,43,43,43	0
55	MG	2A	3560	1/1	0.97	0.13	30,30,30,30	0
55	MG	1X	102	1/1	0.97	0.05	31,31,31,31	0
55	MG	1A	3259	1/1	0.97	0.29	36,36,36,36	0
55	MG	2A	3564	1/1	0.97	0.09	40,40,40,40	0
55	MG	1A	3955	1/1	0.97	0.14	50,50,50,50	0
55	MG	1A	4086	1/1	0.97	0.06	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	1X	106	1/1	0.97	0.08	47,47,47,47	0
55	MG	1A	3636	1/1	0.97	0.13	15,15,15,15	0
55	MG	2A	3014	1/1	0.97	0.09	38,38,38,38	0
55	MG	2A	3780	1/1	0.97	0.05	53,53,53,53	0
55	MG	2a	3071	1/1	0.97	0.14	51,51,51,51	0
55	MG	1Y	202	1/1	0.97	0.19	45,45,45,45	0
55	MG	1A	3568	1/1	0.97	0.05	25,25,25,25	0
55	MG	2A	3572	1/1	0.97	0.15	27,27,27,27	0
55	MG	1A	3960	1/1	0.97	0.07	36,36,36,36	0
55	MG	1A	4091	1/1	0.97	0.12	24,24,24,24	0
55	MG	1A	4092	1/1	0.97	0.06	41,41,41,41	0
55	MG	2A	3788	1/1	0.97	0.05	73,73,73,73	0
55	MG	1A	4093	1/1	0.97	0.07	41,41,41,41	0
55	MG	1A	3189	1/1	0.97	0.06	43,43,43,43	0
55	MG	1A	3507	1/1	0.97	0.13	27,27,27,27	0
55	MG	1A	3029	1/1	0.97	0.25	30,30,30,30	0
55	MG	1A	3643	1/1	0.97	0.09	43,43,43,43	0
55	MG	2A	3027	1/1	0.97	0.13	31,31,31,31	0
55	MG	2A	3028	1/1	0.97	0.07	41,41,41,41	0
55	MG	11	101	1/1	0.97	0.11	34,34,34,34	0
55	MG	1A	3573	1/1	0.97	0.08	28,28,28,28	0
55	MG	1A	3082	1/1	0.97	0.09	29,29,29,29	0
55	MG	2A	3387	1/1	0.97	0.18	29,29,29,29	0
55	MG	2A	3032	1/1	0.97	0.10	42,42,42,42	0
55	MG	2A	3206	1/1	0.97	0.05	38,38,38,38	0
55	MG	2A	3804	1/1	0.97	0.09	46,46,46,46	0
55	MG	2A	3805	1/1	0.97	0.06	54,54,54,54	0
55	MG	1A	3575	1/1	0.97	0.12	32,32,32,32	0
55	MG	1A	3192	1/1	0.97	0.09	32,32,32,32	0
55	MG	2A	3809	1/1	0.97	0.07	43,43,43,43	0
55	MG	2A	3810	1/1	0.97	0.13	38,38,38,38	0
55	MG	1A	3856	1/1	0.97	0.18	40,40,40,40	0
55	MG	1A	3119	1/1	0.97	0.10	30,30,30,30	0
55	MG	2a	3100	1/1	0.97	0.11	57,57,57,57	0
55	MG	1A	3749	1/1	0.97	0.12	37,37,37,37	0
55	MG	13	103	1/1	0.97	0.07	41,41,41,41	0
55	MG	1A	3974	1/1	0.97	0.09	44,44,44,44	0
55	MG	2A	3818	1/1	0.97	0.12	41,41,41,41	0
55	MG	2A	3397	1/1	0.97	0.10	25,25,25,25	0
55	MG	1A	3453	1/1	0.97	0.35	46,46,46,46	0
55	MG	2A	3216	1/1	0.97	0.06	50,50,50,50	0
55	MG	1A	3351	1/1	0.97	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3651	1/1	0.97	0.09	29,29,29,29	0
55	MG	1A	3753	1/1	0.97	0.07	48,48,48,48	0
