



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:15 PM EDT

PDB ID : 10PX / pdb_000010px
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with benzoxaborole derivative of azithromycin (AZI-BB2), mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.45Å resolution
Authors : Chen, C.-W.; Volynkina, I.A.; Bortyazh, M.O.; Tereshchenkov, A.G.; Karakchieva, A.O.; Lukianov, D.A.; Komarova, E.S.; Tupikin, A.E.; Skvortsov, D.A.; Tevyashova, A.N.; Tikhomirov, A.S.; Tashlitsky, V.N.; Kabilov, M.R.; Shchekotikhin, A.E.; Dontsova, O.A.; Sergiev, P.V.; Polikanov, Y.S.
Deposited on : 2026-02-01
Resolution : 2.45 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	:	9.0.015 (Gargrove)

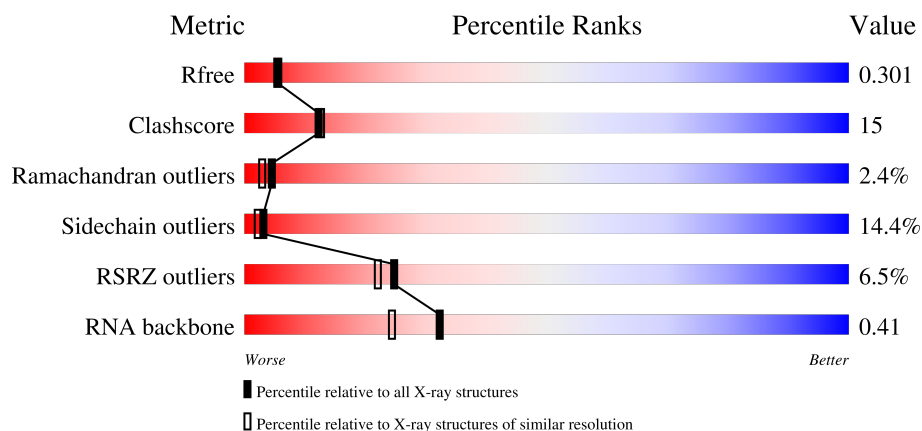
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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	

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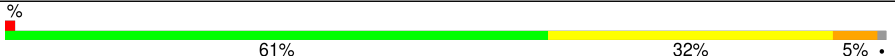
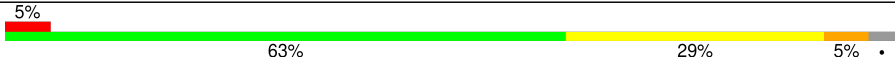
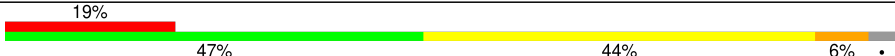
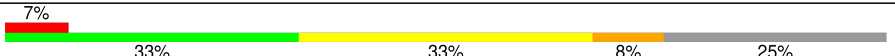
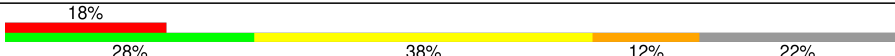
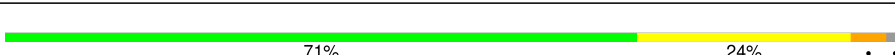
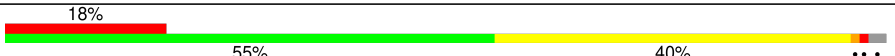
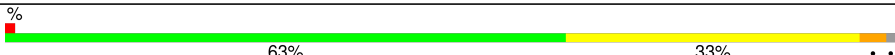
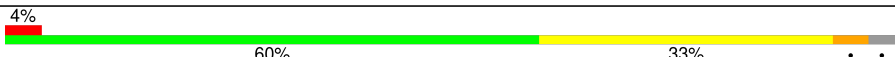
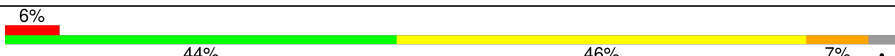
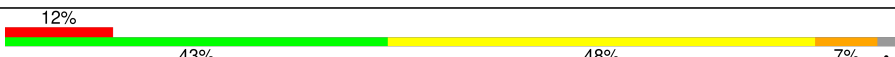
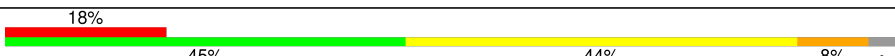
Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	2A	2915	
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	

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

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Mol	Chain	Length	Quality of chain
26	24	71	
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	

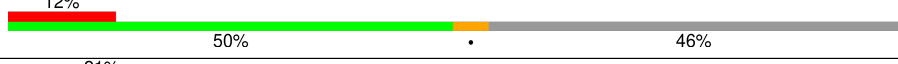
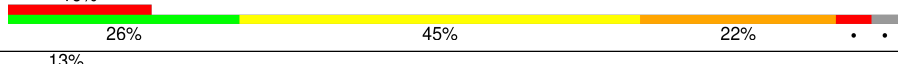
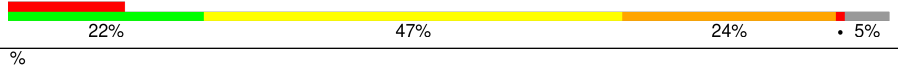
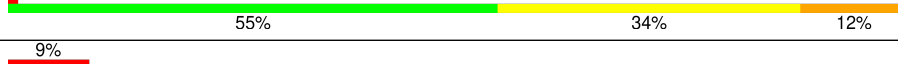
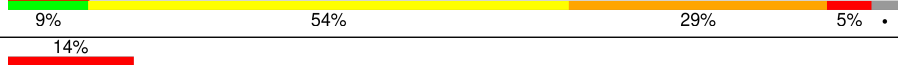
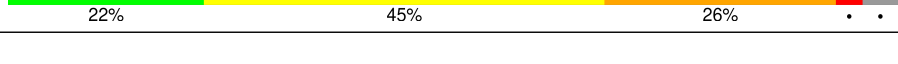
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Mol	Chain	Length	Quality of chain
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	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

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Mol	Chain	Length	Quality of chain
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	29	101	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-PHE-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1603	722	287	518	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNA^{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNA^{phe}.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1099	Total	Mg	0	0
			1099	1099		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	13	Total	Mg	0	0
			13	13		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	12	Total	Mg	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	5	Total 5	Mg 5	0	0
57	1P	3	Total 3	Mg 3	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	4	Total 4	Mg 4	0	0
57	1U	10	Total 10	Mg 10	0	0
57	1V	10	Total 10	Mg 10	0	0
57	1W	8	Total 8	Mg 8	0	0
57	1X	7	Total 7	Mg 7	0	0
57	1Y	3	Total 3	Mg 3	0	0
57	1Z	4	Total 4	Mg 4	0	0
57	10	8	Total 8	Mg 8	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	15	9	Total 9	Mg 9	0	0
57	16	2	Total 2	Mg 2	0	0
57	17	7	Total 7	Mg 7	0	0
57	18	5	Total 5	Mg 5	0	0
57	1a	213	Total 213	Mg 213	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	2	Total 2	Mg 2	0	0
57	1n	3	Total 3	Mg 3	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	2	Total 2	Mg 2	0	0
57	1w	8	Total 8	Mg 8	0	0
57	1x	14	Total 14	Mg 14	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	883	Total 883	Mg 883	0	0
57	2B	20	Total 20	Mg 20	0	0
57	2D	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	3	Total 3	Mg 3	0	0
57	2Q	3	Total 3	Mg 3	0	0
57	2R	3	Total 3	Mg 3	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	1	Total 1	Mg 1	0	0
57	25	5	Total 5	Mg 5	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	4	Total 4	Mg 4	0	0
57	29	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2a	234	Total Mg 234 234	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	1	Total Mg 1 1	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	2	Total Mg 2 2	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	4	Total Mg 4 4	0	0
57	2m	1	Total Mg 1 1	0	0
57	2p	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	2	Total Mg 2 2	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	3	Total Mg 3 3	0	0
57	2w	9	Total Mg 9 9	0	0
57	2x	6	Total Mg 6 6	0	0
57	2y	6	Total Mg 6 6	0	0

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

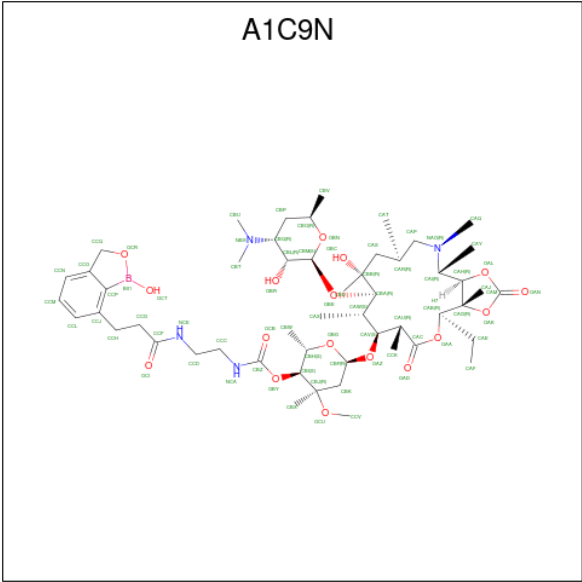
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0

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

- Molecule 59 is AZI-BB2 (CCD ID: A1C9N) (formula: C₅₂H₈₅BN₄O₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total B C N O 74 1 52 4 17	0	0
59	2A	1	Total B C N O 74 1 52 4 17	0	0

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

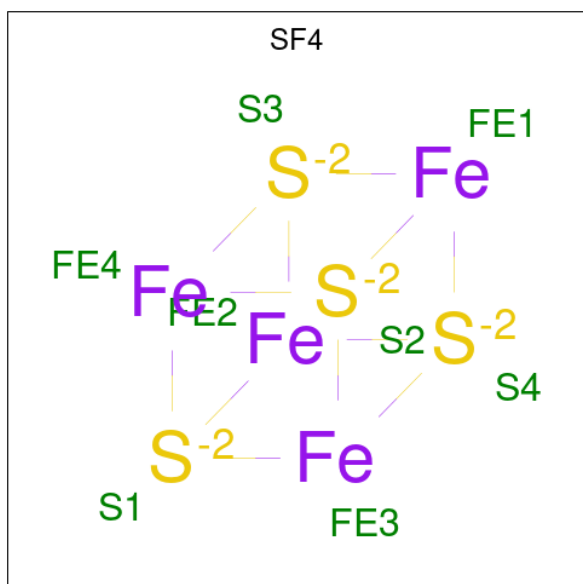
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0

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

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1997	Total 1997	O 1997	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1B	63	Total 63	O 63	0	0
62	1D	30	Total 30	O 30	0	0
62	1E	31	Total 31	O 31	0	0
62	1F	16	Total 16	O 16	0	0
62	1G	5	Total 5	O 5	0	0
62	1H	2	Total 2	O 2	0	0
62	1I	1	Total 1	O 1	0	0
62	1N	8	Total 8	O 8	0	0
62	1O	5	Total 5	O 5	0	0
62	1P	24	Total 24	O 24	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	11	Total 11	O 11	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	9	Total 9	O 9	0	0
62	1U	9	Total 9	O 9	0	0
62	1V	9	Total 9	O 9	0	0
62	1W	8	Total 8	O 8	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	4	Total 4	O 4	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	11	14	Total 14	O 14	0	0
62	12	2	Total 2	O 2	0	0
62	13	3	Total 3	O 3	0	0
62	15	6	Total 6	O 6	0	0
62	16	4	Total 4	O 4	0	0
62	17	9	Total 9	O 9	0	0
62	18	10	Total 10	O 10	0	0
62	1a	379	Total 379	O 379	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	7	Total 7	O 7	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	13	Total 13	O 13	0	0
62	1x	15	Total 15	O 15	0	0
62	1y	2	Total 2	O 2	0	0
62	2A	1156	Total 1156	O 1156	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2B	24	Total 24	O 24	0	0
62	2D	22	Total 22	O 22	0	0
62	2E	14	Total 14	O 14	0	0
62	2F	12	Total 12	O 12	0	0
62	2I	3	Total 3	O 3	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	3	Total 3	O 3	0	0
62	2P	12	Total 12	O 12	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	6	Total 6	O 6	0	0
62	2T	5	Total 5	O 5	0	0
62	2U	3	Total 3	O 3	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	1	Total 1	O 1	0	0
62	2X	3	Total 3	O 3	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	3	Total 3	O 3	0	0
62	21	12	Total 12	O 12	0	0
62	23	2	Total 2	O 2	0	0
62	25	2	Total 2	O 2	0	0
62	27	4	Total 4	O 4	0	0

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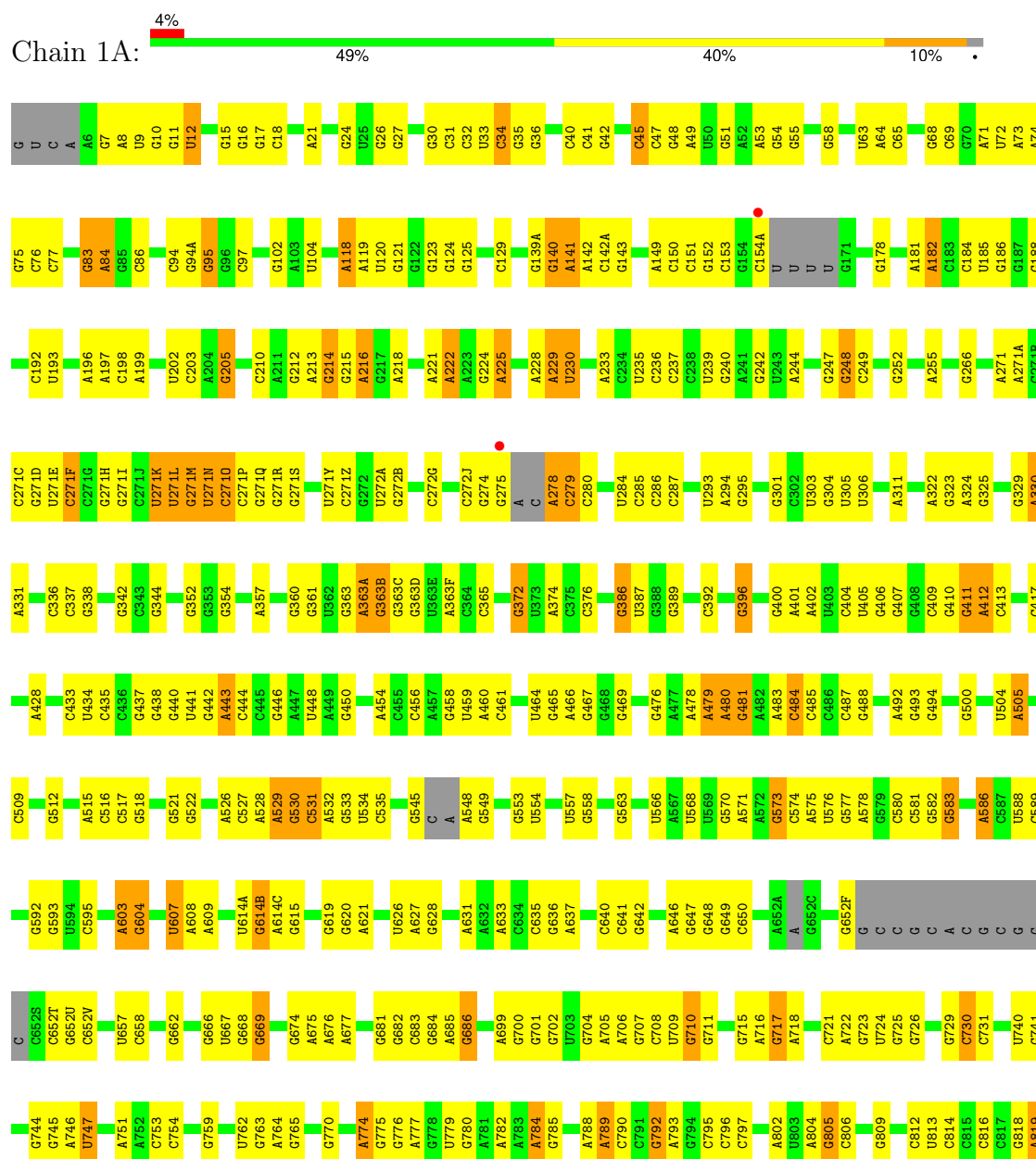
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	267	Total 267	O 267	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0
62	2f	1	Total 1	O 1	0	0
62	2j	3	Total 3	O 3	0	0
62	2l	6	Total 6	O 6	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	2	Total 2	O 2	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	6	Total 6	O 6	0	0
62	2y	8	Total 8	O 8	0	0

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



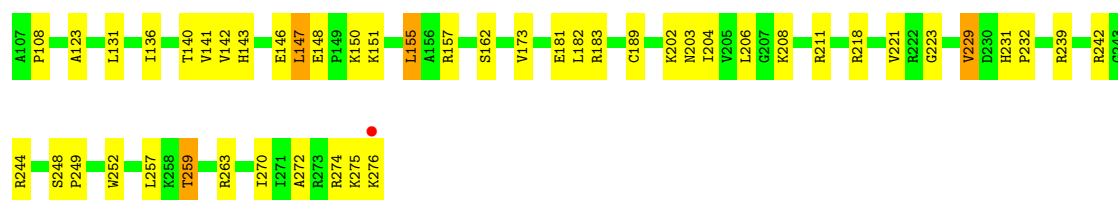
A1971	A1889	C1782	A1669	G1568	A1477	G1388	A1213	A1128	U1066	C993	A900	A820
A1972	A1890	A1783	C1670	A1569	G1482	G1389	C1224	A1129	A1067	C994	A901	A821
G1985	C1891	A1784	U1673	A1570	G1484	U1394	G1225	U1130	A1068	C995	A902	A824
A1986	A1786	A1785	C1674	A1571	G1485	U1395	G1226	U1131	A1069	A996	C902	A824
G1699	G1699	A1767	C1675	A1572	G1486	U1396	G1229	U1133	A1070	C997	C904	C825
A1900	A1900	A1676	A1676	U1578	G1487	U1399	G1230	G1135	A1071	C998	U907	U826
U1991	U1991	A1677	G1677	A1579	G1488	C1399	G1230	G1136	C1072	U999	U907	U827
G1903	G1903	C1790	G1677	A1580	G1489	G1400	G1230	G1137	A1073	A1000	U828	U828
G1904	G1904	A1791	G1681	G1581	A1490	G1401	G1236	G1138	G1074	G1003	A910	A829
C1905	C1905	U1794	G1682	A1583	C1493	C1402	G1236	G1139	C1075	C912	A910	A830
G1906	G1906	C1795	G1683	A1584	A1494	C1403	G1237	C1140	C1076	U913	C912	A831
G1907	G1907	U1796	C1684	A1586	A1495	U1405	G1238	C1141	A1077	U913	U913	U839
C1908	C1908	C1797	C1685	A1587	A1496	U1406	G1239	U1141	U1078	C1005	C914	U839
G2000	G2000	U1798	C1686	A1588	A1497	U1407	G1240	U1142	C1079	C1006	C915	C840
A2001	A2001	G1799	G1687	C1588	U1497	U1408	U1240	U1142	C1080	C1007	C915	C840
G2002	G2002	U1688	G1688	C1589	U1497	C1409	G1244	A1142A	C1081	G1011	U922	A841
A2005	A2005	G1801	U1688	G1593	C1502	C1409	G1244	A1143	U1082	G1012	C923	A842
G2012	G2012	A1802	U1683	G1594	U1503	C1411	G1248	A1148	U1083	C1013	C931	C846
A2013	A2013	C1804	G1696	G1595	C1504	A1412	U1249	G1149	A1085	A1020	G932	U847
A2014	A2014	U1805	A1700	C1599	A1508	G1416	G1250	C1150	A1086	U1021	G942	C848
U2017	U2017	C1806	A1701	A1603	C1509	C1417	G1251	G1151	U1087	G1022	G942	A849
G2018	G2018	A1810	G1719	C1607	A1509A	G1418	C1251	C1152	A1088	U1023	C945	C856
A2019	A2019	G1811	U1720	A1608	A1509B	C1419	G1252	C1153	U1089	G1024	A945	C857
A2020	A2020	C1812	G1721	C1610	G1510	A1419	G1254	A1156	U1090	G1025	G946	U858
C2021	C2021	G1813	U1722	A1610	C1511	U1420	G1256	C1161	C1092	U1026	G947	C859
G2023	G2023	C1814	U1738	A1618	C1513	G1426	C1261	C1162	U1093	A1027	C950	U860
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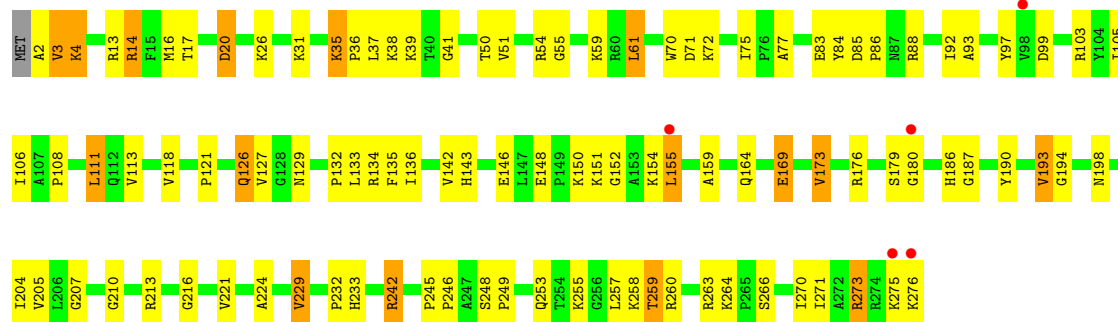


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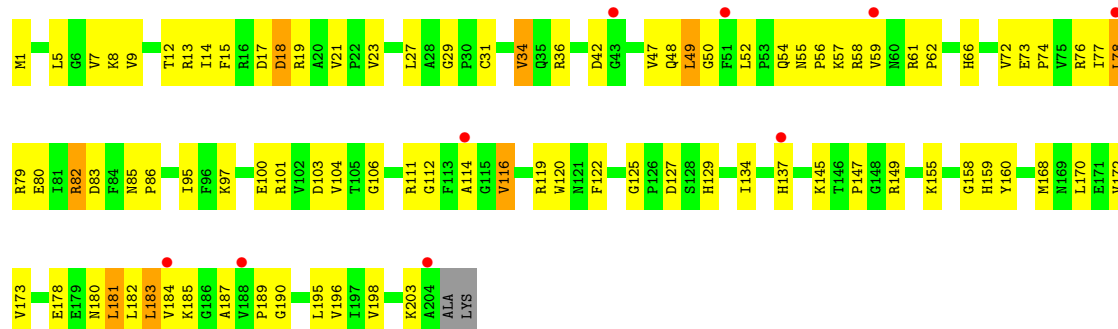
• Molecule 3: 50S ribosomal protein L2