55	MG	1a	1736	1/1	0.97	0.27	39,39,39,39	0
55	MG	16	101	1/1	0.97	0.04	42,42,42,42	0
55	MG	1A	3194	1/1	0.97	0.18	35,35,35,35	0
55	MG	1A	3139	1/1	0.97	0.06	37,37,37,37	0
55	MG	1A	3866	1/1	0.97	0.17	45,45,45,45	0
55	MG	2A	3225	1/1	0.97	0.09	54,54,54,54	0
55	MG	1A	3867	1/1	0.97	0.10	37,37,37,37	0
55	MG	2A	3052	1/1	0.97	0.06	30,30,30,30	0
55	MG	1A	3582	1/1	0.97	0.04	32,32,32,32	0
55	MG	1A	3758	1/1	0.97	0.09	34,34,34,34	0
55	MG	2A	3055	1/1	0.97	0.07	34,34,34,34	0
55	MG	1A	3045	1/1	0.97	0.08	37,37,37,37	0
55	MG	2a	3123	1/1	0.97	0.22	46,46,46,46	0
55	MG	2A	3057	1/1	0.97	0.07	40,40,40,40	0
55	MG	1A	3459	1/1	0.97	0.40	37,37,37,37	0
55	MG	1A	3141	1/1	0.97	0.07	32,32,32,32	0
55	MG	18	106	1/1	0.97	0.10	55,55,55,55	0
55	MG	1A	3661	1/1	0.97	0.09	46,46,46,46	0
55	MG	1A	3269	1/1	0.97	0.12	52,52,52,52	0
55	MG	1B	208	1/1	0.97	0.06	54,54,54,54	0
55	MG	2A	3064	1/1	0.97	0.16	47,47,47,47	0
55	MG	2a	3132	1/1	0.97	0.32	45,45,45,45	0
55	MG	2A	3065	1/1	0.97	0.11	48,48,48,48	0
55	MG	1A	3142	1/1	0.97	0.12	15,15,15,15	0
55	MG	1A	3273	1/1	0.97	0.08	36,36,36,36	0
55	MG	2A	3243	1/1	0.97	0.14	39,39,39,39	0
55	MG	1A	3037	1/1	0.97	0.06	28,28,28,28	0
55	MG	1A	3769	1/1	0.97	0.04	42,42,42,42	0
55	MG	2A	3246	1/1	0.97	0.09	51,51,51,51	0
55	MG	1B	213	1/1	0.97	0.20	44,44,44,44	0
55	MG	1A	3412	1/1	0.97	0.10	33,33,33,33	0
55	MG	2A	3857	1/1	0.97	0.18	36,36,36,36	0
55	MG	2A	3433	1/1	0.97	0.23	47,47,47,47	0
55	MG	1a	1761	1/1	0.97	0.04	49,49,49,49	0
55	MG	2A	3251	1/1	0.97	0.06	50,50,50,50	0
55	MG	1A	3030	1/1	0.97	0.09	39,39,39,39	0
55	MG	1A	3467	1/1	0.97	0.29	46,46,46,46	0
55	MG	1A	3882	1/1	0.97	0.08	47,47,47,47	0
55	MG	2A	3439	1/1	0.97	0.08	64,64,64,64	0
55	MG	1B	219	1/1	0.97	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3773	1/1	0.97	0.19	29,29,29,29	0
55	MG	1a	1767	1/1	0.97	0.05	32,32,32,32	0
55	MG	2a	3153	1/1	0.97	0.11	36,36,36,36	0
55	MG	1A	3593	1/1	0.97	0.23	53,53,53,53	0
55	MG	2a	3155	1/1	0.97	0.13	58,58,58,58	0
55	MG	2A	3444	1/1	0.97	0.09	18,18,18,18	0
55	MG	1A	3048	1/1	0.97	0.05	32,32,32,32	0
55	MG	1a	1771	1/1	0.97	0.08	64,64,64,64	0
55	MG	1A	3009	1/1	0.97	0.06	28,28,28,28	0
55	MG	1A	3363	1/1	0.97	0.18	36,36,36,36	0
55	MG	1A	3779	1/1	0.97	0.11	28,28,28,28	0
55	MG	1A	3280	1/1	0.97	0.24	45,45,45,45	0
55	MG	1a	1777	1/1	0.97	0.06	45,45,45,45	0
55	MG	1A	3105	1/1	0.97	0.18	31,31,31,31	0
55	MG	1a	1779	1/1	0.97	0.09	49,49,49,49	0
55	MG	1A	3151	1/1	0.97	0.14	38,38,38,38	0
55	MG	2A	3455	1/1	0.97	0.05	56,56,56,56	0
55	MG	1A	3894	1/1	0.97	0.08	26,26,26,26	0
55	MG	2D	301	1/1	0.97	0.05	31,31,31,31	0
55	MG	2a	3170	1/1	0.97	0.13	36,36,36,36	0
55	MG	2A	3657	1/1	0.97	0.09	44,44,44,44	0
55	MG	2A	3658	1/1	0.97	0.05	58,58,58,58	0
55	MG	1A	3178	1/1	0.97	0.10	31,31,31,31	0
55	MG	1A	3106	1/1	0.97	0.10	35,35,35,35	0
55	MG	1A	3535	1/1	0.97	0.09	41,41,41,41	0
55	MG	2A	3097	1/1	0.97	0.07	43,43,43,43	0
55	MG	2E	306	1/1	0.97	0.14	42,42,42,42	0
55	MG	2a	3178	1/1	0.97	0.15	43,43,43,43	0
55	MG	1A	3536	1/1	0.97	0.17	56,56,56,56	0
55	MG	1A	3209	1/1	0.97	0.08	27,27,27,27	0
55	MG	1D	302	1/1	0.97	0.07	23,23,23,23	0
55	MG	2A	3279	1/1	0.97	0.10	40,40,40,40	0
55	MG	2A	3667	1/1	0.97	0.07	46,46,46,46	0
55	MG	1A	3107	1/1	0.97	0.13	31,31,31,31	0
55	MG	1D	305	1/1	0.97	0.07	33,33,33,33	0
55	MG	2a	3186	1/1	0.97	0.16	50,50,50,50	0
55	MG	1A	3424	1/1	0.97	0.14	29,29,29,29	0
55	MG	1A	3691	1/1	0.97	0.07	24,24,24,24	0
55	MG	1a	1634	1/1	0.97	0.14	58,58,58,58	0
55	MG	1A	3211	1/1	0.97	0.33	33,33,33,33	0
55	MG	1A	3693	1/1	0.97	0.06	26,26,26,26	0
55	MG	1A	3801	1/1	0.97	0.11	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3110	1/1	0.97	0.09	56,56,56,56	0
55	MG	1A	3694	1/1	0.97	0.09	19,19,19,19	0
55	MG	1A	3026	1/1	0.97	0.11	32,32,32,32	0
55	MG	1A	3696	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3374	1/1	0.97	0.05	31,31,31,31	0
55	MG	1A	3006	1/1	0.97	0.07	50,50,50,50	0
55	MG	1A	3700	1/1	0.97	0.05	23,23,23,23	0
55	MG	1A	3611	1/1	0.97	0.11	12,12,12,12	0
55	MG	2a	3201	1/1	0.97	0.06	55,55,55,55	0
55	MG	1E	308	1/1	0.97	0.13	16,16,16,16	0
55	MG	2A	3686	1/1	0.97	0.05	49,49,49,49	0
55	MG	1A	3811	1/1	0.97	0.07	43,43,43,43	0
55	MG	2A	3298	1/1	0.97	0.07	43,43,43,43	0
55	MG	1A	4036	1/1	0.97	0.07	45,45,45,45	0
55	MG	2A	3121	1/1	0.97	0.14	39,39,39,39	0
55	MG	1a	1809	1/1	0.97	0.14	49,49,49,49	0
55	MG	1E	311	1/1	0.97	0.05	43,43,43,43	0
55	MG	1a	1651	1/1	0.97	0.13	41,41,41,41	0
55	MG	1A	3484	1/1	0.97	0.04	35,35,35,35	0