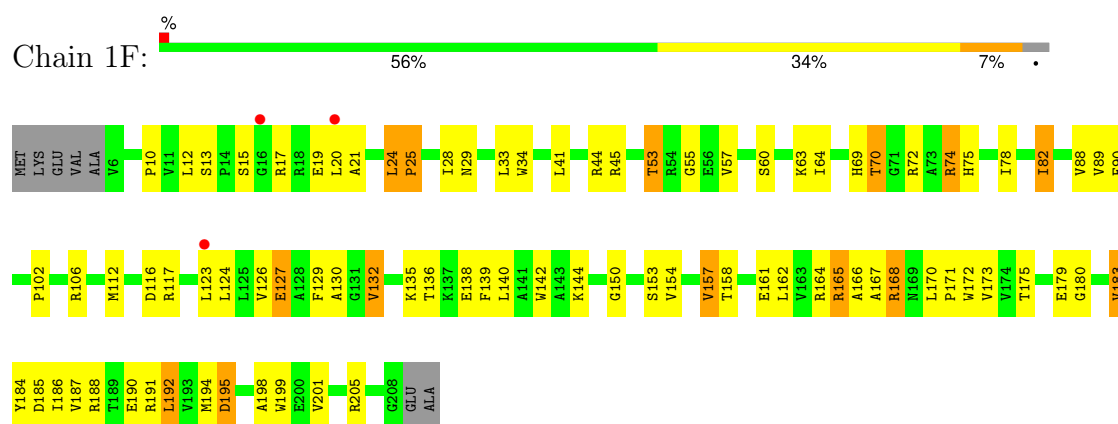
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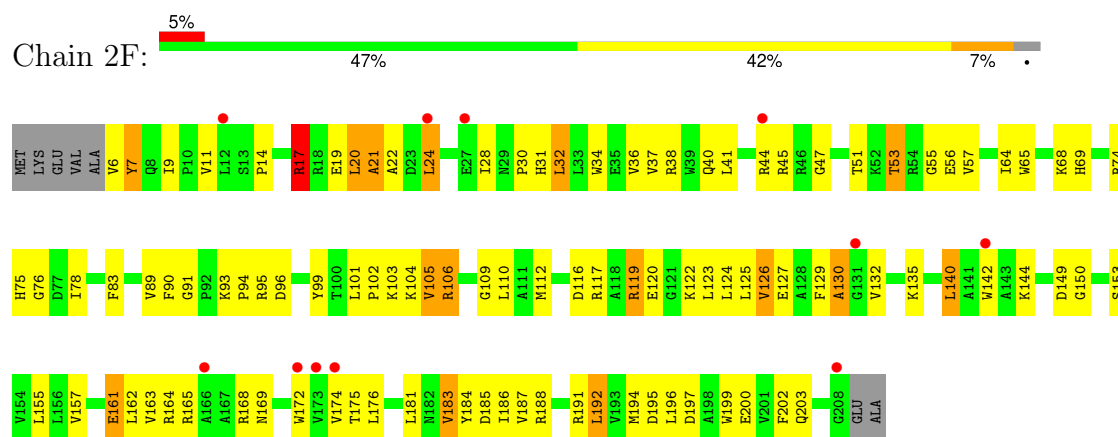
• Molecule 4: 50S ribosomal protein L3



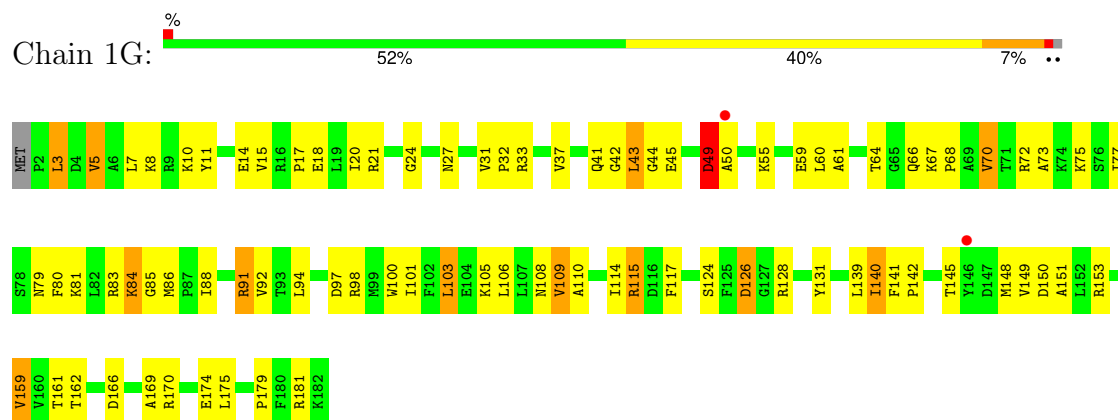
• Molecule 5: 50S ribosomal protein L4



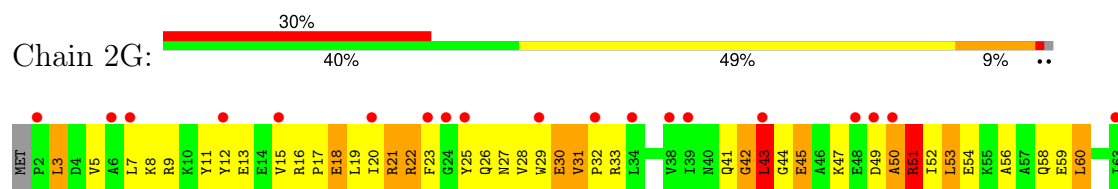
• Molecule 5: 50S ribosomal protein L4

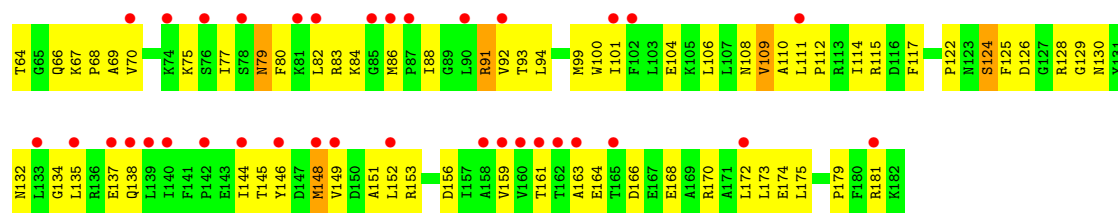


• Molecule 6: 50S ribosomal protein L5

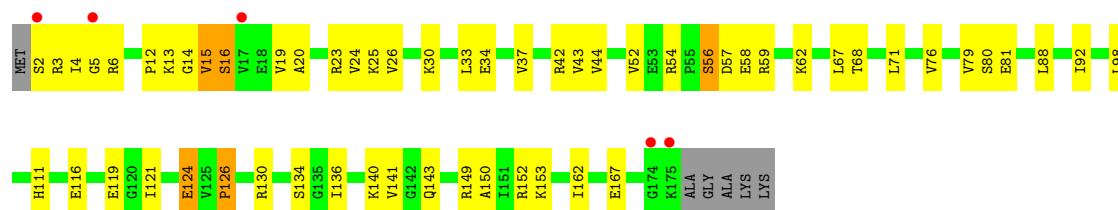


• Molecule 6: 50S ribosomal protein L5

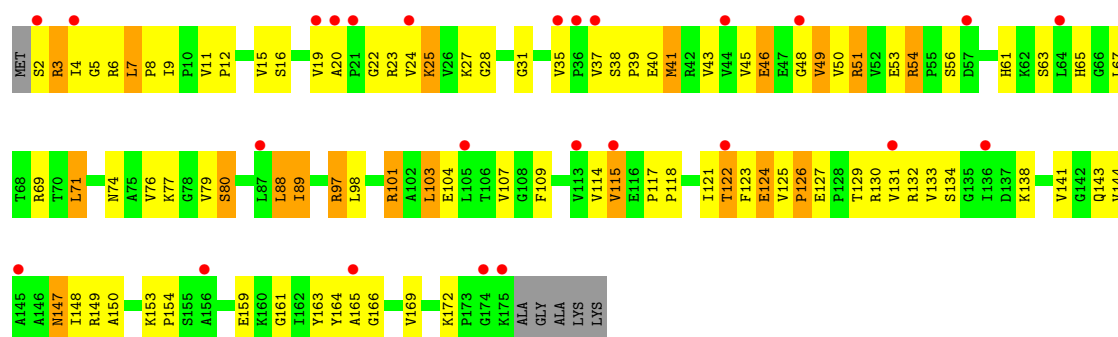




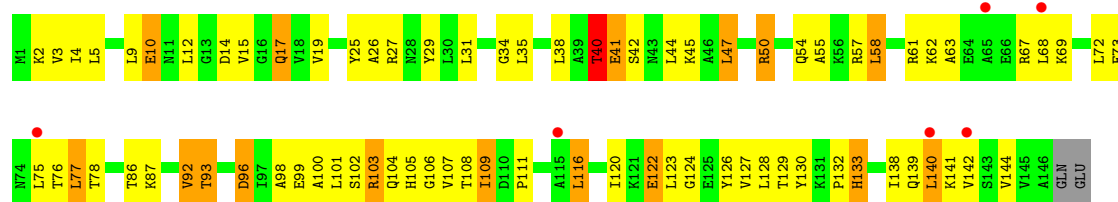
• Molecule 7: 50S ribosomal protein L6



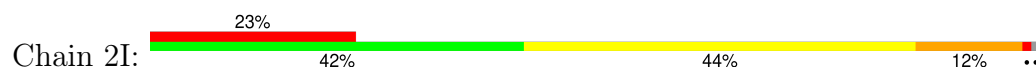
• Molecule 7: 50S ribosomal protein L6

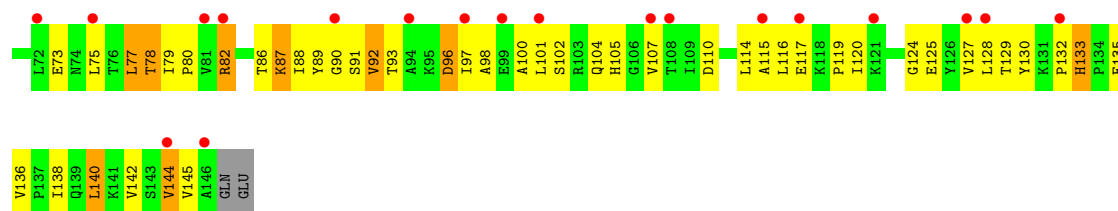


• Molecule 8: 50S ribosomal protein L9

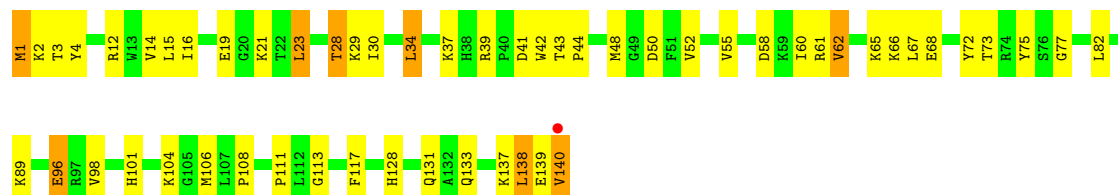


• Molecule 8: 50S ribosomal protein L9

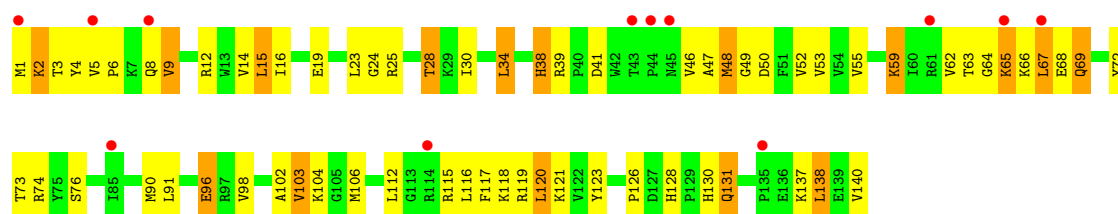




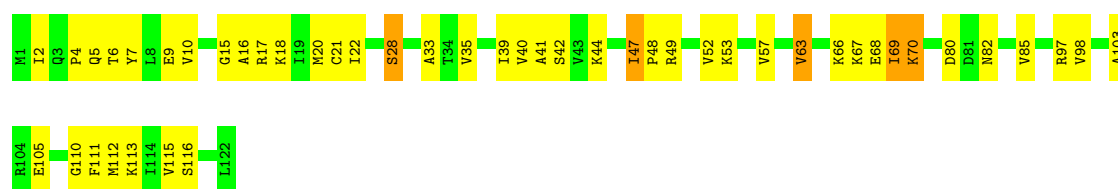
• Molecule 9: 50S ribosomal protein L13



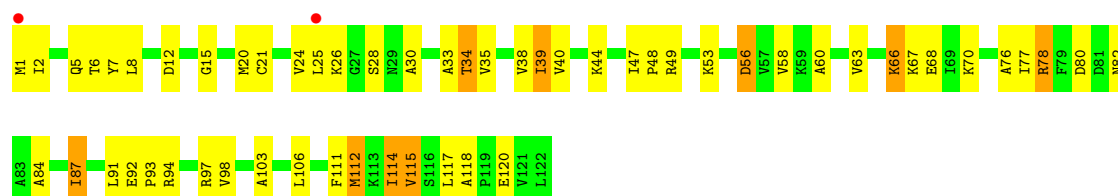
• Molecule 9: 50S ribosomal protein L13



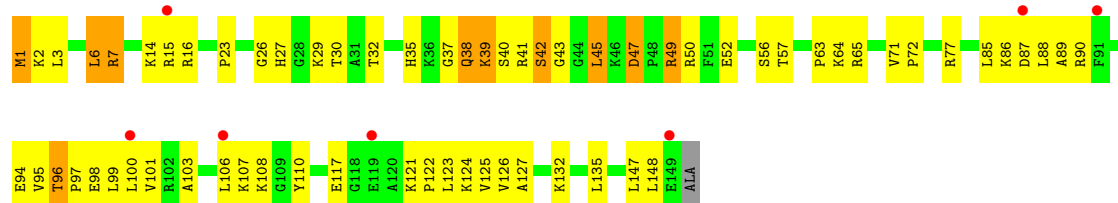
• Molecule 10: 50S ribosomal protein L14



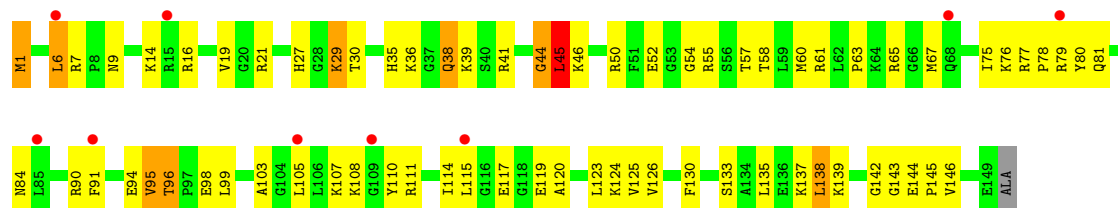
• Molecule 10: 50S ribosomal protein L14



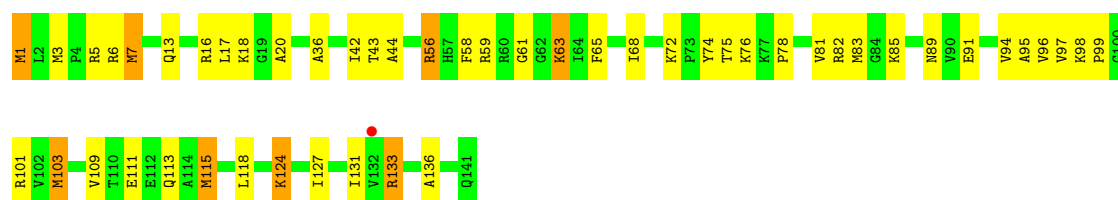
• Molecule 11: 50S ribosomal protein L15



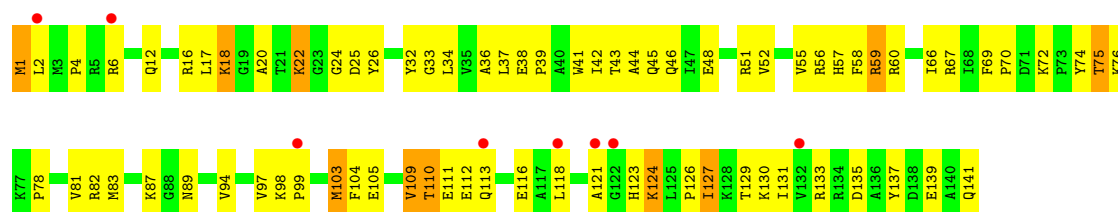
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16

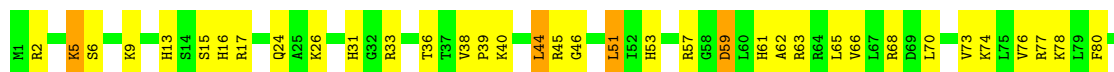


• Molecule 13: 50S ribosomal protein L17

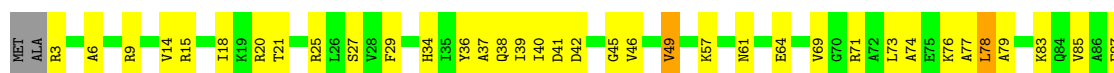




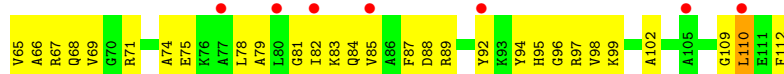
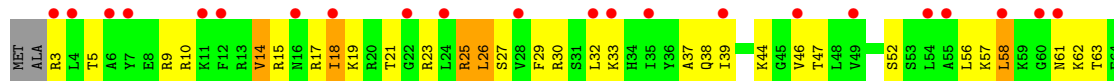
- Molecule 13: 50S ribosomal protein L17



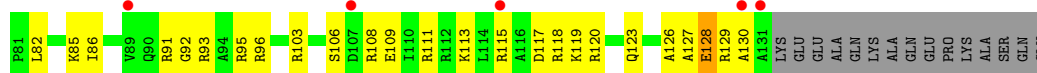
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

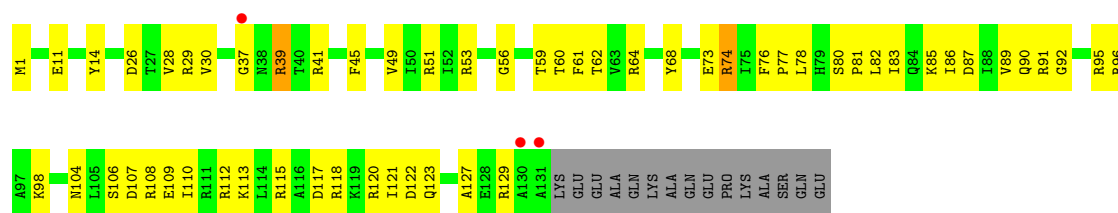


- Molecule 15: 50S ribosomal protein L19



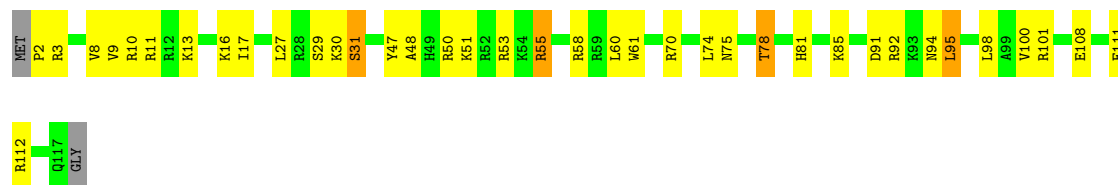
- Molecule 15: 50S ribosomal protein L19





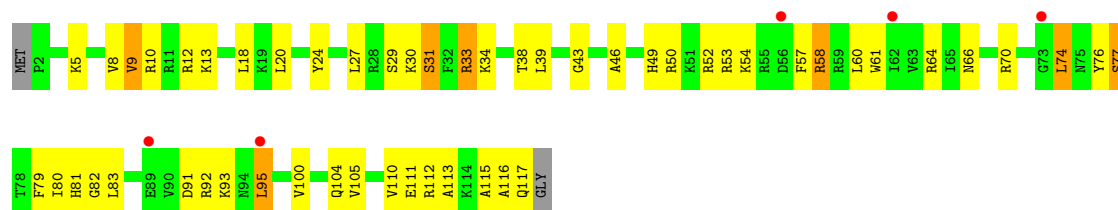
• Molecule 16: 50S ribosomal protein L20

Chain 1U: 66% 29% . .



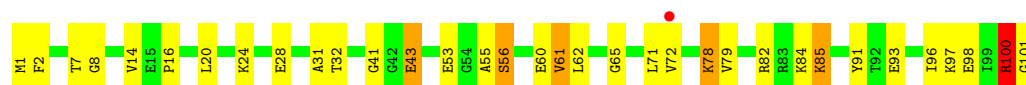
• Molecule 16: 50S ribosomal protein L20

Chain 2U: 4% 53% 39% 6% .



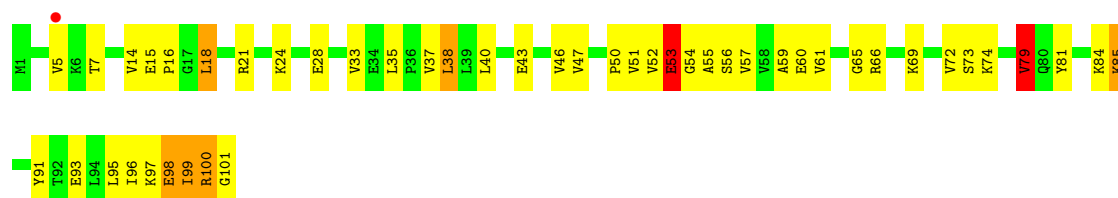
• Molecule 17: 50S ribosomal protein L21

Chain 1V: 66% 28% 5% .



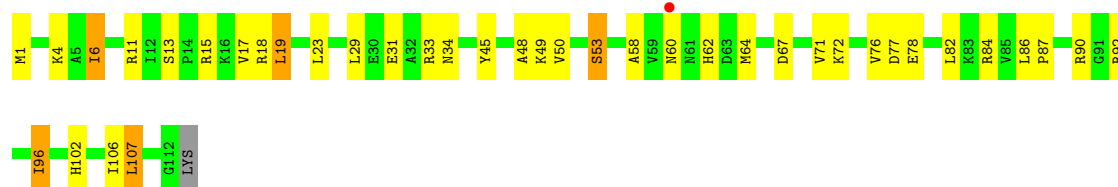
• Molecule 17: 50S ribosomal protein L21

Chain 2V: 53% 39% 6% .

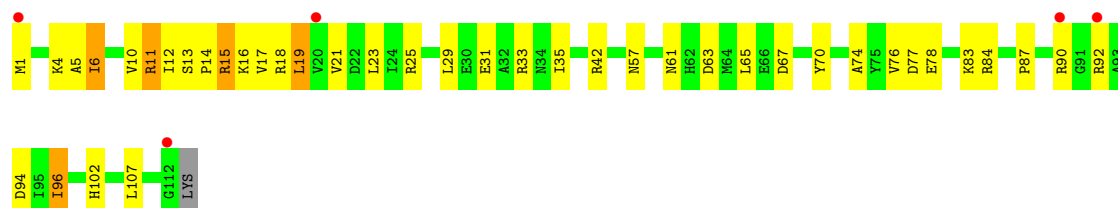


• Molecule 18: 50S ribosomal protein L22

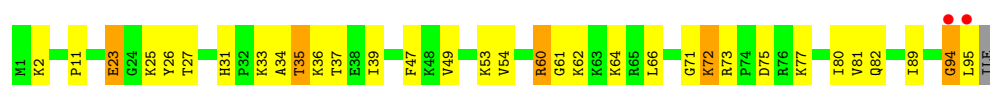
Chain 1W: 65% 30% . .