55	MG	1A	3813	1/1	0.97	0.06	41,41,41,41	0
55	MG	1A	4039	1/1	0.97	0.07	38,38,38,38	0
55	MG	1F	306	1/1	0.97	0.28	20,20,20,20	0
55	MG	2A	3702	1/1	0.97	0.05	45,45,45,45	0
55	MG	1F	307	1/1	0.97	0.08	33,33,33,33	0
55	MG	1A	3183	1/1	0.97	0.09	46,46,46,46	0
55	MG	1A	3815	1/1	0.97	0.08	16,16,16,16	0
55	MG	1A	3816	1/1	0.97	0.13	42,42,42,42	0
55	MG	1A	3817	1/1	0.97	0.08	50,50,50,50	0
55	MG	2A	3709	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3706	1/1	0.97	0.08	15,15,15,15	0
55	MG	2A	3502	1/1	0.97	0.06	48,48,48,48	0
55	MG	1A	4046	1/1	0.97	0.04	66,66,66,66	0
55	MG	2A	3504	1/1	0.97	0.11	35,35,35,35	0
55	MG	1A	3924	1/1	0.97	0.09	38,38,38,38	0
55	MG	1A	4048	1/1	0.97	0.06	40,40,40,40	0
55	MG	1A	4049	1/1	0.97	0.11	53,53,53,53	0
55	MG	1A	3378	1/1	0.97	0.16	41,41,41,41	0
55	MG	1A	3076	1/1	0.97	0.14	40,40,40,40	0
55	MG	2A	3510	1/1	0.97	0.08	36,36,36,36	0
56	ZN	2n	501	1/1	0.97	0.05	100,100,100,100	0
55	MG	1A	4055	1/1	0.97	0.13	38,38,38,38	0
55	MG	1A	3927	1/1	0.97	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	3328	1/1	0.98	0.20	40,40,40,40	0
55	MG	1A	3629	1/1	0.98	0.07	32,32,32,32	0
55	MG	1A	3738	1/1	0.98	0.06	34,34,34,34	0
55	MG	2A	3016	1/1	0.98	0.05	40,40,40,40	0
55	MG	2A	3249	1/1	0.98	0.05	59,59,59,59	0
55	MG	1A	3143	1/1	0.98	0.03	28,28,28,28	0
55	MG	2E	305	1/1	0.98	0.14	38,38,38,38	0
55	MG	1B	218	1/1	0.98	0.07	20,20,20,20	0
55	MG	1A	3396	1/1	0.98	0.16	31,31,31,31	0
55	MG	1A	3959	1/1	0.98	0.08	40,40,40,40	0
55	MG	1A	4044	1/1	0.98	0.06	57,57,57,57	0
55	MG	1B	222	1/1	0.98	0.09	28,28,28,28	0
55	MG	1A	3097	1/1	0.98	0.08	30,30,30,30	0
55	MG	1A	3682	1/1	0.98	0.07	33,33,33,33	0
55	MG	1A	3075	1/1	0.98	0.04	11,11,11,11	0
55	MG	1A	3684	1/1	0.98	0.05	44,44,44,44	0
55	MG	2A	3756	1/1	0.98	0.04	53,53,53,53	0
55	MG	2A	3497	1/1	0.98	0.06	41,41,41,41	0
55	MG	1a	1776	1/1	0.98	0.09	40,40,40,40	0
55	MG	2A	3261	1/1	0.98	0.08	43,43,43,43	0
55	MG	1A	3886	1/1	0.98	0.07	28,28,28,28	0
55	MG	2A	3263	1/1	0.98	0.07	50,50,50,50	0
55	MG	1A	3887	1/1	0.98	0.03	31,31,31,31	0
55	MG	2A	3763	1/1	0.98	0.15	49,49,49,49	0
55	MG	1A	4051	1/1	0.98	0.04	41,41,41,41	0
55	MG	1A	3301	1/1	0.98	0.05	32,32,32,32	0
55	MG	2Q	204	1/1	0.98	0.23	43,43,43,43	0
55	MG	1A	3146	1/1	0.98	0.20	21,21,21,21	0
55	MG	1A	3968	1/1	0.98	0.07	40,40,40,40	0
55	MG	2A	3634	1/1	0.98	0.08	52,52,52,52	0
55	MG	1A	3214	1/1	0.98	0.11	36,36,36,36	0
55	MG	1A	3970	1/1	0.98	0.04	71,71,71,71	0
55	MG	1A	3402	1/1	0.98	0.11	35,35,35,35	0
55	MG	1A	3366	1/1	0.98	0.11	39,39,39,39	0
55	MG	2A	3511	1/1	0.98	0.10	51,51,51,51	0
55	MG	1A	3639	1/1	0.98	0.08	21,21,21,21	0
55	MG	1A	3099	1/1	0.98	0.10	14,14,14,14	0
55	MG	1D	306	1/1	0.98	0.13	45,45,45,45	0
55	MG	1A	3148	1/1	0.98	0.04	31,31,31,31	0
55	MG	1A	3113	1/1	0.98	0.10	34,34,34,34	0
55	MG	1A	3754	1/1	0.98	0.09	30,30,30,30	0
55	MG	1A	3978	1/1	0.98	0.06	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	1687	1/1	0.98	0.16	52,52,52,52	0
55	MG	2A	3048	1/1	0.98	0.05	52,52,52,52	0
55	MG	1A	3562	1/1	0.98	0.08	17,17,17,17	0
55	MG	1A	3275	1/1	0.98	0.34	28,28,28,28	0
55	MG	1D	313	1/1	0.98	0.18	30,30,30,30	0
55	MG	2A	3786	1/1	0.98	0.04	72,72,72,72	0
55	MG	1A	3698	1/1	0.98	0.08	39,39,39,39	0
55	MG	1A	3012	1/1	0.98	0.06	28,28,28,28	0
55	MG	1E	303	1/1	0.98	0.14	27,27,27,27	0
55	MG	2A	3790	1/1	0.98	0.05	59,59,59,59	0
55	MG	2a	3003	1/1	0.98	0.17	49,49,49,49	0
55	MG	1A	3061	1/1	0.98	0.08	31,31,31,31	0
55	MG	1A	3701	1/1	0.98	0.06	18,18,18,18	0
55	MG	2A	3530	1/1	0.98	0.16	41,41,41,41	0
55	MG	1A	3986	1/1	0.98	0.06	24,24,24,24	0
55	MG	2A	3532	1/1	0.98	0.17	42,42,42,42	0
55	MG	1A	3116	1/1	0.98	0.06	30,30,30,30	0
55	MG	1A	3153	1/1	0.98	0.09	49,49,49,49	0
55	MG	1A	3281	1/1	0.98	0.14	36,36,36,36	0
55	MG	1a	1700	1/1	0.98	0.06	42,42,42,42	0
55	MG	1A	3175	1/1	0.98	0.05	20,20,20,20	0
55	MG	1A	3909	1/1	0.98	0.07	37,37,37,37	0
55	MG	1A	3707	1/1	0.98	0.12	18,18,18,18	0
55	MG	1F	302	1/1	0.98	0.15	33,33,33,33	0
55	MG	2A	3668	1/1	0.98	0.08	36,36,36,36	0
55	MG	1F	303	1/1	0.98	0.09	30,30,30,30	0
55	MG	1A	3224	1/1	0.98	0.10	35,35,35,35	0
55	MG	1a	1817	1/1	0.98	0.04	68,68,68,68	0
55	MG	1A	3653	1/1	0.98	0.05	40,40,40,40	0
55	MG	2A	3811	1/1	0.98	0.14	35,35,35,35	0
55	MG	1A	3379	1/1	0.98	0.06	16,16,16,16	0
55	MG	1A	3711	1/1	0.98	0.04	31,31,31,31	0
55	MG	2A	3814	1/1	0.98	0.06	48,48,48,48	0
55	MG	1A	3176	1/1	0.98	0.05	24,24,24,24	0
55	MG	2A	3073	1/1	0.98	0.24	43,43,43,43	0
55	MG	1A	3010	1/1	0.98	0.07	24,24,24,24	0