- Molecule 18: 50S ribosomal protein L22



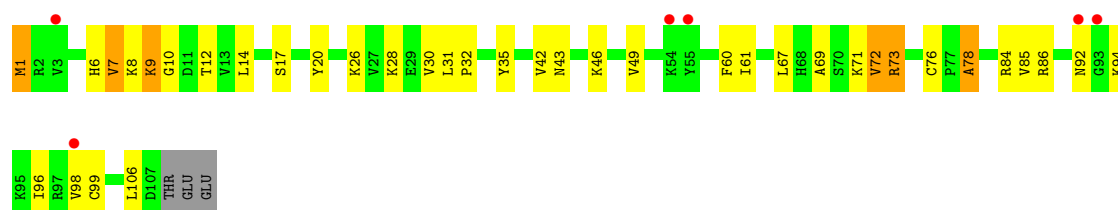
- Molecule 19: 50S ribosomal protein L23



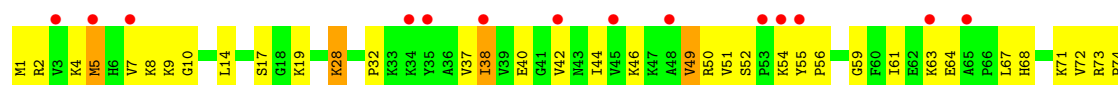
- Molecule 19: 50S ribosomal protein L23

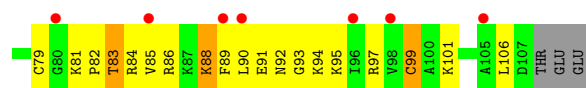


- Molecule 20: 50S ribosomal protein L24

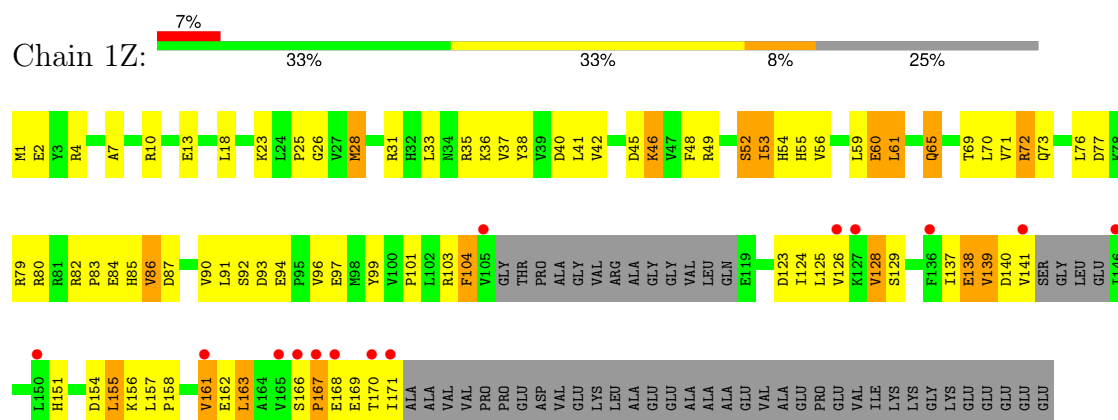


- Molecule 20: 50S ribosomal protein L24

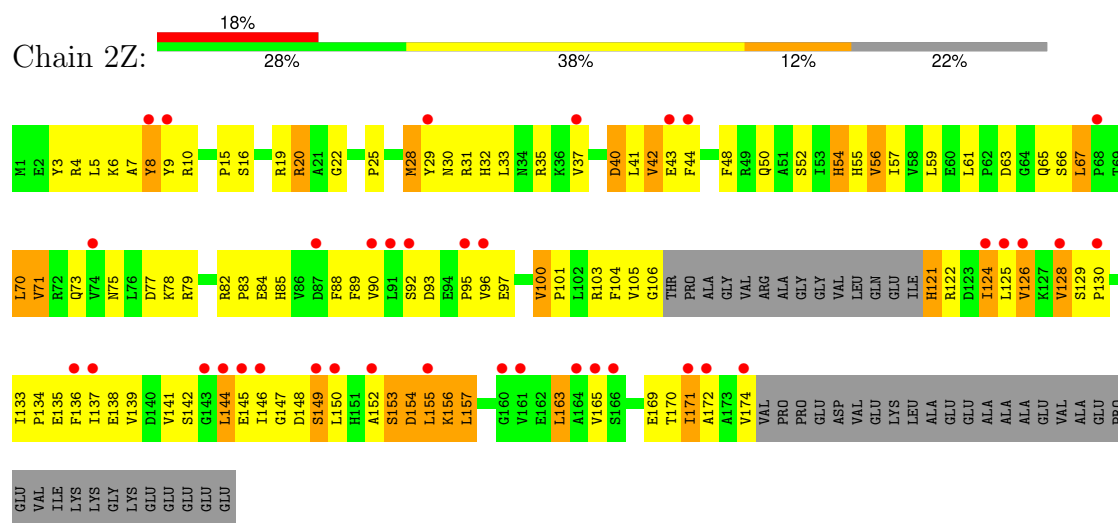




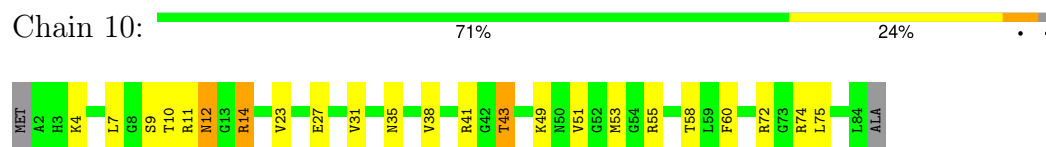
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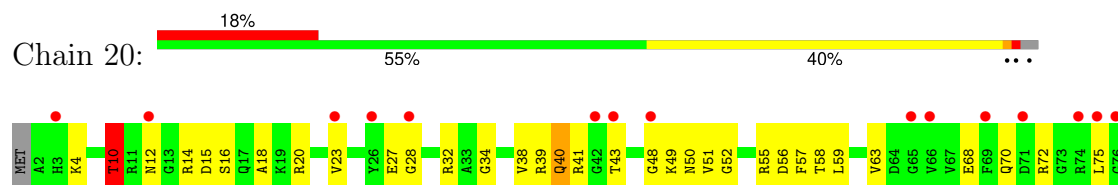
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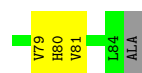


• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

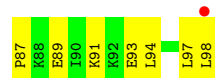
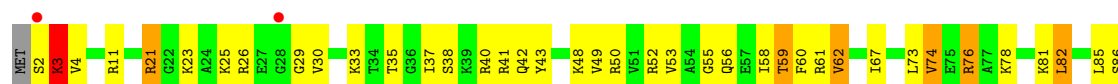




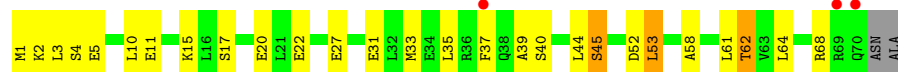
- Molecule 23: 50S ribosomal protein L28



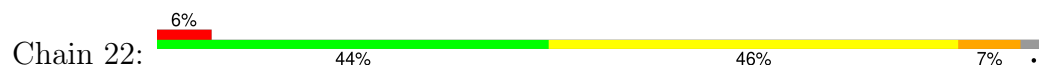
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



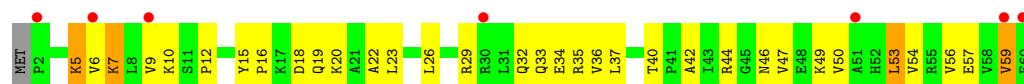
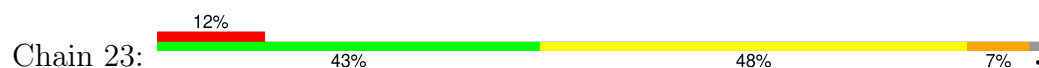
- Molecule 24: 50S ribosomal protein L29



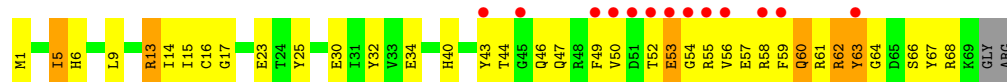
- Molecule 25: 50S ribosomal protein L30



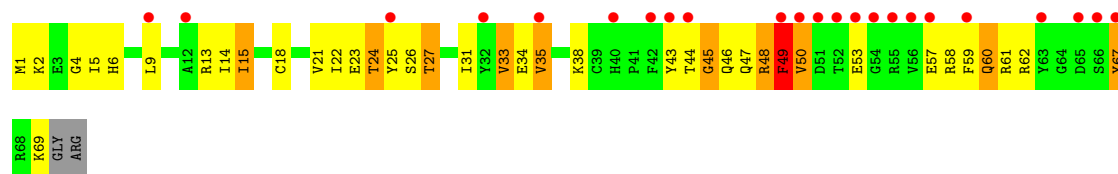
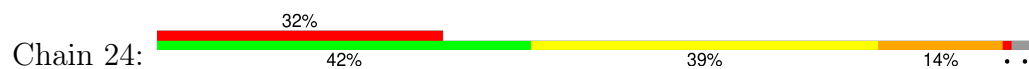
- Molecule 25: 50S ribosomal protein L30



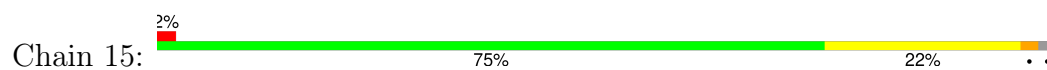
- Molecule 26: 50S ribosomal protein L31



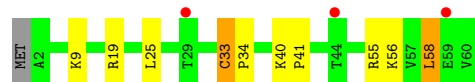
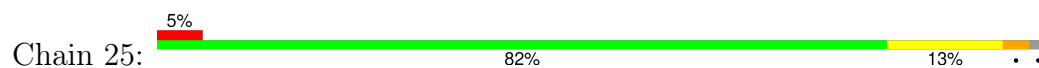
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

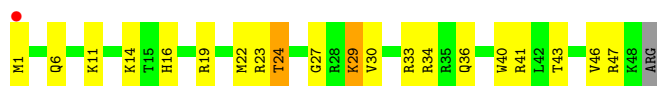


- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34





- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



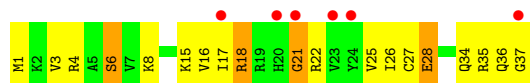
- Molecule 30: 50S ribosomal protein L35



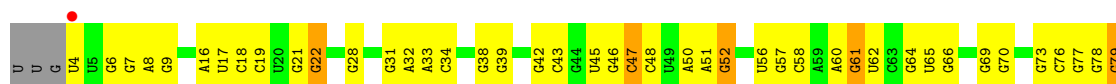
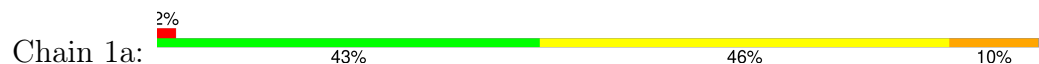
- Molecule 31: 50S ribosomal protein L36



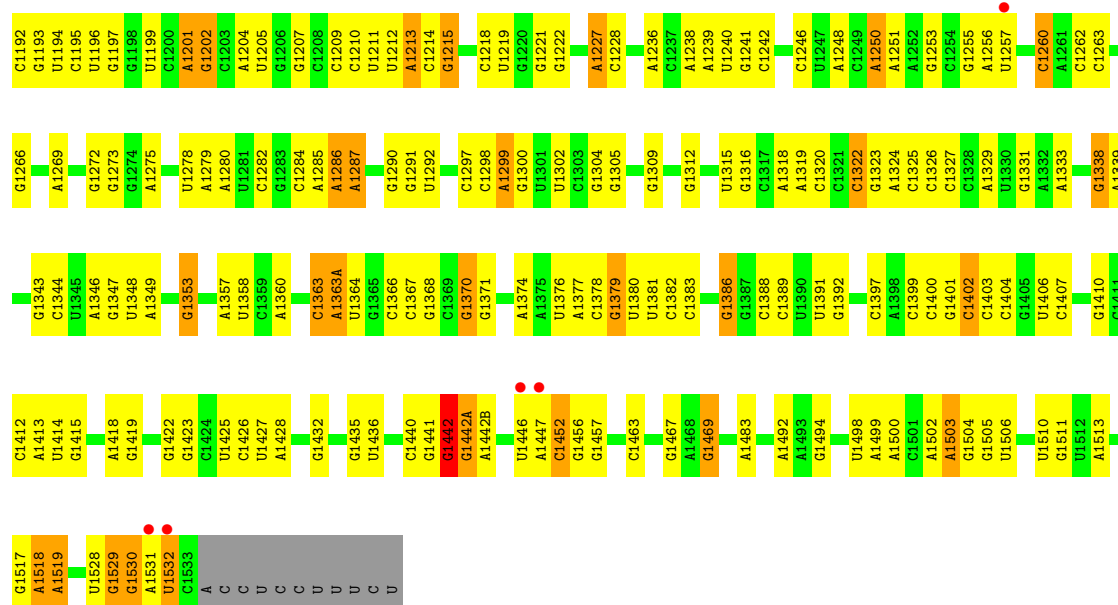
- Molecule 31: 50S ribosomal protein L36