55	MG	1A	3774	1/1	0.98	0.05	37,37,37,37	0
55	MG	2A	3309	1/1	0.98	0.06	63,63,63,63	0
55	MG	1A	3457	1/1	0.98	0.05	21,21,21,21	0
55	MG	2A	3428	1/1	0.98	0.16	32,32,32,32	0
55	MG	1A	3200	1/1	0.98	0.06	22,22,22,22	0
55	MG	1A	4003	1/1	0.98	0.04	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	2A	3825	1/1	0.98	0.05	42,42,42,42	0
55	MG	1A	3660	1/1	0.98	0.09	22,22,22,22	0
55	MG	1A	4095	1/1	0.98	0.05	31,31,31,31	0
55	MG	1A	3201	1/1	0.98	0.09	32,32,32,32	0
55	MG	2A	3687	1/1	0.98	0.07	53,53,53,53	0
55	MG	1a	1617	1/1	0.98	0.07	63,63,63,63	0
55	MG	1A	3718	1/1	0.98	0.07	19,19,19,19	0
55	MG	2A	3561	1/1	0.98	0.09	46,46,46,46	0
55	MG	1A	3118	1/1	0.98	0.08	26,26,26,26	0
55	MG	2A	3692	1/1	0.98	0.08	54,54,54,54	0
55	MG	1A	3782	1/1	0.98	0.08	38,38,38,38	0
55	MG	1A	3783	1/1	0.98	0.07	26,26,26,26	0
55	MG	1A	3720	1/1	0.98	0.07	31,31,31,31	0
55	MG	1A	3663	1/1	0.98	0.03	23,23,23,23	0
55	MG	1A	3786	1/1	0.98	0.09	38,38,38,38	0
55	MG	2A	3091	1/1	0.98	0.14	37,37,37,37	0
55	MG	2A	3700	1/1	0.98	0.06	51,51,51,51	0
55	MG	1A	3787	1/1	0.98	0.07	13,13,13,13	0
55	MG	2A	3843	1/1	0.98	0.14	37,37,37,37	0
55	MG	1A	3664	1/1	0.98	0.06	18,18,18,18	0
55	MG	1A	3665	1/1	0.98	0.07	25,25,25,25	0
55	MG	1A	3724	1/1	0.98	0.11	12,12,12,12	0
55	MG	1A	3230	1/1	0.98	0.18	44,44,44,44	0
55	MG	1A	3792	1/1	0.98	0.07	20,20,20,20	0
55	MG	1A	3864	1/1	0.98	0.11	43,43,43,43	0
55	MG	2A	3708	1/1	0.98	0.04	36,36,36,36	0
55	MG	1A	4111	1/1	0.98	0.04	51,51,51,51	0
55	MG	1Q	207	1/1	0.98	0.18	39,39,39,39	0
55	MG	1A	3386	1/1	0.98	0.22	23,23,23,23	0
55	MG	1A	3090	1/1	0.98	0.09	29,29,29,29	0
55	MG	1A	3795	1/1	0.98	0.06	21,21,21,21	0
55	MG	1A	3941	1/1	0.98	0.05	54,54,54,54	0
55	MG	2A	3105	1/1	0.98	0.05	30,30,30,30	0
55	MG	1A	4025	1/1	0.98	0.08	25,25,25,25	0
55	MG	1A	3728	1/1	0.98	0.04	31,31,31,31	0
55	MG	1U	201	1/1	0.98	0.26	33,33,33,33	0
55	MG	2A	3460	1/1	0.98	0.20	48,48,48,48	0
55	MG	1A	3943	1/1	0.98	0.07	39,39,39,39	0
55	MG	1U	203	1/1	0.98	0.02	22,22,22,22	0
55	MG	1B	202	1/1	0.98	0.09	35,35,35,35	0
55	MG	1A	4028	1/1	0.98	0.04	44,44,44,44	0
55	MG	1A	3080	1/1	0.98	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	2A	3466	1/1	0.98	0.31	42,42,42,42	0
55	MG	1A	3015	1/1	0.98	0.06	33,33,33,33	0