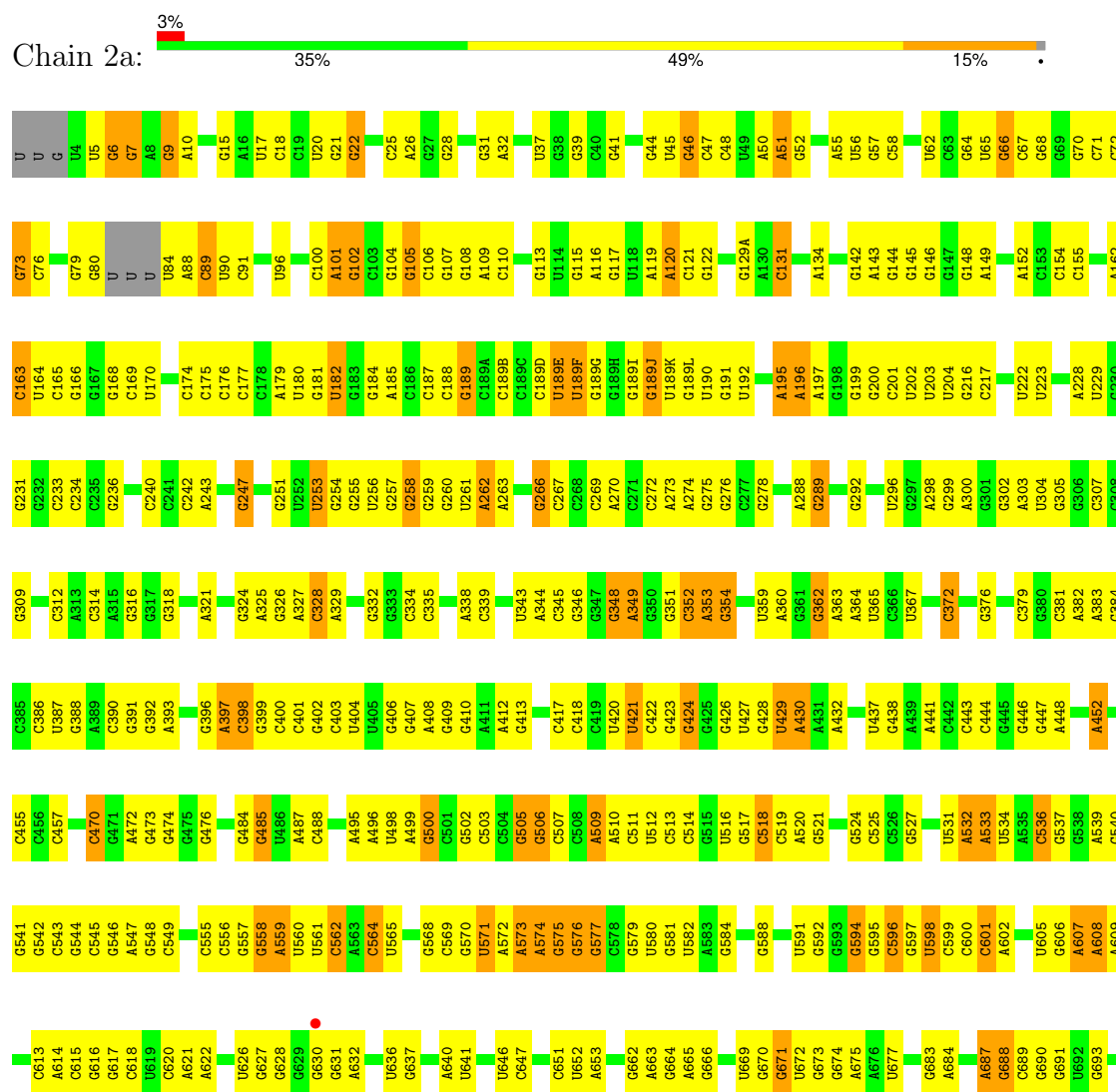
- Molecule 32: 16S Ribosomal RNA

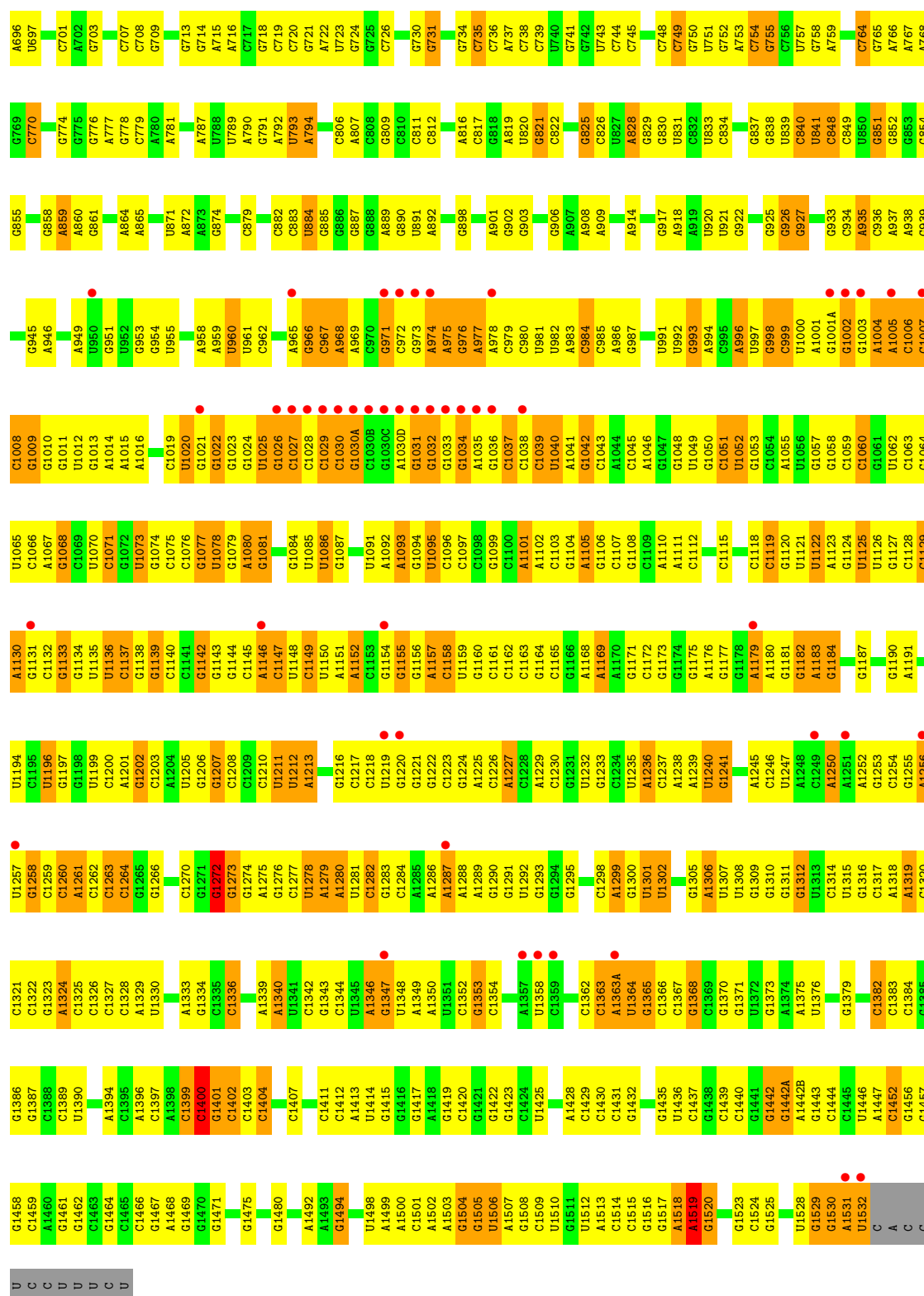


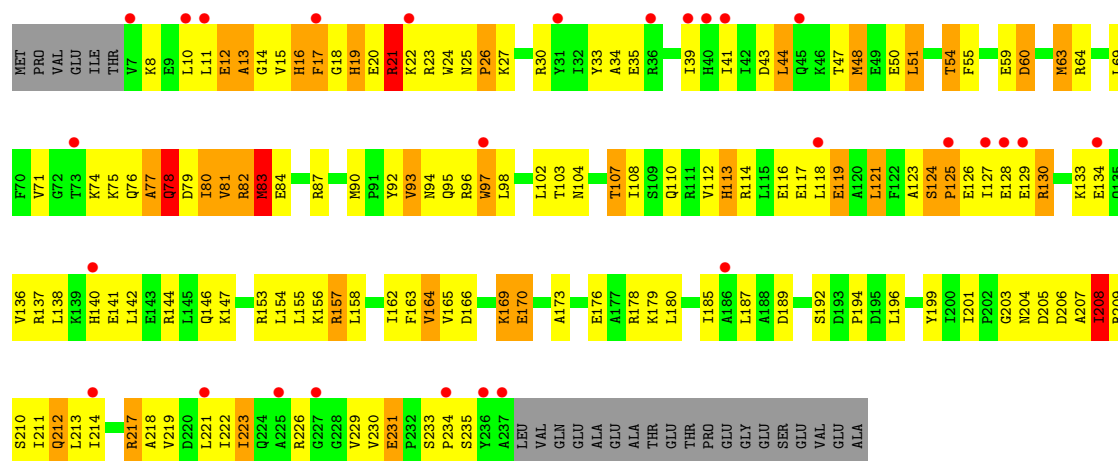
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C1119	G1036	A975	G809	G718	A642	U561	C488	A408	G324	G166	G166	U
U1122	C1037	G976	C812	U723	A648	U560	C489	G409	A325	G167	G167	U
A1123	C1038	A977	U813	G724	G649	C562	G492	G410	C326	G168	G168	U
A1123	C1039	A978	U814	G724	G650	A563	G493	G411	G327	C169	C169	A
U1125	C1040	A979	A815	G724	G651	C564	U494	A412	A246	U170	U170	C
U1125	A1041	C980	A916	A728	U652	G567	U495	G413	A329	A171	A171	U90
C1129	C1042	U981	C917	A729	U653	U568	A496	G416	G331	A172	A172	C91
C1129	A1043	U982	C917	G730	A653	C569	U498	G417	G332	U173	U173	C92
A1130	C1044	G731	G821	G731	C656	U570	U499	G418	G333	C174	C174	U96
G1131	G984	G732	G821	G732	C657	U571	G500	C419	C339	C175	C175	G97
G1132	C985	G733	C824	C734	G658	A572	C501	C422	C340	C176	C176	G98
G1133	A919	C735	G825	C735	G659	A573	G502	G423	U340	C177	C177	U99
G1134	U920	C736	G826	C736	U660	A574	C503	G424	C341	U178	U178	C100
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U1136	A923	U827	A828	C738	G664	G576	G505	G426	U343	G181	G181	G102
U1137	G924	C739	G829	C739	U665	G577	A509	U427	A344	U182	U182	C103
C1138	C925	U740	G829	U740	A665	C578	A510	U428	C345	G183	G183	G104
G1139	G926	G741	U833	G741	U667	G579	C511	G429	G346	G184	G184	G105
C1140	U927	G742	C834	G742	G667	U580	U512	U430	G347	A185	A185	C106
C1141	G997	U743	U835	U743	G674	C581	C513	A431	G348	G189	G189	A109
U1143	A923	C744	U836	C744	A675	U582	C514	A432	G350	G110	G110	G110
C1144	G924	C745	G837	C745	A676	C583	G515	C433	C351	G111	G111	G111
C1145	C931	U749	G838	U749	A677	U584	U516	U434	C352	G112	G112	G112
A1146	C932	G755	G839	G755	A678	G585	G517	G435	C353	G113	G113	G113
U1065	G933	G760	U840	G760	A679	C592	C518	C436	C354	U114	U114	U114
C1066	C934	G761	C948	G761	U678	C596	C519	U437	C355	G115	G115	G115
U1067	G939	G762	C949	G762	C679	C597	A520	G438	A356	A116	A116	A116
U1068	C940	G763	U850	G763	C680	C598	C521	A439	C357	G1891	G1891	G1891
C1007	G945	U766	G851	U766	G683	C599	A522	A441	U367	U189L	U189L	A120
C1008	A946	A767	G852	A767	A687	C607	A523	C442	G371	G192	G192	C121
G1011	C948	A768	G853	A768	G688	A608	G524	C443	G372	G193	G193	C122
A1014	A949	G769	U859	G769	C689	G609	G527	C444	A373	C194	C194	C123
A1015	U950	C770	A860	C770	C690	A614	G530	G445	G376	A195	A195	G131
A1016	G951	G771	G861	G771	G691	C613	U531	G446	G377	C196	C196	C132
G1017	U952	U772	A864	U772	U692	A614	A532	G447	A288	G197	G197	U133
U1020	G953	G773	A865	G773	C693	C618	A533	A448	G289	A196	A196	A134
G1021	G954	G774	C866	G774	A694	U619	C536	A452	U296	G198	G198	G142
U1022	U955	A777	C867	A777	A695	C620	G537	C457	G297	G199	G199	A143
G1023	U957	C784	G867	C784	A696	C621	G538	C488	A298	G200	G200	G144
G1024	A958	U787	U871	U787	G697	C624	A539	G460	G299	C201	C201	G145
U1025	U960	A787	U872	A787	A698	C625	G540	A461	A300	U202	U202	G146
G1026	U961	U788	A872	U788	A699	U626	G541	C470	G301	U203	U203	G147
C1027	C962	U789	C875	U789	G703	G627	G542	G471	G309	U204	U204	G148
C1028	G963	A790	G876	A790	C707	G628	G543	A472	G310	G216	G216	A149
C1029	A964	G791	C877	G791	C708	U629	C545	G473	C311	C217	C217	C150
C1030	U965	U792	G877	U792	C709	C630	G546	G474	C312	C218	C218	A151
G1030A	G966	U793	G881	U793	G709	C631	A547	G475	C313	C219	C219	G155
C1030B	C967	A794	G881	A794	G710	A632	G550	C479	G314	U222	U222	C155
G1030C	C968	C795	G890	C795	G711	U636	C555	A482	G318	G159	G159	G159
A1030D	A969	C796	U891	C796	A712	G637	C556	G483	G319	A160	A160	A160
G1031	C970	G796	A892	G796	G713	G638	C557	G484	C320	A161	A161	A161
C1107	G971	G799	C893	G799	A715	U639	C558	G485	U404	A162	A162	C163
G1033	C972		G894				G557		U405	U229	U229	



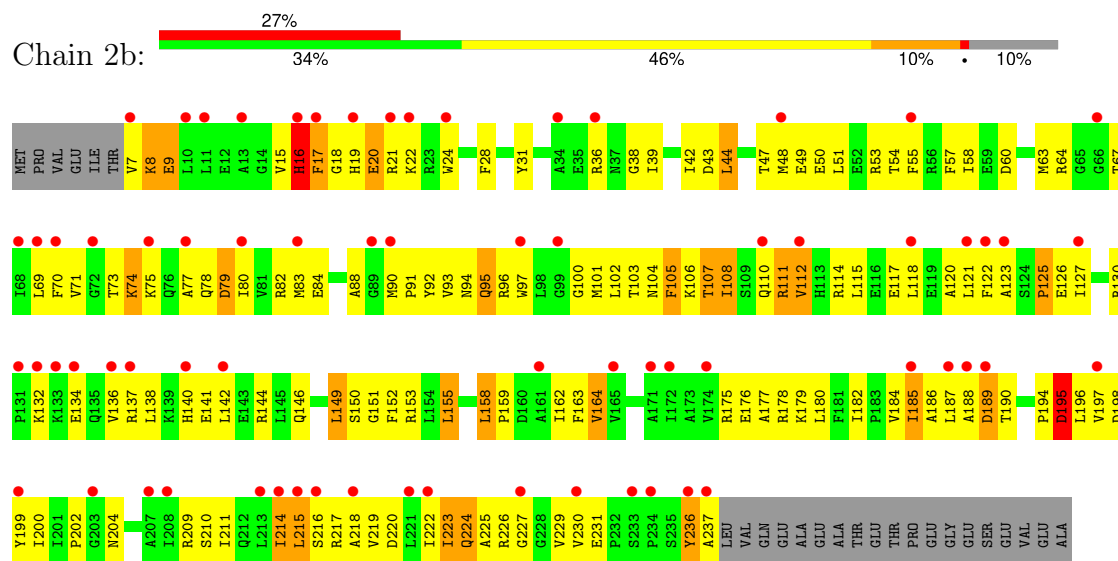
• Molecule 32: 16S Ribosomal RNA



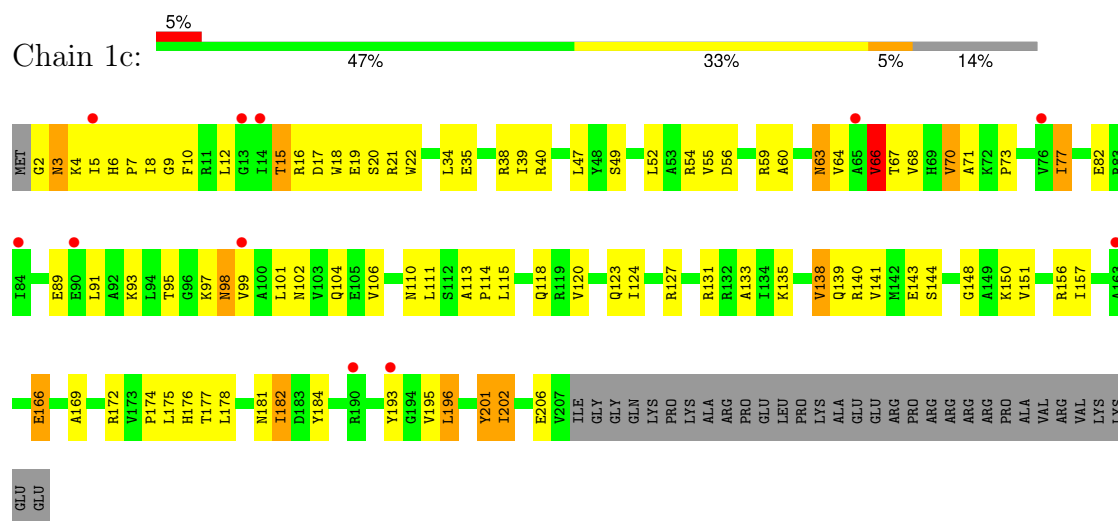




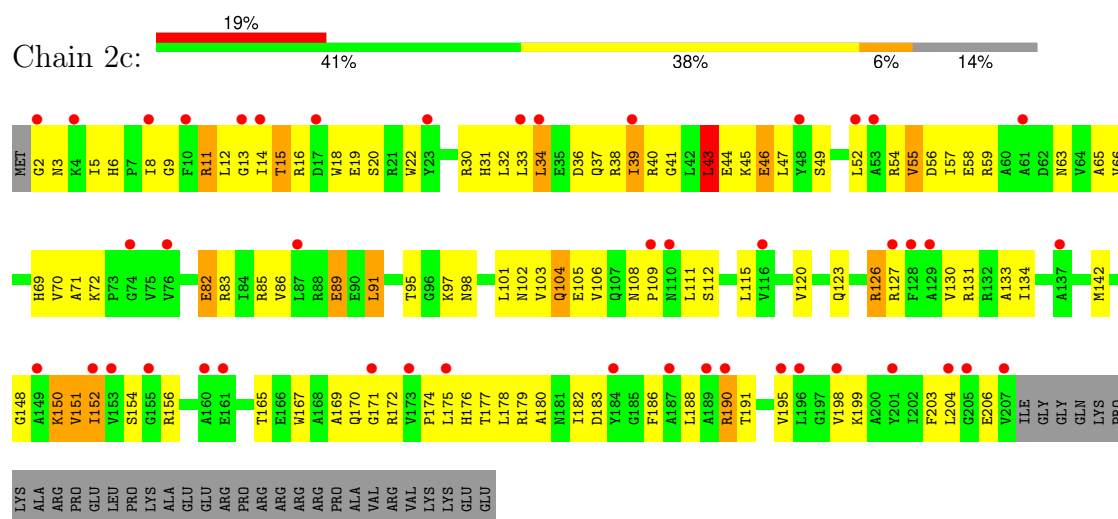
• Molecule 33: 30S ribosomal protein S2



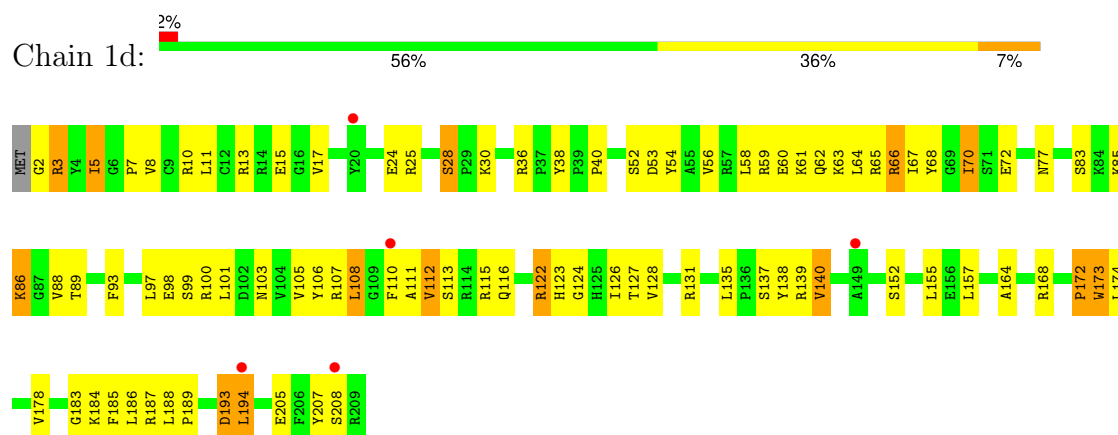
• Molecule 34: 30S ribosomal protein S3



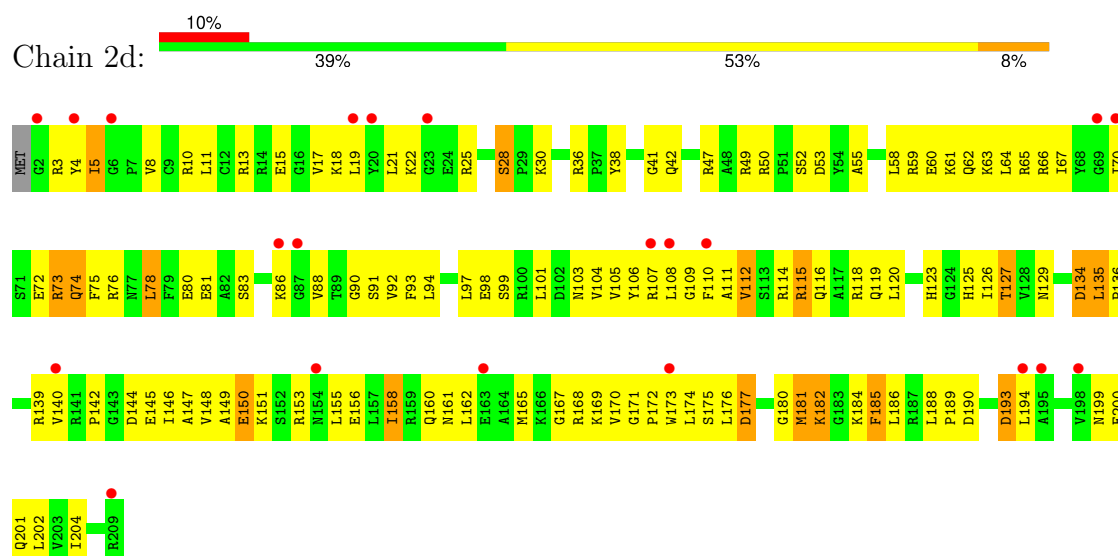
• Molecule 34: 30S ribosomal protein S3



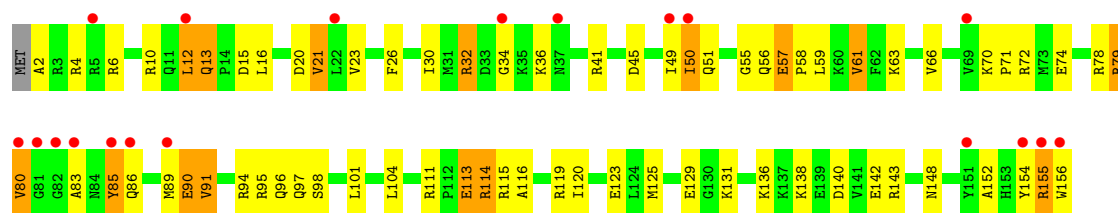
• Molecule 35: 30S ribosomal protein S4



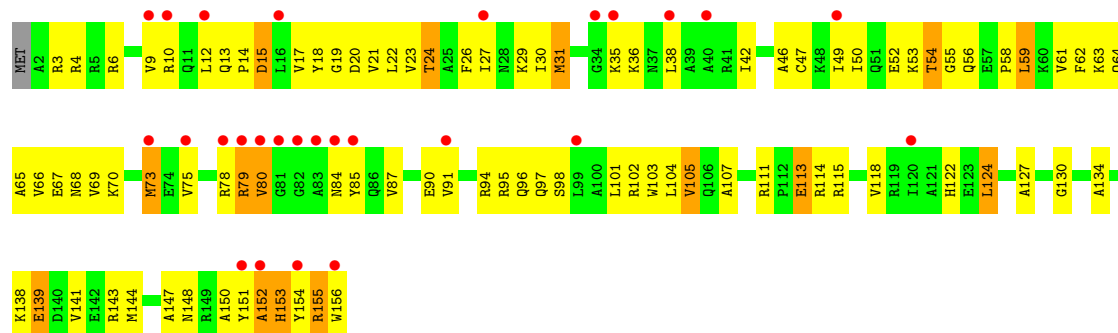
• Molecule 35: 30S ribosomal protein S4



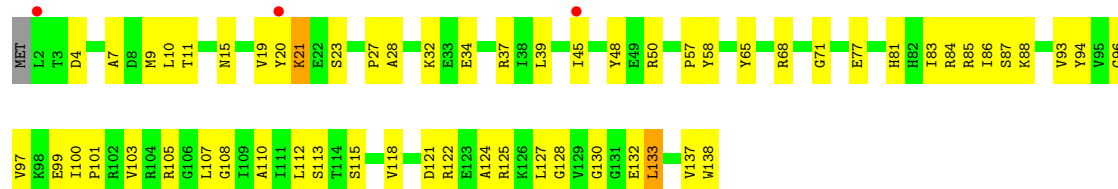
• Molecule 36: 30S ribosomal protein S5



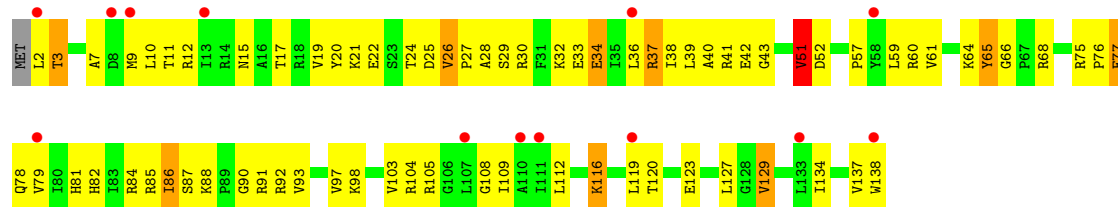
• Molecule 38: 30S ribosomal protein S7



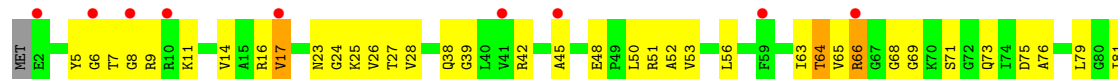
• Molecule 39: 30S ribosomal protein S8

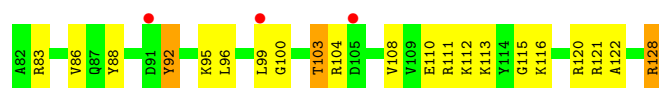


• Molecule 39: 30S ribosomal protein S8

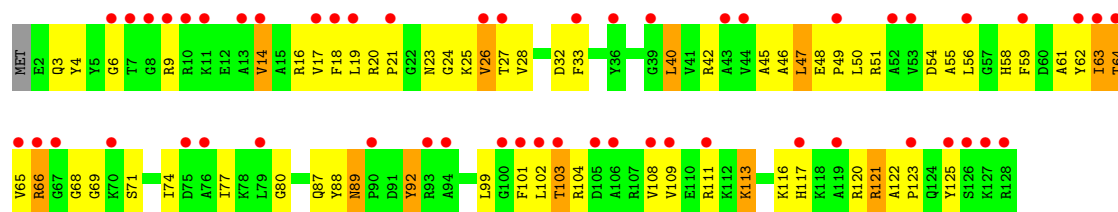
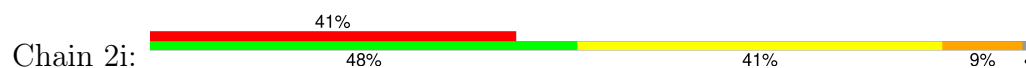


• Molecule 40: 30S ribosomal protein S9

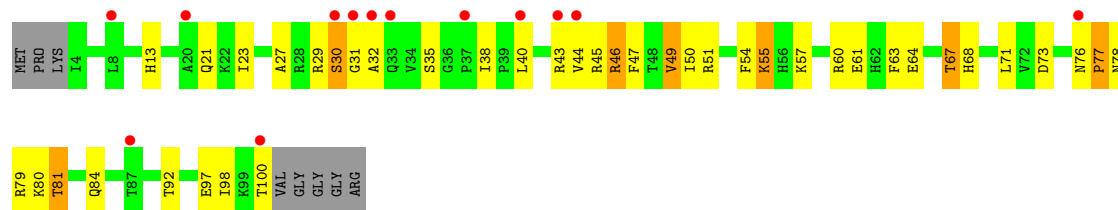




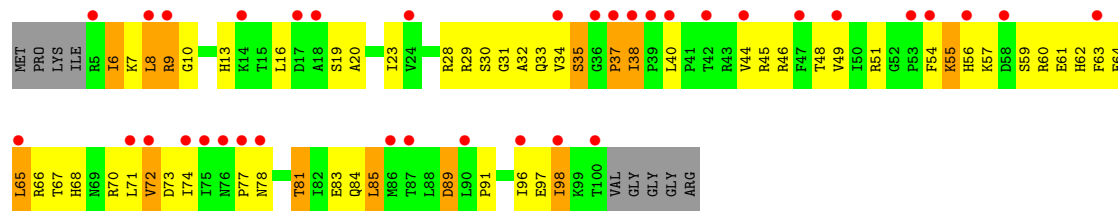
• Molecule 40: 30S ribosomal protein S9



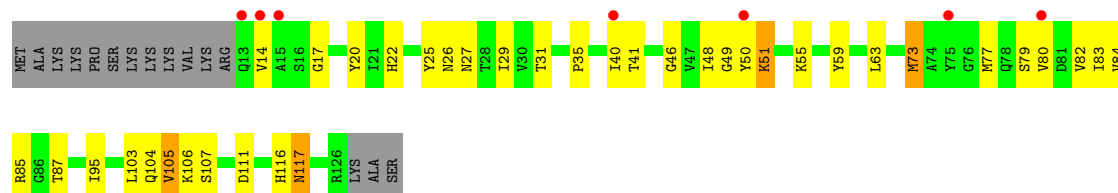
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11

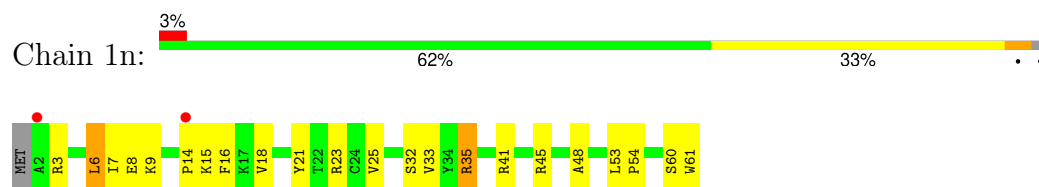


• Molecule 42: 30S ribosomal protein S11

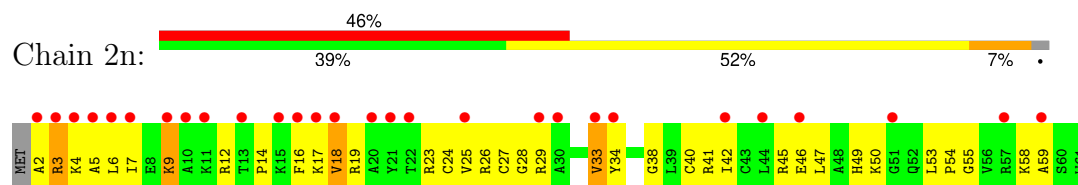




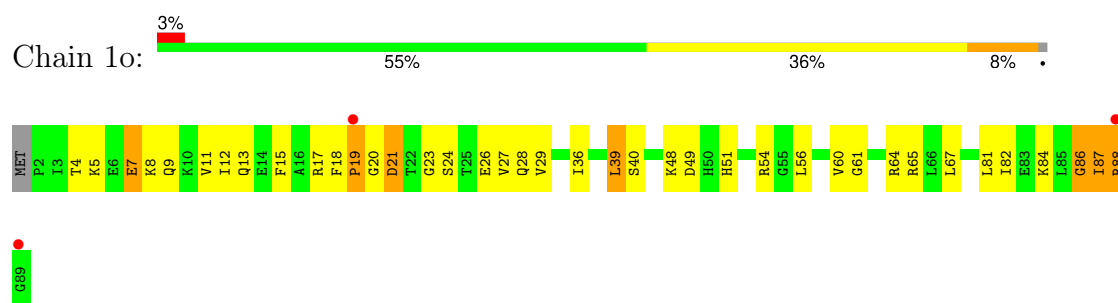
- Molecule 45: 30S ribosomal protein S14 type Z