55	MG	1a	1648	1/1	0.98	0.16	36,36,36,36	0
55	MG	1B	206	1/1	0.98	0.12	40,40,40,40	0
55	MG	1A	3544	1/1	0.98	0.10	30,30,30,30	0
55	MG	1A	3003	1/1	0.98	0.07	22,22,22,22	0
55	MG	2A	3004	1/1	0.98	0.04	43,43,43,43	0
55	MG	1A	4033	1/1	0.98	0.04	36,36,36,36	0
55	MG	1A	3802	1/1	0.98	0.04	32,32,32,32	0
55	MG	1A	3023	1/1	0.98	0.07	35,35,35,35	0
55	MG	1a	1756	1/1	0.98	0.04	41,41,41,41	0
55	MG	1A	3034	1/1	0.98	0.09	24,24,24,24	0
56	ZN	14	501	1/1	0.98	0.07	109,109,109,109	0
55	MG	1a	1759	1/1	0.98	0.06	40,40,40,40	0
55	MG	2A	3126	1/1	0.98	0.16	34,34,34,34	0
55	MG	1a	1760	1/1	0.98	0.14	39,39,39,39	0
55	MG	1A	3085	1/1	0.98	0.07	24,24,24,24	0
58	SF4	1d	501	8/8	0.98	0.05	57,70,76,77	0
58	SF4	2d	303	8/8	0.98	0.05	58,77,87,92	0
55	MG	1A	4070	1/1	0.99	0.07	19,19,19,19	0
55	MG	1A	3985	1/1	0.99	0.05	24,24,24,24	0
55	MG	1A	3689	1/1	0.99	0.09	28,28,28,28	0
55	MG	2A	3822	1/1	0.99	0.11	26,26,26,26	0
55	MG	1A	3690	1/1	0.99	0.16	35,35,35,35	0
55	MG	1A	3640	1/1	0.99	0.05	28,28,28,28	0
55	MG	1A	3490	1/1	0.99	0.12	28,28,28,28	0
55	MG	1A	3990	1/1	0.99	0.06	56,56,56,56	0
55	MG	1A	3846	1/1	0.99	0.03	28,28,28,28	0
55	MG	1A	3666	1/1	0.99	0.07	22,22,22,22	0
55	MG	2A	3694	1/1	0.99	0.06	24,24,24,24	0
55	MG	1A	3953	1/1	0.99	0.03	19,19,19,19	0
55	MG	2A	3186	1/1	0.99	0.15	40,40,40,40	0
55	MG	2A	3187	1/1	0.99	0.05	53,53,53,53	0
55	MG	1A	3491	1/1	0.99	0.16	29,29,29,29	0
55	MG	1A	3437	1/1	0.99	0.03	36,36,36,36	0
55	MG	1a	1757	1/1	0.99	0.12	47,47,47,47	0
55	MG	1A	3956	1/1	0.99	0.08	24,24,24,24	0
55	MG	2P	202	1/1	0.99	0.06	48,48,48,48	0
55	MG	1A	3405	1/1	0.99	0.13	40,40,40,40	0
55	MG	1A	3272	1/1	0.99	0.13	22,22,22,22	0
55	MG	1A	4085	1/1	0.99	0.04	39,39,39,39	0
55	MG	1A	3014	1/1	0.99	0.05	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1A	4087	1/1	0.99	0.04	37,37,37,37	0
55	MG	2A	3075	1/1	0.99	0.03	29,29,29,29	0
55	MG	1A	3135	1/1	0.99	0.10	25,25,25,25	0
55	MG	2A	3514	1/1	0.99	0.08	26,26,26,26	0
55	MG	1A	3923	1/1	0.99	0.05	29,29,29,29	0
55	MG	2A	3580	1/1	0.99	0.10	45,45,45,45	0
55	MG	2A	3018	1/1	0.99	0.05	32,32,32,32	0
55	MG	1A	3019	1/1	0.99	0.10	28,28,28,28	0
55	MG	1A	3276	1/1	0.99	0.08	38,38,38,38	0
55	MG	1a	1768	1/1	0.99	0.05	40,40,40,40	0