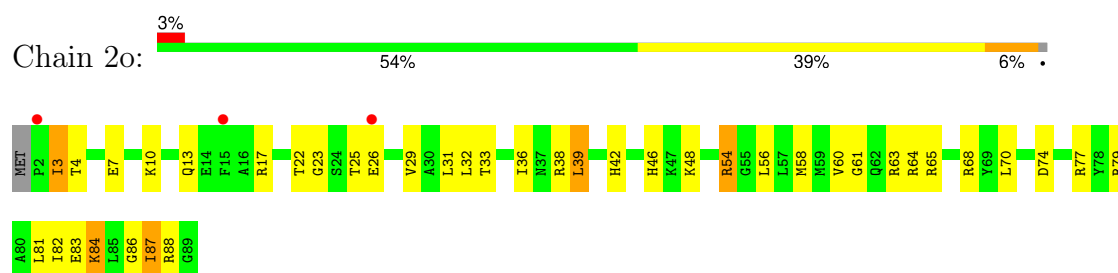
- Molecule 45: 30S ribosomal protein S14 type Z



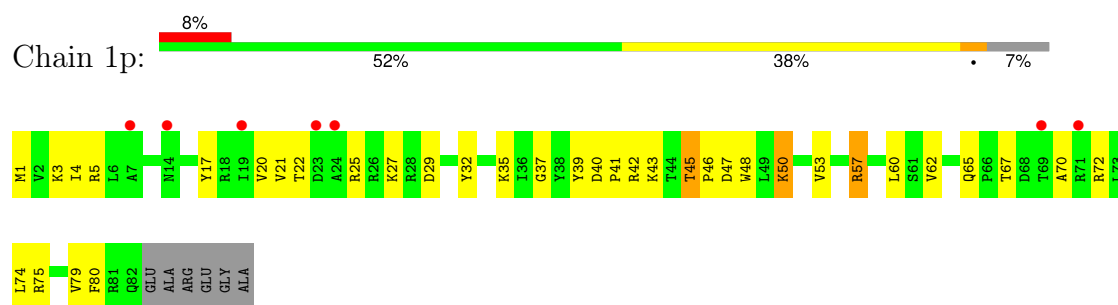
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

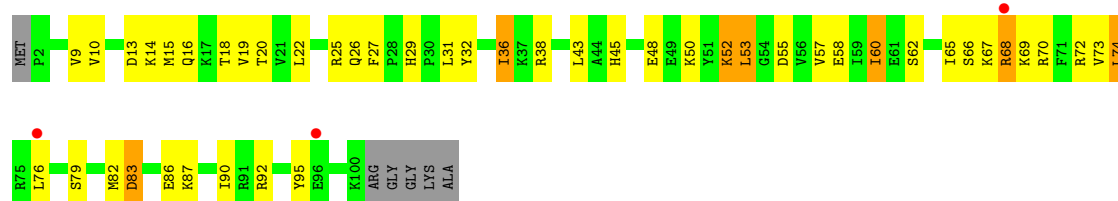


- Molecule 47: 30S ribosomal protein S16





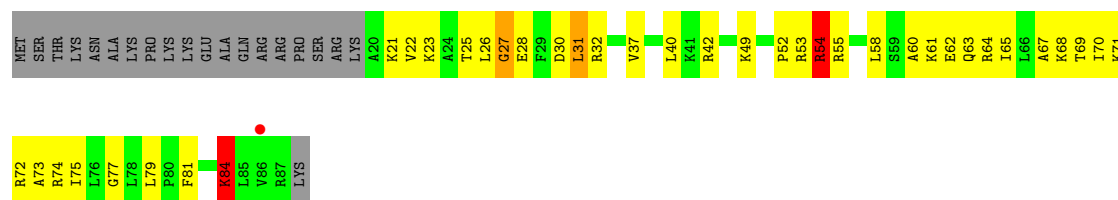
- Molecule 48: 30S ribosomal protein S17



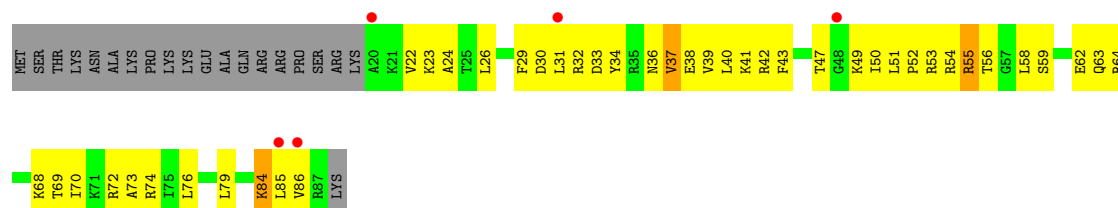
- Molecule 48: 30S ribosomal protein S17



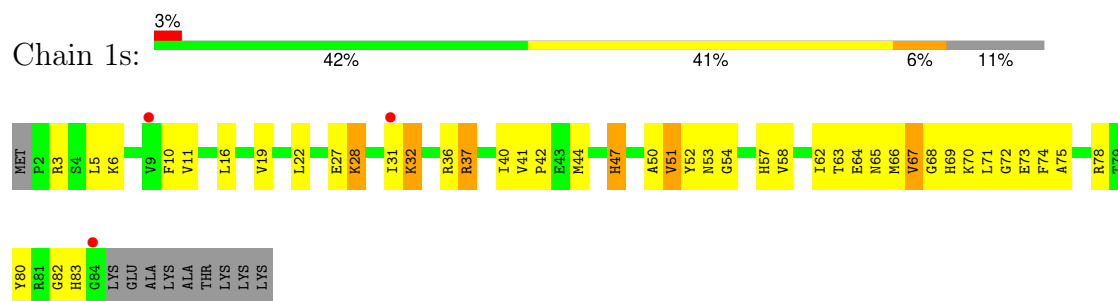
- Molecule 49: 30S ribosomal protein S18



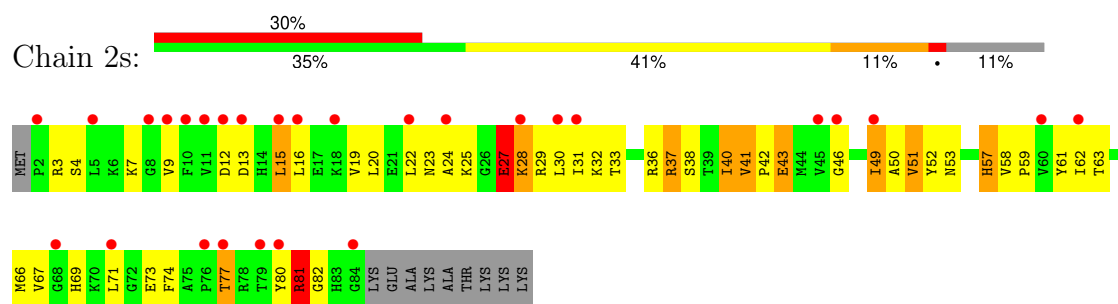
- Molecule 49: 30S ribosomal protein S18



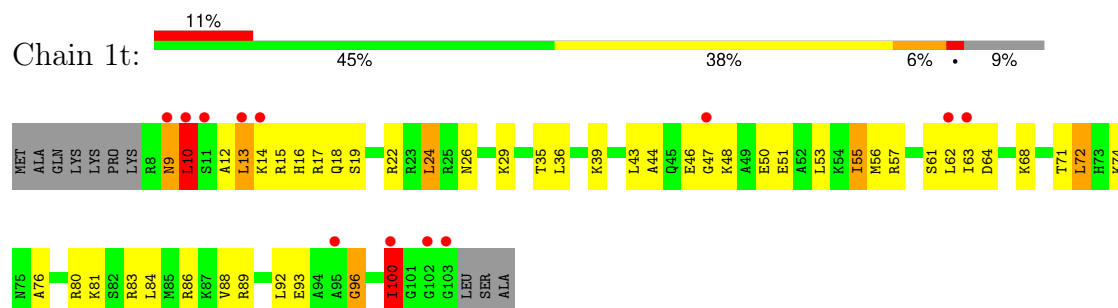
- Molecule 50: 30S ribosomal protein S19



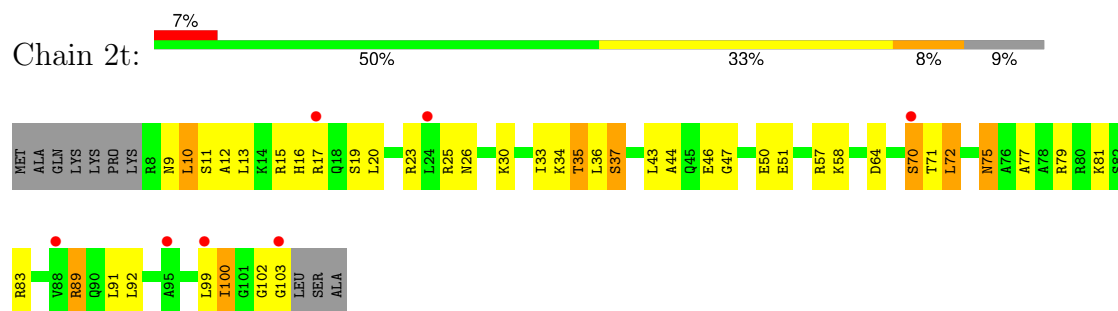
- Molecule 50: 30S ribosomal protein S19



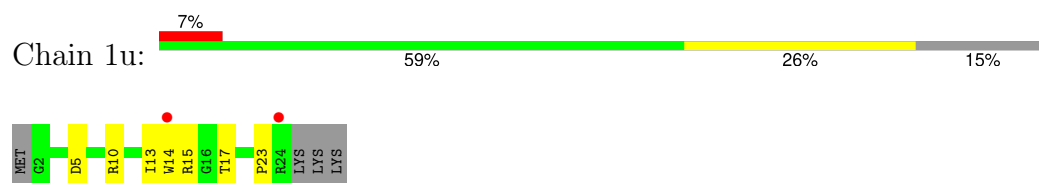
- Molecule 51: 30S ribosomal protein S20



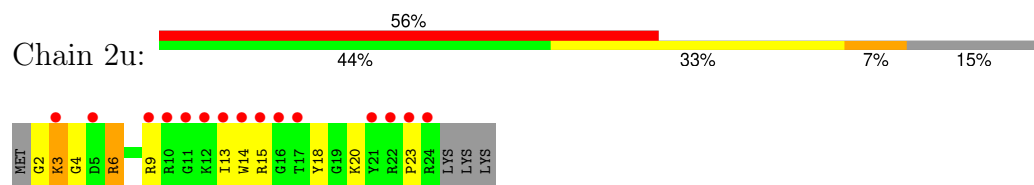
- Molecule 51: 30S ribosomal protein S20



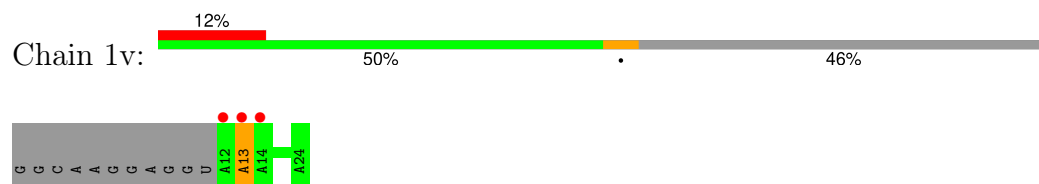
- Molecule 52: 30S ribosomal protein Thx



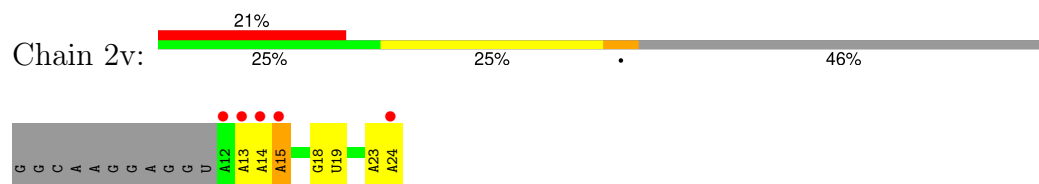
- Molecule 52: 30S ribosomal protein Thx



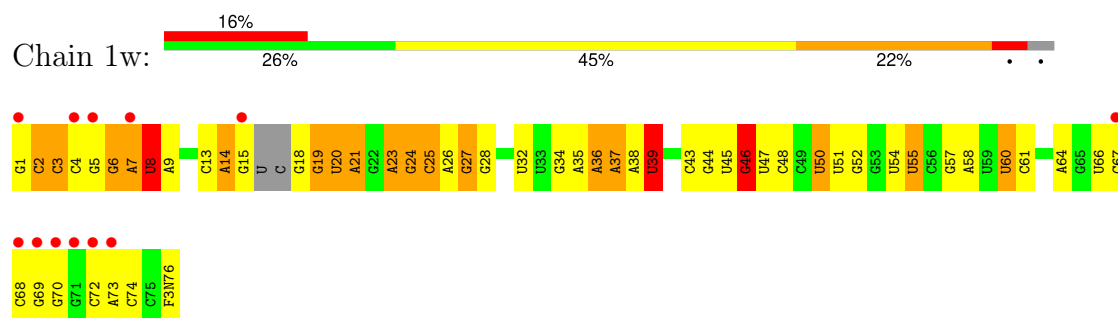
- Molecule 53: MET-PHE-mRNA



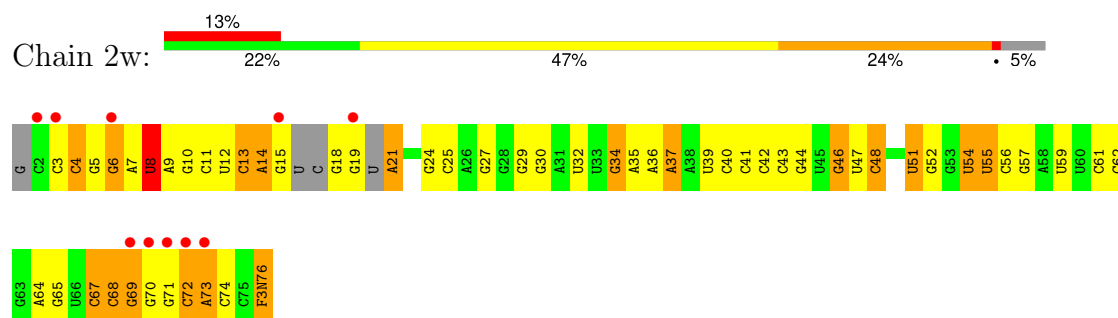
- Molecule 53: MET-PHE-mRNA



- Molecule 54: A-site Aminoacylated Phe-tRNAphe

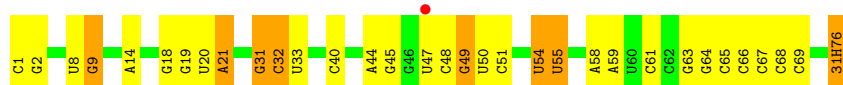


- Molecule 54: A-site Aminoacylated Phe-tRNAphe

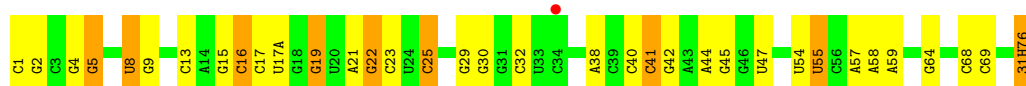


- Molecule 55: P-site Aminoacylated fMet-tRNAmet

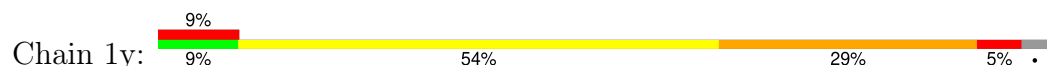




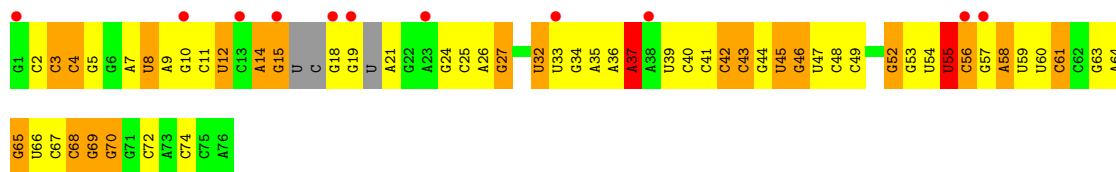
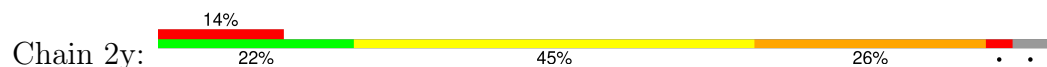
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



- Molecule 56: E-site Deacylated tRNA^{phe}



- Molecule 56: E-site Deacylated tRNA^{phe}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.22Å 446.66Å 615.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.11 – 2.45 121.11 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (121.11-2.45) 99.9 (121.11-2.45)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.245 , 0.300 0.247 , 0.301	Depositor DCC
R_{free} test set	103653 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	300377	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: UR3, 0TD, 4SU, ZN, OMC, F3N, 2MG, SF4, 4OC, A1C9N, MIA, M2G, OMG, MG, G7M, 31H, 5MC, 2MA, 5MU, MA6, PSU, K, OMU

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	0.54	0/69011	0.74	5/107720 (0.0%)
1	2A	0.41	0/67295	0.63	2/105042 (0.0%)
2	1B	0.46	0/2882	0.68	0/4494
2	2B	0.37	0/2879	0.58	0/4487
3	1D	0.57	0/2186	0.79	3/2944 (0.1%)
3	2D	0.43	0/2186	0.67	0/2944
4	1E	0.49	0/1592	0.76	0/2149
4	2E	0.43	0/1592	0.64	0/2149
5	1F	0.51	0/1619	0.72	0/2193
5	2F	0.38	0/1615	0.65	0/2188
6	1G	0.41	0/1448	0.67	0/1957
6	2G	0.38	0/1453	0.63	0/1963
7	1H	0.43	0/1356	0.65	0/1834
7	2H	0.34	0/1356	0.53	0/1834
8	1I	0.39	0/1112	0.62	0/1514
8	2I	0.37	0/1079	0.66	0/1475
9	1N	0.49	0/1144	0.71	0/1543
9	2N	0.37	0/1144	0.66	0/1543
10	1O	0.50	0/943	0.70	0/1269
10	2O	0.41	0/943	0.71	0/1269
11	1P	0.50	0/1152	0.78	0/1533
11	2P	0.39	0/1152	0.72	0/1533
12	1Q	0.52	0/1143	0.74	0/1527
12	2Q	0.40	0/1143	0.67	0/1527
13	1R	0.55	0/982	0.81	0/1312
13	2R	0.43	0/982	0.66	0/1312
14	1S	0.43	0/883	0.69	0/1176
14	2S	0.38	0/880	0.62	0/1172
15	1T	0.46	0/1105	0.67	0/1477
15	2T	0.39	0/1097	0.64	0/1468
16	1U	0.53	0/977	0.72	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.39	0/977	0.58	0/1301
17	1V	0.51	0/782	0.67	0/1049
17	2V	0.36	0/782	0.62	0/1049
18	1W	0.54	0/897	0.73	0/1205
18	2W	0.43	0/897	0.63	0/1205
19	1X	0.53	0/764	0.80	0/1025
19	2X	0.39	0/764	0.65	0/1025
20	1Y	0.45	0/819	0.67	0/1095
20	2Y	0.40	0/819	0.64	0/1095
21	1Z	0.41	0/1267	0.65	0/1717
21	2Z	0.41	0/1299	0.66	0/1763
22	10	0.53	0/662	0.85	2/881 (0.2%)
22	20	0.40	0/662	0.65	0/881
23	11	0.51	0/762	0.72	0/1014
23	21	0.40	0/762	0.64	0/1014
24	12	0.46	0/590	0.64	0/781
24	22	0.41	0/590	0.57	0/781
25	13	0.50	0/474	0.71	0/635
25	23	0.35	0/469	0.62	0/630
26	14	0.46	0/565	0.79	0/761
26	24	0.42	0/545	0.64	0/737
27	15	0.58	0/469	0.78	0/635
27	25	0.45	0/469	0.74	0/635
28	16	0.51	0/460	0.73	0/613
28	26	0.40	0/456	0.66	0/608
29	17	0.61	0/426	0.83	0/561
29	27	0.49	0/426	0.69	0/561
30	18	0.50	0/525	0.69	0/691
30	28	0.39	0/525	0.59	0/691
31	19	0.57	0/310	0.83	0/407
31	29	0.38	0/310	0.60	0/407
32	1a	0.40	0/35795	0.61	4/55864 (0.0%)
32	2a	0.37	0/35886	0.59	4/56005 (0.0%)
33	1b	0.40	0/1881	0.71	0/2542
33	2b	0.41	0/1860	0.67	0/2518
34	1c	0.38	0/1572	0.63	1/2126 (0.0%)
34	2c	0.38	0/1566	0.60	0/2119
35	1d	0.37	0/1685	0.63	0/2262
35	2d	0.39	0/1704	0.65	0/2284
36	1e	0.40	0/1145	0.63	0/1543
36	2e	0.37	0/1149	0.67	0/1548
37	1f	0.44	0/823	0.62	0/1115
37	2f	0.38	0/829	0.56	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.38	0/1250	0.59	0/1679
38	2g	0.38	0/1254	0.55	0/1683
39	1h	0.36	0/1108	0.60	0/1494
39	2h	0.35	0/1108	0.56	0/1494
40	1i	0.38	0/1002	0.70	0/1346
40	2i	0.39	0/997	0.63	0/1343
41	1j	0.36	0/722	0.59	0/982
41	2j	0.41	0/727	0.66	0/988
42	1k	0.37	0/844	0.65	0/1145
42	2k	0.34	0/848	0.53	0/1149
43	1l	0.42	0/937	0.65	0/1260
43	2l	0.36	0/937	0.61	0/1260
44	1m	0.39	0/969	0.62	0/1302
44	2m	0.41	0/961	0.66	0/1291
45	1n	0.36	0/501	0.68	0/664
45	2n	0.31	0/501	0.59	0/664
46	1o	0.41	0/739	0.63	0/985
46	2o	0.34	0/739	0.56	0/985
47	1p	0.35	0/697	0.61	0/939
47	2p	0.41	0/693	0.62	0/935
48	1q	0.39	0/836	0.59	0/1117
48	2q	0.36	0/836	0.61	0/1117
49	1r	0.44	0/560	0.64	0/746
49	2r	0.36	0/560	0.61	0/746
50	1s	0.37	0/667	0.65	0/900
50	2s	0.41	0/661	0.69	0/893
51	1t	0.37	0/730	0.66	0/965
51	2t	0.37	0/729	0.68	0/965
52	1u	0.36	0/203	0.61	0/266
52	2u	0.49	0/203	0.68	0/266
53	1v	0.45	0/310	0.56	0/480
53	2v	0.40	0/310	0.52	0/480
54	1w	0.46	1/1581 (0.1%)	0.62	0/2458
54	2w	0.47	2/1531 (0.1%)	0.61	0/2379
55	1x	0.47	0/1723	0.66	0/2684
55	2x	0.41	1/1723 (0.1%)	0.60	0/2684
56	1y	0.50	2/1606 (0.1%)	0.62	0/2497
56	2y	0.54	2/1583 (0.1%)	0.61	0/2459
All	All	0.44	8/316636 (0.0%)	0.66	21/474041 (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
5	2F	0	1
6	1G	0	1
22	10	0	1
25	13	0	1
26	14	0	1
33	1b	0	2
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	O3'-P	6.24	1.62	1.56
54	2w	8	4SU	O3'-P	6.11	1.62	1.56
54	2w	46	G7M	O3'-P	5.87	1.62	1.56
55	2x	8	4SU	O3'-P	5.84	1.62	1.56
56	2y	8	4SU	O3'-P	5.78	1.62	1.56