55	MG	1A	3702	1/1	0.99	0.09	14,14,14,14	0
55	MG	1A	3289	1/1	0.99	0.06	33,33,33,33	0
55	MG	1A	3760	1/1	0.99	0.06	24,24,24,24	0
55	MG	2X	102	1/1	0.99	0.10	52,52,52,52	0
55	MG	1A	3761	1/1	0.99	0.08	14,14,14,14	0
55	MG	1A	3066	1/1	0.99	0.07	26,26,26,26	0
55	MG	1A	3173	1/1	0.99	0.03	24,24,24,24	0
55	MG	2A	3210	1/1	0.99	0.12	35,35,35,35	0
55	MG	1A	3222	1/1	0.99	0.11	28,28,28,28	0
55	MG	1A	4052	1/1	0.99	0.04	24,24,24,24	0
55	MG	1A	4053	1/1	0.99	0.04	29,29,29,29	0
55	MG	1A	3933	1/1	0.99	0.03	24,24,24,24	0
55	MG	1A	3022	1/1	0.99	0.04	29,29,29,29	0
55	MG	1A	3830	1/1	0.99	0.06	31,31,31,31	0
55	MG	2A	3034	1/1	0.99	0.09	36,36,36,36	0
55	MG	1e	202	1/1	0.99	0.09	56,56,56,56	0
55	MG	1A	3078	1/1	0.99	0.03	30,30,30,30	0
55	MG	1B	235	1/1	0.99	0.04	23,23,23,23	0
55	MG	1A	3656	1/1	0.99	0.06	20,20,20,20	0
55	MG	1A	3799	1/1	0.99	0.04	41,41,41,41	0
55	MG	1a	1785	1/1	0.99	0.06	51,51,51,51	0
55	MG	1D	303	1/1	0.99	0.09	43,43,43,43	0
55	MG	2A	3803	1/1	0.99	0.06	29,29,29,29	0
55	MG	1A	3059	1/1	0.99	0.05	28,28,28,28	0
55	MG	1A	3468	1/1	0.99	0.08	46,46,46,46	0
55	MG	1A	3271	1/1	0.99	0.11	26,26,26,26	0
55	MG	1Q	206	1/1	0.99	0.04	35,35,35,35	0
55	MG	2A	3808	1/1	0.99	0.04	45,45,45,45	0
55	MG	1a	1635	1/1	0.99	0.10	30,30,30,30	0
55	MG	1A	4020	1/1	0.99	0.04	26,26,26,26	0
55	MG	1A	3403	1/1	0.99	0.07	38,38,38,38	0
56	ZN	1Y	205	1/1	0.99	0.02	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	1A	3571	1/1	0.99	0.09	32,32,32,32	0
56	ZN	15	106	1/1	0.99	0.03	46,46,46,46	0
56	ZN	16	102	1/1	0.99	0.04	41,41,41,41	0
56	ZN	19	102	1/1	0.99	0.05	41,41,41,41	0
56	ZN	1n	103	1/1	0.99	0.03	69,69,69,69	0
56	ZN	2Y	501	1/1	0.99	0.02	77,77,77,77	0
55	MG	1A	3375	1/1	0.99	0.04	26,26,26,26	0
56	ZN	26	102	1/1	0.99	0.07	54,54,54,54	0
56	ZN	29	501	1/1	0.99	0.05	61,61,61,61	0
55	MG	1A	3530	1/1	0.99	0.12	19,19,19,19	0
55	MG	1a	1797	1/1	0.99	0.08	58,58,58,58	0
55	MG	1A	4068	1/1	0.99	0.07	23,23,23,23	0
55	MG	1a	1799	1/1	0.99	0.07	68,68,68,68	0
55	MG	1A	3807	1/1	0.99	0.08	36,36,36,36	0
56	ZN	25	103	1/1	1.00	0.02	52,52,52,52	0
55	MG	1A	3821	1/1	1.00	0.08	21,21,21,21	0
55	MG	1A	3906	1/1	1.00	0.04	17,17,17,17	0
55	MG	1A	3781	1/1	1.00	0.03	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.