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1992	G	C2'-C3'-O3'	7.48	120.72	109.50
1	1A	1992	G	C2'-C3'-O3'	7.39	120.58	109.50
32	1a	266	G	C2'-C3'-O3'	6.41	119.11	109.50
1	1A	2629	A	P-O3'-C3'	6.18	129.47	120.20
3	1D	98	VAL	N-CA-C	-6.18	104.92	112.76

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	10	12	ASN	Peptide
25	13	53	LEU	Peptide
26	14	67	TYR	Peptide
6	1G	50	ALA	Peptide
33	1b	125	PRO	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	31189	1084	0
1	2A	60322	0	30421	1282	0
2	1B	2577	0	1305	54	0
2	2B	2575	0	1303	74	0
3	1D	2136	0	2218	58	0
3	2D	2136	0	2218	86	0
4	1E	1559	0	1618	64	0
4	2E	1559	0	1618	63	0
5	1F	1584	0	1625	58	0
5	2F	1580	0	1619	79	0
6	1G	1423	0	1436	63	0
6	2G	1428	0	1438	93	0
7	1H	1330	0	1407	30	0
7	2H	1330	0	1407	62	0
8	1I	1097	0	1140	49	0
8	2I	1064	0	1082	57	1
9	1N	1117	0	1184	34	0
9	2N	1117	0	1184	50	0
10	1O	933	0	996	30	0
10	2O	933	0	996	43	0
11	1P	1135	0	1212	71	0
11	2P	1135	0	1212	62	0
12	1Q	1122	0	1179	41	0
12	2Q	1122	0	1179	60	0
13	1R	968	0	1033	41	0
13	2R	968	0	1033	44	0
14	1S	873	0	927	29	0
14	2S	870	0	923	54	0
15	1T	1091	0	1151	33	0
15	2T	1083	0	1136	44	0
16	1U	959	0	1019	30	0
16	2U	959	0	1019	41	0
17	1V	771	0	830	21	0
17	2V	771	0	830	34	0
18	1W	886	0	940	24	0
18	2W	886	0	940	28	0
19	1X	750	0	814	31	0
19	2X	750	0	814	28	0
20	1Y	806	0	881	23	0
20	2Y	806	0	881	40	0
21	1Z	1240	0	1240	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1271	0	1273	82	0
22	10	653	0	674	23	0
22	20	653	0	674	30	0
23	11	755	0	826	27	0
23	21	755	0	826	37	0
24	12	588	0	643	20	0
24	22	588	0	643	32	0
25	13	469	0	518	10	0
25	23	464	0	514	20	0
26	14	552	0	533	24	0
26	24	532	0	503	50	0
27	15	455	0	465	13	0
27	25	455	0	464	8	0
28	16	453	0	473	15	0
28	26	449	0	469	20	0
29	17	418	0	467	20	0
29	27	418	0	467	21	0
30	18	517	0	582	19	0
30	28	517	0	582	23	0
31	19	307	0	335	13	0
31	29	307	0	335	13	0
32	1a	32246	0	16294	640	1
32	2a	32327	0	16338	822	0
33	1b	1846	0	1867	105	0
33	2b	1825	0	1828	105	0
34	1c	1548	0	1535	73	0
34	2c	1542	0	1517	82	0
35	1d	1655	0	1672	67	0
35	2d	1674	0	1714	90	0
36	1e	1129	0	1185	64	0
36	2e	1133	0	1191	60	0
37	1f	810	0	804	49	0
37	2f	816	0	808	37	0
38	1g	1231	0	1238	55	0
38	2g	1235	0	1249	84	0
39	1h	1088	0	1126	36	0
39	2h	1088	0	1126	55	0
40	1i	983	0	986	38	0
40	2i	978	0	965	53	0
41	1j	709	0	650	28	0
41	2j	714	0	672	47	0
42	1k	829	0	825	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	836	43	0
43	1l	932	0	981	31	0
43	2l	932	0	979	30	0
44	1m	958	0	1002	49	0
44	2m	950	0	988	78	0
45	1n	492	0	529	17	0
45	2n	492	0	529	46	0
46	1o	728	0	760	22	0
46	2o	728	0	760	29	0
47	1p	681	0	697	26	0
47	2p	677	0	686	37	0
48	1q	823	0	891	43	0
48	2q	823	0	891	38	0
49	1r	555	0	618	28	0
49	2r	555	0	618	38	0
50	1s	652	0	662	34	0
50	2s	646	0	644	53	0
51	1t	728	0	798	42	0
51	2t	727	0	796	33	0
52	1u	199	0	208	5	0
52	2u	199	0	208	8	0
53	1v	277	0	140	2	0
53	2v	277	0	140	6	0
54	1w	1603	0	828	53	0
54	2w	1555	0	797	38	0
55	1x	1656	0	848	20	0
55	2x	1656	0	849	23	0
56	1y	1585	0	803	62	0
56	2y	1565	0	794	56	0
57	10	8	0	0	0	0
57	11	5	0	0	0	0
57	12	2	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	9	0	0	0	0
57	16	2	0	0	0	0
57	17	7	0	0	0	0
57	18	5	0	0	0	0
57	1A	1099	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1F	12	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	5	0	0	0	0
57	1P	3	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	4	0	0	0	0
57	1S	3	0	0	0	0
57	1T	4	0	0	0	0
57	1U	10	0	0	0	0
57	1V	10	0	0	0	0
57	1W	8	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	4	0	0	0	0
57	1a	213	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1k	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	2	0	0	0	0
57	1n	3	0	0	0	0
57	1t	1	0	0	0	0
57	1v	2	0	0	0	0
57	1w	8	0	0	0	0
57	1x	14	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	1	0	0	0	0
57	25	5	0	0	0	0
57	27	2	0	0	0	0
57	28	4	0	0	0	0
57	29	1	0	0	0	0
57	2A	883	0	0	0	0
57	2B	20	0	0	0	0
57	2D	8	0	0	0	0
57	2E	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	3	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	3	0	0	0	0
57	2T	3	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	3	0	0	0	0
57	2X	2	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	234	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	2	0	0	0	0
57	2k	1	0	0	0	0
57	2l	4	0	0	0	0
57	2m	1	0	0	0	0
57	2p	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	3	0	0	0	0
57	2w	9	0	0	0	0
57	2x	6	0	0	0	0
57	2y	6	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	74	0	0	1	0
59	2A	74	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	10	0	0	1	0
62	11	14	0	0	0	0
62	12	2	0	0	0	0
62	13	3	0	0	1	0
62	15	6	0	0	1	0
62	16	4	0	0	0	0
62	17	9	0	0	3	0
62	18	10	0	0	0	0
62	1A	1997	0	0	151	0
62	1B	63	0	0	3	0
62	1D	30	0	0	1	0
62	1E	31	0	0	4	0
62	1F	16	0	0	1	0
62	1G	5	0	0	1	0
62	1H	2	0	0	1	0
62	1I	1	0	0	0	0
62	1N	8	0	0	1	0
62	1O	5	0	0	0	0
62	1P	24	0	0	6	0
62	1Q	8	0	0	0	0
62	1R	11	0	0	0	0
62	1S	5	0	0	0	0
62	1T	9	0	0	0	0
62	1U	9	0	0	0	0
62	1V	9	0	0	0	0
62	1W	8	0	0	1	0
62	1X	5	0	0	0	0
62	1Y	4	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	379	0	0	30	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	13	0	0	1	0
62	1x	15	0	0	1	0
62	1y	2	0	0	0	0
62	20	3	0	0	0	0
62	21	12	0	0	1	0
62	23	2	0	0	0	0
62	25	2	0	0	0	0
62	27	4	0	0	0	0
62	28	3	0	0	1	0
62	29	1	0	0	0	0
62	2A	1156	0	0	135	0
62	2B	24	0	0	4	0
62	2D	22	0	0	3	0
62	2E	14	0	0	6	0
62	2F	12	0	0	0	0
62	2I	3	0	0	0	0
62	2N	1	0	0	0	0
62	2O	3	0	0	0	0
62	2P	12	0	0	3	0
62	2Q	1	0	0	0	0
62	2R	6	0	0	0	0
62	2T	5	0	0	0	0
62	2U	3	0	0	1	0
62	2V	1	0	0	0	0
62	2W	1	0	0	0	0
62	2X	3	0	0	2	0
62	2Z	1	0	0	0	0
62	2a	267	0	0	22	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2f	1	0	0	0	0
62	2j	3	0	0	1	0
62	2l	6	0	0	1	0
62	2o	1	0	0	0	0
62	2p	2	0	0	0	0
62	2t	2	0	0	0	0
62	2v	2	0	0	0	0
62	2w	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2x	6	0	0	0	0
62	2y	8	0	0	0	0
All	All	300377	0	196733	7374	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7374 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.15	1.37
1:1A:1082:U:N3	1:1A:1086:A:N6	1.94	1.13
54:1w:27:G:H1	54:1w:43:C:N4	1.50	1.08
54:1w:3:C:H42	54:1w:70:G:H1	1.05	1.02
32:2a:664:G:H22	32:2a:741:G:H1	1.07	1.01

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:357:G:O2'	8:2I:89:TYR:O[2_655]	2.19	0.01

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%)	253 (93%)	20 (7%)	0	100	100
3	2D	273/276 (99%)	243 (89%)	27 (10%)	3 (1%)	11	12
4	1E	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	12	14
4	2E	202/206 (98%)	178 (88%)	18 (9%)	6 (3%)	3	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	192 (96%)	7 (4%)	2 (1%)	12	14
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	6	4
6	1G	179/182 (98%)	151 (84%)	24 (13%)	4 (2%)	5	3
6	2G	179/182 (98%)	148 (83%)	25 (14%)	6 (3%)	3	1
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	27
7	2H	172/180 (96%)	147 (86%)	23 (13%)	2 (1%)	10	11
8	1I	144/148 (97%)	112 (78%)	28 (19%)	4 (3%)	4	2
8	2I	144/148 (97%)	110 (76%)	27 (19%)	7 (5%)	1	0
9	1N	138/140 (99%)	125 (91%)	10 (7%)	3 (2%)	5	3
9	2N	138/140 (99%)	123 (89%)	12 (9%)	3 (2%)	5	3
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	20
11	1P	147/150 (98%)	123 (84%)	18 (12%)	6 (4%)	2	1
11	2P	147/150 (98%)	121 (82%)	20 (14%)	6 (4%)	2	1
12	1Q	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	8
12	2Q	139/141 (99%)	120 (86%)	17 (12%)	2 (1%)	9	8
13	1R	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	14	17
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	17
14	2S	108/112 (96%)	90 (83%)	12 (11%)	6 (6%)	1	0
15	1T	129/146 (88%)	117 (91%)	10 (8%)	2 (2%)	7	7
15	2T	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	16	20
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	105 (92%)	8 (7%)	1 (1%)	14	17
17	1V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	2
17	2V	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	3	2
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	103 (94%)	6 (6%)	1 (1%)	14	17
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	5	3
19	2X	93/96 (97%)	82 (88%)	10 (11%)	1 (1%)	11	12
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	14
21	1Z	148/206 (72%)	125 (84%)	18 (12%)	5 (3%)	3	1
21	2Z	156/206 (76%)	122 (78%)	27 (17%)	7 (4%)	2	0
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	72 (89%)	7 (9%)	2 (2%)	4	3
23	11	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	12
23	21	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	11	12
24	12	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
24	22	68/72 (94%)	60 (88%)	8 (12%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	3	1
26	14	67/71 (94%)	48 (72%)	15 (22%)	4 (6%)	1	0
26	24	67/71 (94%)	48 (72%)	12 (18%)	7 (10%)	0	0
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	45 (88%)	5 (10%)	1 (2%)	6	4
29	17	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	7
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	29	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	3	2
33	1b	229/256 (90%)	174 (76%)	36 (16%)	19 (8%)	0	0
33	2b	229/256 (90%)	166 (72%)	45 (20%)	18 (8%)	1	0
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24	32
34	2c	204/239 (85%)	167 (82%)	31 (15%)	6 (3%)	3	2
35	1d	206/209 (99%)	178 (86%)	24 (12%)	4 (2%)	6	5
35	2d	206/209 (99%)	174 (84%)	25 (12%)	7 (3%)	3	1
36	1e	146/162 (90%)	132 (90%)	12 (8%)	2 (1%)	9	8
36	2e	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	87 (89%)	9 (9%)	2 (2%)	6	4
38	1g	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	4	2
38	2g	153/156 (98%)	127 (83%)	17 (11%)	9 (6%)	1	0
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	109 (81%)	24 (18%)	2 (2%)	8	7
40	1i	125/128 (98%)	100 (80%)	24 (19%)	1 (1%)	16	20
40	2i	125/128 (98%)	100 (80%)	23 (18%)	2 (2%)	7	7
41	1j	95/105 (90%)	77 (81%)	14 (15%)	4 (4%)	2	0
41	2j	94/105 (90%)	78 (83%)	7 (7%)	9 (10%)	0	0
42	1k	112/129 (87%)	99 (88%)	9 (8%)	4 (4%)	2	1
42	2k	112/129 (87%)	93 (83%)	12 (11%)	7 (6%)	1	0
43	1l	119/132 (90%)	104 (87%)	15 (13%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	6 (5%)	2 (2%)	7	6
44	1m	121/126 (96%)	106 (88%)	15 (12%)	0	100	100
44	2m	120/126 (95%)	90 (75%)	26 (22%)	4 (3%)	3	1
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	6
46	1o	86/89 (97%)	74 (86%)	7 (8%)	5 (6%)	1	0
46	2o	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	10	11
47	1p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
47	2p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	9	9
48	1q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	12	14
48	2q	97/105 (92%)	79 (81%)	14 (14%)	4 (4%)	2	1
49	1r	66/88 (75%)	55 (83%)	7 (11%)	4 (6%)	1	0
49	2r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	7
50	1s	81/93 (87%)	68 (84%)	10 (12%)	3 (4%)	2	1
50	2s	81/93 (87%)	62 (76%)	14 (17%)	5 (6%)	1	0
51	1t	94/106 (89%)	79 (84%)	9 (10%)	6 (6%)	1	0
51	2t	94/106 (89%)	73 (78%)	16 (17%)	5 (5%)	1	0
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0	0
All	All	11370/12128 (94%)	9876 (87%)	1219 (11%)	275 (2%)	4	3

5 of 275 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1I	107	VAL
11	1P	38	GLN
11	1P	39	LYS
20	1Y	78	ALA
21	1Z	53	ILE

5.3.2 Protein sidechains [i](#)

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%)	196 (91%)	19 (9%)	9	10
3	2D	215/218 (99%)	194 (90%)	21 (10%)	7	7
4	1E	164/166 (99%)	142 (87%)	22 (13%)	4	3
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	5
5	1F	160/166 (96%)	134 (84%)	26 (16%)	2	1
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3	3
6	1G	143/156 (92%)	124 (87%)	19 (13%)	4	3
6	2G	143/156 (92%)	117 (82%)	26 (18%)	2	1
7	1H	144/148 (97%)	126 (88%)	18 (12%)	4	4
7	2H	144/148 (97%)	115 (80%)	29 (20%)	1	0
8	1I	113/124 (91%)	84 (74%)	29 (26%)	0	0
8	2I	105/124 (85%)	74 (70%)	31 (30%)	0	0
9	1N	118/119 (99%)	103 (87%)	15 (13%)	4	4
9	2N	118/119 (99%)	92 (78%)	26 (22%)	1	0
10	1O	100/100 (100%)	88 (88%)	12 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	2O	100/100 (100%)	87 (87%)	13 (13%)	4	3
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9	11
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	6
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7	7
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	4	3
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	7
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	5
14	1S	86/88 (98%)	72 (84%)	14 (16%)	2	1
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	3
15	1T	115/127 (91%)	100 (87%)	15 (13%)	4	3
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	8
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	8
16	2U	93/94 (99%)	81 (87%)	12 (13%)	4	3
17	1V	80/82 (98%)	69 (86%)	11 (14%)	3	3
17	2V	80/82 (98%)	65 (81%)	15 (19%)	1	0
18	1W	90/92 (98%)	77 (86%)	13 (14%)	3	2
18	2W	90/92 (98%)	79 (88%)	11 (12%)	5	4
19	1X	77/78 (99%)	71 (92%)	6 (8%)	11	14
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11	14
20	1Y	85/91 (93%)	72 (85%)	13 (15%)	3	2
20	2Y	85/91 (93%)	69 (81%)	16 (19%)	1	0
21	1Z	135/179 (75%)	111 (82%)	24 (18%)	2	1
21	2Z	137/179 (76%)	105 (77%)	32 (23%)	1	0
22	10	65/67 (97%)	61 (94%)	4 (6%)	16	23
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	23
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	16
23	21	80/83 (96%)	64 (80%)	16 (20%)	1	0
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	9
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	6
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	3
25	23	50/52 (96%)	43 (86%)	7 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	1
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	0
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	41
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	26
28	16	51/52 (98%)	43 (84%)	8 (16%)	2	1
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	4
29	17	41/42 (98%)	34 (83%)	7 (17%)	2	1
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	17
30	18	54/55 (98%)	48 (89%)	6 (11%)	6	5
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	5
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	52
31	29	34/34 (100%)	28 (82%)	6 (18%)	2	1
33	1b	192/220 (87%)	156 (81%)	36 (19%)	1	0
33	2b	187/220 (85%)	152 (81%)	35 (19%)	1	0
34	1c	142/188 (76%)	123 (87%)	19 (13%)	4	3
34	2c	140/188 (74%)	115 (82%)	25 (18%)	2	1
35	1d	169/181 (93%)	143 (85%)	26 (15%)	2	2
35	2d	173/181 (96%)	139 (80%)	34 (20%)	1	0
36	1e	113/123 (92%)	95 (84%)	18 (16%)	2	1
36	2e	114/123 (93%)	92 (81%)	22 (19%)	1	0
37	1f	84/90 (93%)	72 (86%)	12 (14%)	3	2
37	2f	85/90 (94%)	66 (78%)	19 (22%)	1	0
38	1g	119/127 (94%)	98 (82%)	21 (18%)	2	1
38	2g	120/127 (94%)	100 (83%)	20 (17%)	2	1
39	1h	114/119 (96%)	102 (90%)	12 (10%)	6	6
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4	3
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	3
40	2i	89/99 (90%)	73 (82%)	16 (18%)	2	1
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	2
41	2j	69/92 (75%)	54 (78%)	15 (22%)	1	0
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	2k	83/99 (84%)	62 (75%)	21 (25%)	0	0
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	17
43	2l	96/108 (89%)	81 (84%)	15 (16%)	2	1
44	1m	93/101 (92%)	80 (86%)	13 (14%)	3	3
44	2m	92/101 (91%)	68 (74%)	24 (26%)	0	0
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2	1
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	13
46	1o	78/80 (98%)	68 (87%)	10 (13%)	4	3
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	5
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	2
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	3
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	8
48	2q	94/97 (97%)	82 (87%)	12 (13%)	4	3
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	6
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	11
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	3
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	1
51	1t	70/82 (85%)	60 (86%)	10 (14%)	3	2
51	2t	70/82 (85%)	60 (86%)	10 (14%)	3	2
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	27
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	27
All	All	9303/10064 (92%)	7961 (86%)	1342 (14%)	3	2

5 of 1342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	2Z	54	HIS
37	2f	70	ASP
22	20	40	GLN
21	2Z	42	VAL
33	2b	142	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
23	21	56	GLN
40	2i	3	GLN
25	23	32	GLN
34	2c	181	ASN
42	2k	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	532 (18%)	36 (1%)
1	2A	2791/2915 (95%)	550 (19%)	26 (0%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	35 (29%)	0
32	1a	1497/1521 (98%)	293 (19%)	0
32	2a	1501/1521 (98%)	359 (23%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	25 (35%)	0
54	2w	69/76 (90%)	27 (39%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	13 (17%)	0
56	1y	72/76 (94%)	35 (48%)	0
56	2y	70/76 (92%)	28 (40%)	0
All	All	9346/9620 (97%)	1927 (20%)	62 (0%)

5 of 1927 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	21	A
1	1A	32	C
1	1A	33	U

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2183	C
1	2A	1653	G
1	1A	2756	U
1	2A	1530	C
1	2A	2126	A

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

88 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	5MC	1A	1942	1,57	19,22,23	1.69	3 (15%)	26,32,35	1.40	3 (11%)
54	PSU	2w	32	54	18,21,22	1.44	2 (11%)	21,30,33	1.82	4 (19%)
54	PSU	2w	55	54	18,21,22	1.42	3 (16%)	21,30,33	2.07	6 (28%)
56	5MU	1y	54	56	19,22,23	1.57	4 (21%)	27,32,35	1.97	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.81	3 (15%)	26,32,35	1.20	4 (15%)
54	5MU	1w	54	54	19,22,23	1.31	4 (21%)	27,32,35	2.29	6 (22%)
54	G7M	2w	46	54	23,26,27	1.56	4 (17%)	34,39,42	1.88	5 (14%)
1	OMG	1A	2251	1,57,55	23,26,27	1.28	3 (13%)	32,38,41	2.10	6 (18%)
56	G7M	1y	46	56	23,26,27	1.71	6 (26%)	34,39,42	2.20	9 (26%)
55	PSU	1x	55	55	18,21,22	1.41	2 (11%)	21,30,33	2.00	3 (14%)
55	31H	2x	76	57,58,55	31,34,35	1.34	4 (12%)	35,47,50	2.02	11 (31%)
54	G7M	1w	46	54	23,26,27	1.57	3 (13%)	34,39,42	1.79	4 (11%)
54	4SU	1w	8	54	18,21,22	1.90	4 (22%)	25,30,33	2.66	7 (28%)
43	0TD	2l	92	43	8,9,10	5.25	2 (25%)	6,11,13	4.63	1 (16%)
56	PSU	1y	32	56	18,21,22	1.42	2 (11%)	21,30,33	2.03	4 (19%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.69	4 (19%)
32	G7M	2a	527	32	23,26,27	1.41	5 (21%)	34,39,42	1.61	4 (11%)
56	PSU	2y	32	56	18,21,22	1.40	3 (16%)	21,30,33	1.99	4 (19%)
54	PSU	1w	39	54	18,21,22	1.18	2 (11%)	21,30,33	2.67	6 (28%)
32	5MC	1a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.48	3 (11%)
56	MIA	2y	37	56	21,24,32	1.72	3 (14%)	30,35,47	1.87	9 (30%)
55	5MU	1x	54	57,55	19,22,23	1.36	3 (15%)	27,32,35	1.75	6 (22%)
1	5MU	1A	1939	1	19,22,23	1.53	5 (26%)	27,32,35	2.75	8 (29%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.52	5 (23%)
56	PSU	2y	55	56	18,21,22	1.36	1 (5%)	21,30,33	2.01	5 (23%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	2.03	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1962	1,57	19,22,23	1.81	3 (15%)	26,32,35	1.52	6 (23%)
56	4SU	2y	8	56	18,21,22	1.74	4 (22%)	25,30,33	2.62	6 (24%)
32	UR3	2a	1498	32	19,22,23	1.28	1 (5%)	26,32,35	1.82	5 (19%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.18	2 (8%)
1	OMC	2A	1920	1	19,22,23	0.73	0	25,31,34	0.97	1 (4%)
32	PSU	2a	516	32	18,21,22	1.38	2 (11%)	21,30,33	2.06	6 (28%)
1	OMU	1A	2552	1,57	19,22,23	1.30	4 (21%)	25,31,34	1.94	6 (24%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	1.94	9 (27%)
32	5MC	1a	967	32	19,22,23	1.83	3 (15%)	26,32,35	1.27	3 (11%)
1	5MU	2A	1939	1,57	19,22,23	1.64	5 (26%)	27,32,35	2.78	8 (29%)
1	5MC	2A	1942	1	19,22,23	1.77	2 (10%)	26,32,35	1.46	4 (15%)
1	OMG	2A	2251	1,57,55	23,26,27	1.26	4 (17%)	32,38,41	1.97	7 (21%)
32	5MC	2a	1407	32	19,22,23	1.85	3 (15%)	26,32,35	1.20	3 (11%)
55	4SU	1x	8	55	18,21,22	2.34	6 (33%)	25,30,33	1.97	6 (24%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	1.95	8 (24%)
55	4SU	2x	8	55	18,21,22	2.22	6 (33%)	25,30,33	1.52	6 (24%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.72	10 (26%)
54	5MU	2w	54	54	19,22,23	1.50	6 (31%)	27,32,35	1.89	7 (25%)
32	5MC	2a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.10	3 (11%)
54	PSU	1w	55	54	18,21,22	1.55	3 (16%)	21,30,33	2.39	5 (23%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	21,30,33	2.15	6 (28%)
32	G7M	1a	527	32	23,26,27	1.66	3 (13%)	34,39,42	1.74	4 (11%)
32	2MG	1a	1207	32	23,26,27	1.33	3 (13%)	33,38,41	2.42	10 (30%)
32	PSU	1a	516	32,57	18,21,22	1.38	2 (11%)	21,30,33	2.07	5 (23%)
56	G7M	2y	46	56	23,26,27	1.66	5 (21%)	34,39,42	1.92	4 (11%)
1	5MU	1A	1915	1	19,22,23	1.41	4 (21%)	27,32,35	2.42	6 (22%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	21,30,33	1.91	4 (19%)
54	4SU	2w	8	54	18,21,22	1.82	5 (27%)	25,30,33	2.51	5 (20%)
55	5MU	2x	54	55	19,22,23	1.48	5 (26%)	27,32,35	2.44	8 (29%)
56	PSU	2y	39	56	18,21,22	1.35	2 (11%)	21,30,33	2.09	4 (19%)
32	2MG	2a	1207	32,57	23,26,27	1.28	3 (13%)	33,38,41	2.09	9 (27%)
1	2MA	2A	2503	1,57	22,25,26	1.54	6 (27%)	32,37,40	2.34	7 (21%)
55	31H	1x	76	57,55	31,34,35	1.19	3 (9%)	35,47,50	2.41	14 (40%)
55	5MC	2x	32	40,55	19,22,23	1.36	2 (10%)	26,32,35	1.38	4 (15%)
32	5MC	2a	1400	32	19,22,23	1.42	2 (10%)	26,32,35	1.05	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	4SU	1y	8	56	18,21,22	1.62	3 (16%)	25,30,33	2.30	5 (20%)
32	UR3	1a	1498	32	19,22,23	1.27	2 (10%)	26,32,35	2.27	6 (23%)
55	5MC	1x	32	55	19,22,23	1.37	3 (15%)	26,32,35	1.38	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.15	10 (30%)
1	5MU	2A	1915	1,57	19,22,23	1.47	6 (31%)	27,32,35	2.20	8 (29%)
32	M2G	2a	966	32	24,27,28	1.36	4 (16%)	33,40,43	1.85	6 (18%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	25,32,35	1.39	5 (20%)
54	F3N	1w	76	1,54	33,36,37	1.69	4 (12%)	41,51,54	1.62	8 (19%)
1	OMU	2A	2552	1,57	19,22,23	1.11	3 (15%)	25,31,34	1.83	5 (20%)
1	PSU	2A	2605	1	18,21,22	1.44	3 (16%)	21,30,33	2.00	4 (19%)
56	5MU	2y	54	56	19,22,23	1.49	4 (21%)	27,32,35	1.57	5 (18%)
32	5MC	1a	1407	32	19,22,23	1.91	3 (15%)	26,32,35	1.21	4 (15%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.06	9 (27%)
54	MIA	2w	37	54	24,27,32	2.10	4 (16%)	32,39,47	2.45	11 (34%)
54	PSU	1w	32	57,54	18,21,22	1.27	1 (5%)	21,30,33	1.61	4 (19%)
1	2MA	1A	2503	1,57	22,25,26	1.28	4 (18%)	32,37,40	2.66	11 (34%)
32	5MC	1a	1400	32	19,22,23	1.39	2 (10%)	26,32,35	1.37	3 (11%)
56	MIA	1y	37	56	21,24,32	1.68	3 (14%)	30,35,47	2.16	6 (20%)
1	PSU	1A	1911	1	18,21,22	1.54	3 (16%)	21,30,33	2.28	4 (19%)
32	4OC	1a	1402	32	20,23,24	0.84	1 (5%)	25,32,35	1.06	1 (4%)
56	PSU	1y	55	56	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
1	5MC	2A	1962	1,57	19,22,23	1.74	3 (15%)	26,32,35	1.33	3 (11%)
54	F3N	2w	76	1,54	33,36,37	1.46	5 (15%)	41,51,54	1.83	9 (21%)
1	PSU	2A	1917	1	18,21,22	1.50	3 (16%)	21,30,33	2.26	5 (23%)
43	0TD	1l	92	43	8,9,10	3.95	1 (12%)	6,11,13	9.18	3 (50%)
1	PSU	1A	2605	1,57	18,21,22	1.44	3 (16%)	21,30,33	2.06	4 (19%)
56	PSU	1y	39	56	18,21,22	1.46	3 (16%)	21,30,33	2.06	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1942	1,57	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	0/7/25/26	0/3/3/3
1	OMG	1A	2251	1,57,55	-	0/9/27/28	0/3/3/3
56	G7M	1y	46	56	-	2/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	31H	2x	76	57,58,55	-	5/22/40/41	0/3/3/3
54	G7M	1w	46	54	-	0/7/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
56	PSU	2y	32	56	-	2/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	2/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	3/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	PSU	2a	516	32	-	2/7/25/26	0/2/2/2
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,57,55	-	0/9/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	1/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3
54	5MU	2w	54	54	-	1/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	2/7/25/26	0/3/3/3
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	4/7/25/26	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,57	-	2/9/27/28	0/3/3/3
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
55	31H	1x	76	57,55	-	4/22/40/41	0/3/3/3
55	5MC	2x	32	40,55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	2A	1915	1,57	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
54	F3N	1w	76	1,54	-	0/19/37/38	0/4/4/4
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	1/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	1,54	-	1/19/37/38	0/4/4/4
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2

The worst 5 of 266 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-11.57	1.70	1.82
43	1l	92	0TD	CB-SB	-10.64	1.71	1.82
43	2l	92	0TD	CB-CA	8.77	1.57	1.54
32	1a	1407	5MC	C5-C4	7.52	1.49	1.44
32	1a	967	5MC	C5-C4	7.04	1.49	1.44

The worst 5 of 490 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	21.91	141.76	102.36
43	2l	92	0TD	CSB-SB-CB	-11.05	82.51	102.36
54	1w	37	MIA	C12-C13-C14	-9.37	110.19	127.01
54	2w	37	MIA	C5-C4-N3	-8.33	118.40	127.18
54	1w	39	PSU	N1-C2-N3	8.04	123.66	115.17

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1942	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	55	PSU	1	0
56	1y	54	5MU	2	0
1	1A	2251	OMG	1	0
56	1y	46	G7M	1	0
55	1x	55	PSU	1	0
55	2x	76	31H	3	0
54	1w	46	G7M	1	0
54	1w	8	4SU	1	0
54	1w	39	PSU	2	0
56	2y	37	MIA	1	0
55	1x	54	5MU	1	0
56	2y	55	PSU	5	0
32	1a	966	M2G	2	0
56	2y	8	4SU	3	0
1	1A	2552	OMU	2	0
32	1a	1518	MA6	2	0
32	1a	967	5MC	2	0
1	2A	2251	OMG	1	0
32	1a	1519	MA6	2	0
55	2x	8	4SU	1	0
54	1w	37	MIA	1	0
54	2w	54	5MU	3	0
32	2a	967	5MC	4	0
54	1w	55	PSU	1	0
1	1A	1915	5MU	1	0
55	2x	55	PSU	2	0
54	2w	8	4SU	2	0
32	2a	1207	2MG	2	0
1	2A	2503	2MA	1	0
55	1x	76	31H	1	0
32	2a	1400	5MC	4	0
56	1y	8	4SU	2	0
55	1x	32	5MC	1	0
32	2a	1519	MA6	3	0
1	2A	1915	5MU	1	0
32	2a	966	M2G	2	0
32	2a	1402	4OC	2	0
1	2A	2552	OMU	1	0
32	2a	1518	MA6	1	0
54	2w	37	MIA	2	0
1	1A	2503	2MA	1	0
56	1y	37	MIA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1402	4OC	2	0
56	1y	55	PSU	1	0
54	2w	76	F3N	2	0
56	1y	39	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2812 ligands modelled in this entry, 2808 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	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
59	A1C9N	1A	4101	-	77,79,79	3.00	12 (15%)	107,118,118	2.38	29 (27%)
59	A1C9N	2A	3885	-	77,79,79	1.97	11 (14%)	107,118,118	2.17	28 (26%)
61	SF4	2d	303	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
61	SF4	1d	302	35	-	-	0/6/5/5
59	A1C9N	1A	4101	-	-	14/82/141/141	1/6/6/6
59	A1C9N	2A	3885	-	-	14/82/141/141	1/6/6/6
61	SF4	2d	303	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)
59	1A	4101	A1C9N	B01-OCR	19.21	1.63	1.39
59	1A	4101	A1C9N	B01-OCT	12.44	1.54	1.35
59	2A	3885	A1C9N	B01-OCT	-8.76	1.22	1.35
59	2A	3885	A1C9N	CCQ-CCO	-6.37	1.41	1.50
59	1A	4101	A1C9N	CAU-CAC	-5.50	1.39	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	4101	A1C9N	B01-OCR-CCQ	-16.14	97.70	110.48
59	2A	3885	A1C9N	B01-OCR-CCQ	-12.64	100.47	110.48
59	1A	4101	A1C9N	OBY-CBZ-NCA	5.88	120.59	111.01
59	2A	3885	A1C9N	OBY-CBZ-NCA	5.40	119.81	111.01
59	2A	3885	A1C9N	CAE-CAB-CAG	-5.36	107.83	115.23

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4101	A1C9N	CBI-CBJ-OCU-CCV
59	1A	4101	A1C9N	CBK-CBJ-OCU-CCV
59	1A	4101	A1C9N	CBX-CBJ-OCU-CCV
59	1A	4101	A1C9N	CBP-CBQ-NBS-CBU
59	2A	3885	A1C9N	CBI-CBJ-OCU-CCV

All (2) ring outliers are listed below:

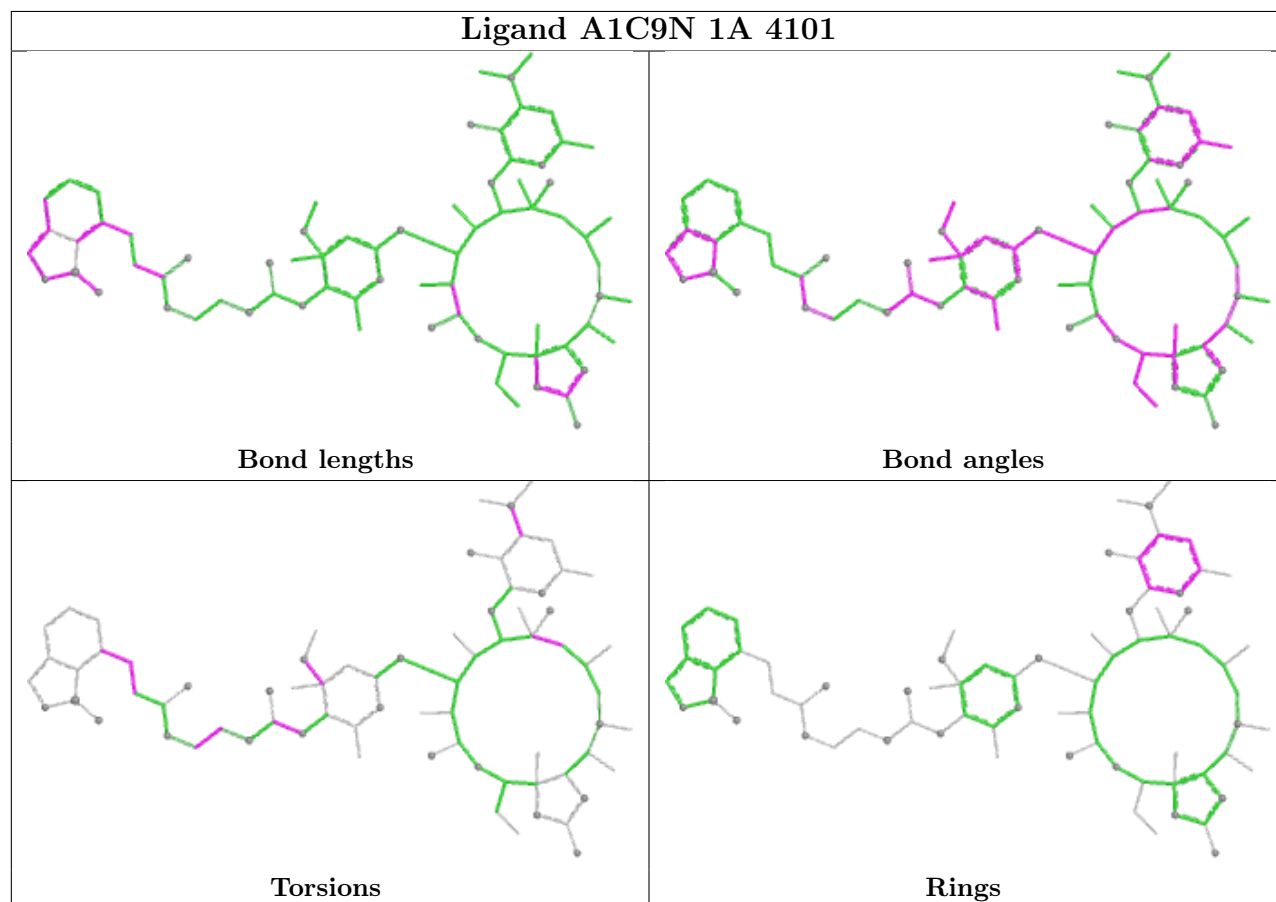
Mol	Chain	Res	Type	Atoms
59	2A	3885	A1C9N	CBL-CBM-CBO-CBP-CBQ-OBN
59	1A	4101	A1C9N	CBL-CBM-CBO-CBP-CBQ-OBN

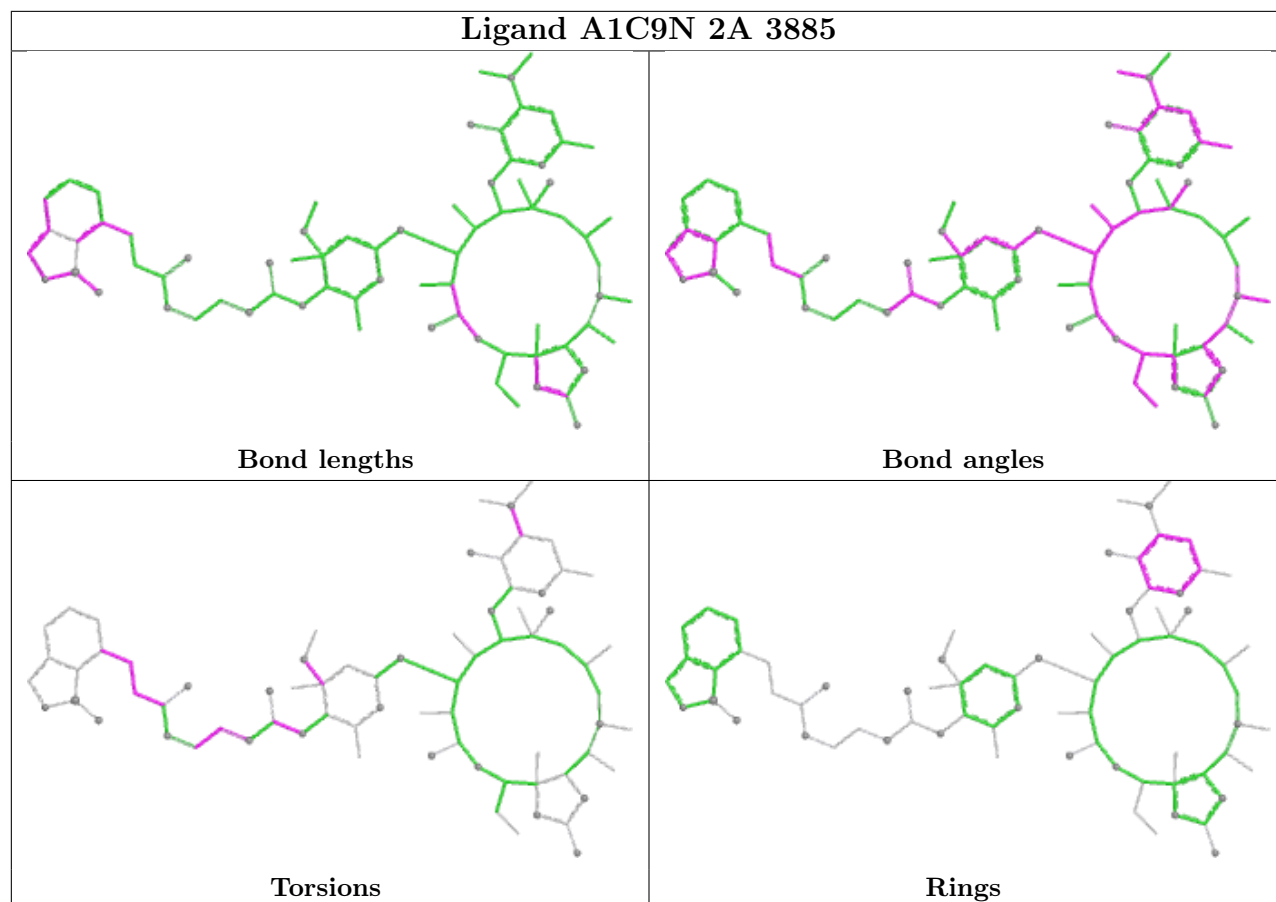
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1A	4101	A1C9N	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.40	115 (4%) 42 41	14, 32, 79, 89	0
1	2A	2789/2915 (95%)	0.14	99 (3%) 47 47	28, 51, 76, 89	0
2	1B	120/121 (99%)	-0.41	0 100 100	25, 41, 53, 76	0
2	2B	120/121 (99%)	0.82	7 (5%) 29 26	52, 65, 73, 75	0
3	1D	275/276 (99%)	-0.00	1 (0%) 88 89	16, 32, 46, 60	0
3	2D	275/276 (99%)	0.46	5 (1%) 67 69	24, 45, 54, 69	0
4	1E	204/206 (99%)	0.19	1 (0%) 87 88	15, 38, 52, 60	0
4	2E	204/206 (99%)	0.66	9 (4%) 39 38	29, 51, 61, 66	0
5	1F	203/210 (96%)	0.21	3 (1%) 72 74	14, 41, 61, 71	0
5	2F	203/210 (96%)	0.90	11 (5%) 31 29	28, 58, 66, 71	0
6	1G	181/182 (99%)	0.67	2 (1%) 78 79	34, 50, 62, 75	0
6	2G	181/182 (99%)	1.66	54 (29%) 1 1	56, 65, 71, 75	0
7	1H	174/180 (96%)	0.60	5 (2%) 53 55	32, 49, 57, 60	0
7	2H	174/180 (96%)	1.32	25 (14%) 6 4	57, 68, 74, 78	0
8	1I	146/148 (98%)	0.82	6 (4%) 41 41	37, 59, 68, 71	0
8	2I	146/148 (98%)	1.47	34 (23%) 2 1	51, 64, 71, 75	0
9	1N	140/140 (100%)	0.12	1 (0%) 84 86	24, 36, 52, 65	0
9	2N	140/140 (100%)	1.06	12 (8%) 16 14	37, 56, 64, 68	0
10	1O	122/122 (100%)	0.10	0 100 100	24, 36, 50, 56	0
10	2O	122/122 (100%)	0.53	2 (1%) 70 73	33, 49, 58, 64	0
11	1P	149/150 (99%)	0.45	7 (4%) 36 35	15, 43, 61, 67	0
11	2P	149/150 (99%)	0.91	9 (6%) 27 24	35, 56, 69, 76	0
12	1Q	141/141 (100%)	0.10	1 (0%) 84 86	22, 35, 47, 58	0
12	2Q	141/141 (100%)	1.02	8 (5%) 29 26	37, 56, 63, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.01	0 100 100	19, 31, 42, 48	0
13	2R	118/118 (100%)	0.56	1 (0%) 82 83	32, 44, 56, 64	0
14	1S	110/112 (98%)	0.30	0 100 100	31, 42, 52, 55	0
14	2S	110/112 (98%)	1.49	29 (26%) 1 1	51, 60, 67, 70	0
15	1T	131/146 (89%)	0.44	6 (4%) 37 36	25, 42, 62, 72	0
15	2T	131/146 (89%)	0.65	3 (2%) 61 63	41, 51, 63, 72	0
16	1U	116/118 (98%)	-0.07	0 100 100	20, 30, 42, 48	0
16	2U	116/118 (98%)	0.81	5 (4%) 40 39	38, 56, 64, 72	0
17	1V	101/101 (100%)	-0.01	1 (0%) 79 80	17, 37, 51, 55	0
17	2V	101/101 (100%)	0.87	1 (0%) 79 80	40, 61, 66, 69	0
18	1W	112/113 (99%)	0.12	1 (0%) 81 82	21, 31, 46, 63	0
18	2W	112/113 (99%)	0.77	5 (4%) 38 37	35, 45, 59, 81	0
19	1X	95/96 (98%)	-0.01	2 (2%) 63 65	19, 32, 53, 69	0
19	2X	95/96 (98%)	0.68	1 (1%) 78 79	39, 51, 61, 67	0
20	1Y	107/110 (97%)	0.52	6 (5%) 30 27	32, 43, 58, 67	0
20	2Y	107/110 (97%)	1.39	21 (19%) 3 2	52, 61, 67, 72	0
21	1Z	154/206 (74%)	0.90	14 (9%) 15 12	34, 54, 67, 75	0
21	2Z	160/206 (77%)	1.51	37 (23%) 2 1	54, 66, 73, 76	0
22	10	83/85 (97%)	0.03	0 100 100	21, 31, 41, 56	0
22	20	83/85 (97%)	1.33	15 (18%) 3 3	38, 53, 60, 62	0
23	11	97/98 (98%)	0.30	1 (1%) 79 80	21, 40, 59, 64	0
23	21	97/98 (98%)	0.68	3 (3%) 51 52	35, 49, 61, 67	0
24	12	70/72 (97%)	0.30	3 (4%) 40 39	28, 43, 52, 68	0
24	22	70/72 (97%)	0.97	4 (5%) 29 26	50, 57, 64, 70	0
25	13	59/60 (98%)	0.09	1 (1%) 69 71	20, 33, 50, 57	0
25	23	59/60 (98%)	1.23	7 (11%) 9 7	46, 57, 69, 72	0
26	14	69/71 (97%)	1.14	13 (18%) 3 2	39, 59, 74, 79	0
26	24	69/71 (97%)	1.77	23 (33%) 1 1	61, 70, 77, 79	0
27	15	59/60 (98%)	-0.03	1 (1%) 69 71	17, 30, 43, 48	0
27	25	59/60 (98%)	0.61	3 (5%) 33 31	28, 45, 57, 62	0
28	16	53/54 (98%)	0.12	0 100 100	26, 36, 46, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.94	5 (9%) 14 11	43, 53, 60, 64	0
29	17	48/49 (97%)	-0.19	1 (2%) 63 65	15, 24, 39, 49	0
29	27	48/49 (97%)	0.36	2 (4%) 40 40	26, 39, 50, 63	0
30	18	64/65 (98%)	-0.01	1 (1%) 70 73	22, 29, 37, 40	0
30	28	64/65 (98%)	0.78	6 (9%) 14 11	37, 48, 54, 57	0
31	19	37/37 (100%)	0.20	1 (2%) 56 57	29, 36, 49, 55	0
31	29	37/37 (100%)	1.40	6 (16%) 4 3	54, 59, 66, 70	0
32	1a	1488/1521 (97%)	0.13	29 (1%) 66 67	29, 53, 76, 88	0
32	2a	1491/1521 (98%)	0.53	48 (3%) 50 51	39, 62, 78, 90	0
33	1b	231/256 (90%)	1.11	28 (12%) 8 7	49, 62, 72, 78	0
33	2b	231/256 (90%)	1.59	69 (29%) 1 1	59, 70, 75, 78	0
34	1c	206/239 (86%)	0.81	11 (5%) 32 30	45, 56, 67, 74	0
34	2c	206/239 (86%)	1.50	45 (21%) 2 2	55, 67, 73, 77	0
35	1d	208/209 (99%)	0.72	5 (2%) 59 62	44, 54, 61, 66	0
35	2d	208/209 (99%)	1.13	21 (10%) 12 10	43, 55, 63, 72	0
36	1e	148/162 (91%)	0.63	5 (3%) 48 48	40, 52, 61, 72	0
36	2e	148/162 (91%)	1.09	12 (8%) 18 16	52, 62, 67, 74	0
37	1f	100/101 (99%)	0.50	1 (1%) 79 80	37, 49, 60, 67	0
37	2f	100/101 (99%)	0.74	3 (3%) 52 53	49, 58, 65, 70	0
38	1g	155/156 (99%)	1.04	19 (12%) 8 7	46, 56, 67, 73	0
38	2g	155/156 (99%)	1.22	27 (17%) 4 3	58, 66, 73, 81	0
39	1h	137/138 (99%)	0.69	3 (2%) 62 64	46, 54, 61, 65	0
39	2h	137/138 (99%)	1.17	13 (9%) 14 11	55, 63, 69, 71	0
40	1i	127/128 (99%)	1.13	12 (9%) 14 11	40, 58, 68, 72	0
40	2i	127/128 (99%)	1.96	53 (41%) 0 0	58, 68, 72, 75	0
41	1j	97/105 (92%)	1.18	13 (13%) 7 6	43, 61, 70, 74	0
41	2j	96/105 (91%)	1.82	36 (37%) 1 0	57, 68, 73, 77	0
42	1k	114/129 (88%)	0.78	7 (6%) 27 24	35, 53, 62, 66	0
42	2k	114/129 (88%)	1.03	9 (7%) 18 16	47, 61, 68, 70	0
43	1l	121/132 (91%)	0.40	4 (3%) 49 50	36, 44, 53, 63	0
43	2l	121/132 (91%)	0.84	6 (4%) 34 32	43, 54, 61, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.01	10 (8%) 18 16	41, 56, 64, 69	0
44	2m	122/126 (96%)	1.77	36 (29%) 1 1	60, 67, 72, 74	0
45	1n	60/61 (98%)	0.77	2 (3%) 49 50	43, 51, 60, 60	0
45	2n	60/61 (98%)	2.09	28 (46%) 0 0	61, 66, 71, 73	0
46	1o	88/89 (98%)	0.81	3 (3%) 48 48	38, 51, 61, 63	0
46	2o	88/89 (98%)	0.98	3 (3%) 48 48	50, 58, 65, 70	0
47	1p	82/88 (93%)	1.17	7 (8%) 16 14	47, 56, 61, 64	0
47	2p	82/88 (93%)	0.92	7 (8%) 16 14	46, 54, 60, 65	0
48	1q	99/105 (94%)	0.99	3 (3%) 52 53	41, 54, 62, 67	0
48	2q	99/105 (94%)	1.04	9 (9%) 15 12	52, 60, 66, 70	0
49	1r	68/88 (77%)	0.49	1 (1%) 72 74	43, 51, 60, 65	0
49	2r	68/88 (77%)	0.88	5 (7%) 20 18	53, 61, 66, 70	0
50	1s	83/93 (89%)	0.81	3 (3%) 46 46	46, 56, 64, 69	0
50	2s	83/93 (89%)	1.71	28 (33%) 1 1	60, 68, 73, 77	0
51	1t	96/106 (90%)	1.08	12 (12%) 8 6	51, 57, 66, 71	0
51	2t	96/106 (90%)	0.98	7 (7%) 21 18	48, 56, 67, 69	0
52	1u	23/27 (85%)	1.26	2 (8%) 16 14	51, 54, 58, 62	0
52	2u	23/27 (85%)	2.55	15 (65%) 0 0	61, 68, 72, 73	0
53	1v	13/24 (54%)	0.57	3 (23%) 2 1	37, 43, 77, 83	0
53	2v	13/24 (54%)	1.47	5 (38%) 1 0	53, 62, 80, 84	0
54	1w	66/76 (86%)	0.97	12 (18%) 3 3	23, 69, 79, 83	0
54	2w	64/76 (84%)	1.16	10 (15%) 5 3	40, 77, 82, 87	0
55	1x	72/77 (93%)	0.22	1 (1%) 73 75	19, 52, 67, 77	0
55	2x	72/77 (93%)	0.58	1 (1%) 73 75	34, 63, 71, 78	0
56	1y	67/76 (88%)	1.28	7 (10%) 11 9	48, 80, 84, 86	0
56	2y	66/76 (86%)	1.53	11 (16%) 4 3	59, 82, 85, 87	0
All	All	20873/21748 (95%)	0.49	1356 (6%) 25 22	14, 53, 73, 90	0

The worst 5 of 1356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	7.4
1	2A	882	G	6.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	6.3
1	2A	883	G	6.1
44	2m	124	PRO	5.8

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
56	G7M	2y	46	24/25	0.49	0.16	67,84,89,96	0
56	PSU	2y	55	20/21	0.59	0.16	75,82,88,102	0
56	G7M	1y	46	24/25	0.60	0.15	76,84,88,94	0
56	4SU	2y	8	20/21	0.65	0.14	73,83,93,99	0
56	5MU	2y	54	21/22	0.67	0.14	66,79,92,103	0
54	G7M	2w	46	24/25	0.68	0.14	69,76,88,94	0
56	MIA	2y	37	22/30	0.69	0.16	68,75,94,99	0
56	4SU	1y	8	20/21	0.70	0.13	79,84,92,103	0
56	MIA	1y	37	22/30	0.71	0.15	63,72,80,94	0
56	PSU	1y	32	20/21	0.71	0.16	70,76,94,100	0
56	5MU	1y	54	21/22	0.73	0.13	66,78,83,96	0
56	PSU	2y	39	20/21	0.74	0.18	72,79,86,94	0
56	PSU	1y	55	20/21	0.75	0.13	71,78,93,93	0
54	G7M	1w	46	24/25	0.75	0.14	57,67,87,98	0
56	PSU	2y	32	20/21	0.77	0.15	62,78,87,90	0
56	PSU	1y	39	20/21	0.81	0.14	68,74,78,79	0
54	4SU	2w	8	20/21	0.82	0.12	68,73,87,88	0
32	2MG	2a	1207	24/25	0.86	0.13	61,66,74,75	0
55	4SU	2x	8	20/21	0.87	0.11	58,62,73,75	0
55	5MU	2x	54	21/22	0.88	0.12	58,67,72,77	0
54	5MU	2w	54	21/22	0.88	0.10	57,66,69,72	0
54	PSU	2w	55	20/21	0.88	0.10	63,69,75,77	0
54	PSU	2w	32	20/21	0.88	0.13	59,64,73,73	0
55	PSU	2x	55	20/21	0.89	0.12	58,63,73,79	0
54	PSU	2w	39	20/21	0.89	0.12	56,65,68,70	0
55	5MC	2x	32	21/22	0.89	0.16	52,57,65,66	0
32	PSU	2a	516	20/21	0.89	0.12	54,60,64,66	0
43	0TD	2l	92	10/11	0.90	0.14	46,53,58,65	0
1	PSU	2A	1917	20/21	0.90	0.11	42,52,59,63	0
54	PSU	1w	55	20/21	0.91	0.10	55,61,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	4SU	1x	8	20/21	0.91	0.12	47,55,62,63	0
54	PSU	1w	32	20/21	0.91	0.12	47,51,58,61	0
1	OMC	2A	1920	21/22	0.92	0.10	46,52,56,57	0
32	5MC	2a	1407	21/22	0.92	0.12	46,52,55,61	0
55	5MU	1x	54	21/22	0.92	0.11	46,54,59,61	0
32	G7M	2a	527	24/25	0.92	0.11	48,56,62,67	0
32	5MC	2a	967	21/22	0.92	0.14	54,61,64,70	0
32	M2G	2a	966	25/26	0.93	0.14	56,62,69,72	0
1	5MU	1A	1915	21/22	0.93	0.11	38,42,50,58	0
55	PSU	1x	55	20/21	0.93	0.09	45,51,59,63	0
32	5MC	2a	1400	21/22	0.93	0.14	46,57,64,70	0
32	5MC	2a	1404	21/22	0.93	0.12	41,53,57,60	0
1	5MC	2A	1942	21/22	0.93	0.11	42,53,59,64	0
54	4SU	1w	8	20/21	0.93	0.11	56,67,72,74	0
1	PSU	2A	1911	20/21	0.93	0.11	44,56,64,66	0
54	5MU	1w	54	21/22	0.94	0.09	45,50,58,66	0
1	5MU	2A	1915	21/22	0.94	0.09	47,56,60,62	0
32	4OC	2a	1402	22/23	0.94	0.11	48,56,58,62	0
32	2MG	1a	1207	24/25	0.94	0.10	43,51,55,65	0
54	MIA	2w	37	25/30	0.94	0.10	50,60,63,65	0
32	MA6	2a	1518	24/25	0.95	0.10	48,54,60,65	0
32	MA6	2a	1519	24/25	0.95	0.12	42,53,57,60	0
1	OMU	2A	2552	21/22	0.95	0.09	34,40,43,47	0
1	OMC	1A	1920	21/22	0.95	0.08	29,37,39,41	0
32	PSU	1a	516	20/21	0.95	0.09	32,47,51,51	0
1	PSU	1A	1911	20/21	0.95	0.08	36,40,47,51	0
43	0TD	1l	92	10/11	0.95	0.09	36,42,45,47	0
54	PSU	1w	39	20/21	0.96	0.08	39,48,51,52	0
32	5MC	1a	1400	21/22	0.96	0.10	28,38,45,49	0
32	4OC	1a	1402	22/23	0.96	0.09	32,38,41,46	0
32	5MC	1a	1404	21/22	0.96	0.08	28,32,37,40	0
32	MA6	1a	1518	24/25	0.96	0.10	32,38,42,42	0
55	5MC	1x	32	21/22	0.96	0.08	35,39,44,49	0
32	MA6	1a	1519	24/25	0.96	0.09	30,37,41,42	0
32	M2G	1a	966	25/26	0.96	0.08	34,41,47,48	0
55	31H	2x	76	32/33	0.96	0.09	26,34,39,49	0
32	UR3	2a	1498	21/22	0.96	0.11	42,51,56,57	0
32	5MC	1a	967	21/22	0.96	0.09	31,41,48,50	0
1	5MC	2A	1962	21/22	0.96	0.10	28,42,48,53	0
1	OMG	2A	2251	24/25	0.96	0.09	29,34,40,42	0
1	5MC	1A	1942	21/22	0.96	0.08	33,38,41,51	0
1	PSU	2A	2605	20/21	0.96	0.08	25,36,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MIA	1w	37	29/30	0.96	0.09	38,46,53,54	0
32	G7M	1a	527	24/25	0.97	0.07	30,35,44,47	0
1	2MA	2A	2503	23/24	0.97	0.07	25,31,39,39	0
32	5MC	1a	1407	21/22	0.97	0.07	26,31,34,40	0
54	F3N	2w	76	33/34	0.97	0.09	27,33,37,42	0
1	OMG	1A	2251	24/25	0.97	0.07	16,21,28,30	0
1	PSU	1A	1917	20/21	0.97	0.08	26,36,45,46	0
55	31H	1x	76	32/33	0.97	0.08	16,21,26,30	10
54	F3N	1w	76	33/34	0.97	0.07	15,19,23,28	0
1	5MC	1A	1962	21/22	0.98	0.07	22,26,38,41	0
1	5MU	1A	1939	21/22	0.98	0.07	20,24,26,27	0
1	5MU	2A	1939	21/22	0.98	0.06	24,33,39,43	0
1	2MA	1A	2503	23/24	0.98	0.06	11,18,23,23	0
1	OMU	1A	2552	21/22	0.98	0.07	20,25,30,33	0
32	UR3	1a	1498	21/22	0.98	0.06	22,32,35,39	0
1	PSU	1A	2605	20/21	0.98	0.07	17,22,27,29	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3246	1/1	0.48	0.32	74,74,74,74	0
57	MG	2a	1818	1/1	0.48	0.20	78,78,78,78	0
57	MG	2a	1788	1/1	0.55	0.25	69,69,69,69	0
57	MG	2A	3506	1/1	0.56	0.33	82,82,82,82	0
57	MG	2A	3562	1/1	0.56	0.20	64,64,64,64	0
57	MG	1A	4008	1/1	0.60	0.13	77,77,77,77	0
57	MG	2A	3884	1/1	0.62	0.24	75,75,75,75	0
57	MG	2a	1618	1/1	0.62	0.24	70,70,70,70	0
57	MG	2A	3730	1/1	0.63	0.18	74,74,74,74	0
57	MG	1A	3292	1/1	0.64	0.32	59,59,59,59	0
57	MG	1A	3467	1/1	0.66	0.27	71,71,71,71	0
57	MG	1a	1613	1/1	0.67	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3948	1/1	0.67	0.13	57,57,57,57	0
57	MG	1A	3516	1/1	0.67	0.28	66,66,66,66	0
57	MG	2a	1624	1/1	0.68	0.34	76,76,76,76	0
57	MG	2a	1711	1/1	0.68	0.34	73,73,73,73	0
57	MG	2A	3289	1/1	0.68	0.19	73,73,73,73	0
57	MG	2A	3004	1/1	0.68	0.27	66,66,66,66	0
57	MG	2a	1822	1/1	0.68	0.20	60,60,60,60	0
57	MG	2A	3607	1/1	0.69	0.18	59,59,59,59	0
57	MG	1A	3978	1/1	0.69	0.22	79,79,79,79	0
57	MG	2A	3761	1/1	0.69	0.25	60,60,60,60	0
57	MG	2a	1629	1/1	0.69	0.21	60,60,60,60	0
57	MG	1B	233	1/1	0.70	0.19	71,71,71,71	0
57	MG	2A	3670	1/1	0.70	0.18	66,66,66,66	0
57	MG	2A	3059	1/1	0.71	0.29	69,69,69,69	0
57	MG	2A	3103	1/1	0.71	0.27	62,62,62,62	0
57	MG	2A	3554	1/1	0.71	0.25	53,53,53,53	0
57	MG	2A	3807	1/1	0.71	0.18	68,68,68,68	0
57	MG	2A	3196	1/1	0.71	0.22	71,71,71,71	0
57	MG	1w	102	1/1	0.71	0.13	73,73,73,73	0
57	MG	2B	202	1/1	0.72	0.23	76,76,76,76	0
57	MG	10	106	1/1	0.72	0.17	46,46,46,46	0
57	MG	1A	4073	1/1	0.72	0.17	57,57,57,57	0
57	MG	2A	3596	1/1	0.72	0.21	76,76,76,76	0
57	MG	2B	212	1/1	0.73	0.32	81,81,81,81	0
57	MG	1A	3884	1/1	0.73	0.15	64,64,64,64	0
57	MG	2A	3501	1/1	0.73	0.14	71,71,71,71	0
57	MG	1A	3887	1/1	0.73	0.21	42,42,42,42	0
57	MG	1A	3858	1/1	0.73	0.16	64,64,64,64	0
57	MG	1A	4094	1/1	0.73	0.18	77,77,77,77	0
57	MG	1x	101	1/1	0.73	0.24	65,65,65,65	0
57	MG	2a	1821	1/1	0.73	0.19	53,53,53,53	0
57	MG	2A	3599	1/1	0.73	0.14	59,59,59,59	0
57	MG	2y	106	1/1	0.73	0.17	73,73,73,73	0
57	MG	1A	3269	1/1	0.74	0.22	65,65,65,65	0
57	MG	1A	3944	1/1	0.74	0.18	40,40,40,40	0
57	MG	29	101	1/1	0.74	0.52	71,71,71,71	0
57	MG	2A	3868	1/1	0.74	0.19	69,69,69,69	0
57	MG	1A	3612	1/1	0.74	0.14	57,57,57,57	0
57	MG	2w	103	1/1	0.74	0.18	62,62,62,62	0
57	MG	2B	201	1/1	0.74	0.22	62,62,62,62	0
57	MG	2A	3344	1/1	0.75	0.16	72,72,72,72	0
57	MG	2a	1771	1/1	0.75	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3955	1/1	0.75	0.17	59,59,59,59	0
57	MG	2a	1798	1/1	0.75	0.17	54,54,54,54	0
57	MG	1A	3838	1/1	0.75	0.22	65,65,65,65	0
57	MG	2A	3243	1/1	0.75	0.19	68,68,68,68	0
57	MG	1a	1676	1/1	0.75	0.31	73,73,73,73	0
57	MG	1a	1743	1/1	0.75	0.20	61,61,61,61	0
57	MG	2A	3322	1/1	0.75	0.23	74,74,74,74	0
57	MG	1A	3675	1/1	0.76	0.11	48,48,48,48	0
57	MG	2A	3192	1/1	0.76	0.18	69,69,69,69	0
57	MG	2A	3414	1/1	0.76	0.13	72,72,72,72	0
57	MG	2A	3262	1/1	0.76	0.34	61,61,61,61	0
57	MG	2A	3606	1/1	0.76	0.12	65,65,65,65	0
57	MG	2j	202	1/1	0.76	0.14	62,62,62,62	0
57	MG	1A	3874	1/1	0.76	0.18	26,26,26,26	0
57	MG	2w	105	1/1	0.76	0.19	77,77,77,77	0
57	MG	2A	3539	1/1	0.76	0.19	54,54,54,54	0
57	MG	1A	3544	1/1	0.77	0.20	67,67,67,67	0
57	MG	1A	4017	1/1	0.77	0.11	38,38,38,38	0
57	MG	2A	3614	1/1	0.77	0.14	55,55,55,55	0
57	MG	1A	4025	1/1	0.77	0.12	59,59,59,59	0
57	MG	2a	1641	1/1	0.77	0.20	64,64,64,64	0
57	MG	2A	3106	1/1	0.77	0.20	73,73,73,73	0
57	MG	1A	3651	1/1	0.77	0.10	35,35,35,35	0
57	MG	2T	203	1/1	0.77	0.21	64,64,64,64	0
57	MG	2A	3348	1/1	0.78	0.16	62,62,62,62	0
57	MG	2a	1644	1/1	0.78	0.33	69,69,69,69	0
57	MG	2A	3370	1/1	0.78	0.28	73,73,73,73	0
57	MG	1A	3805	1/1	0.78	0.14	53,53,53,53	0
57	MG	1w	105	1/1	0.78	0.13	73,73,73,73	0
57	MG	2A	3283	1/1	0.78	0.24	63,63,63,63	0
57	MG	1A	3986	1/1	0.78	0.29	77,77,77,77	0
57	MG	1A	3551	1/1	0.78	0.13	61,61,61,61	0
57	MG	2A	3747	1/1	0.78	0.18	57,57,57,57	0
57	MG	2a	1610	1/1	0.78	0.18	69,69,69,69	0
57	MG	2p	101	1/1	0.78	0.17	53,53,53,53	0
57	MG	1A	3695	1/1	0.78	0.10	30,30,30,30	0
57	MG	2A	3768	1/1	0.78	0.13	56,56,56,56	0
57	MG	2A	3779	1/1	0.78	0.23	60,60,60,60	0
57	MG	2A	3461	1/1	0.79	0.22	64,64,64,64	0
57	MG	1A	4057	1/1	0.79	0.13	47,47,47,47	0
57	MG	2a	1695	1/1	0.79	0.25	66,66,66,66	0
57	MG	1A	4021	1/1	0.79	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3102	1/1	0.79	0.29	66,66,66,66	0
57	MG	2A	3687	1/1	0.79	0.15	62,62,62,62	0
57	MG	2B	211	1/1	0.79	0.20	64,64,64,64	0
57	MG	2A	3713	1/1	0.79	0.12	58,58,58,58	0
57	MG	1A	3646	1/1	0.79	0.14	54,54,54,54	0
57	MG	1A	4097	1/1	0.79	0.17	65,65,65,65	0
57	MG	2A	3750	1/1	0.79	0.15	64,64,64,64	0
57	MG	2A	3568	1/1	0.79	0.17	50,50,50,50	0
57	MG	2A	3110	1/1	0.79	0.13	65,65,65,65	0
57	MG	2A	3446	1/1	0.79	0.20	54,54,54,54	0
57	MG	2x	104	1/1	0.79	0.20	60,60,60,60	0
57	MG	2a	1630	1/1	0.79	0.33	67,67,67,67	0
57	MG	2a	1620	1/1	0.80	0.19	61,61,61,61	0
57	MG	1A	3428	1/1	0.80	0.20	66,66,66,66	0
57	MG	1A	3965	1/1	0.80	0.09	18,18,18,18	0
57	MG	1a	1804	1/1	0.80	0.12	39,39,39,39	0
57	MG	2A	3410	1/1	0.80	0.17	71,71,71,71	0
57	MG	2A	3412	1/1	0.80	0.12	61,61,61,61	0
57	MG	2A	3809	1/1	0.80	0.16	61,61,61,61	0
57	MG	2A	3820	1/1	0.80	0.14	58,58,58,58	0
57	MG	2a	1743	1/1	0.80	0.27	68,68,68,68	0
57	MG	1A	4048	1/1	0.80	0.11	24,24,24,24	0
57	MG	1A	4009	1/1	0.80	0.15	57,57,57,57	0
57	MG	2A	3663	1/1	0.80	0.16	76,76,76,76	0
57	MG	2A	3272	1/1	0.80	0.13	76,76,76,76	0
57	MG	1A	3418	1/1	0.80	0.21	65,65,65,65	0
57	MG	2A	3689	1/1	0.80	0.14	65,65,65,65	0
57	MG	2B	216	1/1	0.80	0.15	69,69,69,69	0
57	MG	2B	220	1/1	0.80	0.25	58,58,58,58	0
57	MG	2v	101	1/1	0.80	0.17	74,74,74,74	0
57	MG	2A	3115	1/1	0.80	0.24	55,55,55,55	0
57	MG	2A	3718	1/1	0.80	0.15	59,59,59,59	0
57	MG	2A	3116	1/1	0.80	0.22	57,57,57,57	0
57	MG	2A	3326	1/1	0.80	0.21	59,59,59,59	0
57	MG	1v	101	1/1	0.81	0.16	59,59,59,59	0
57	MG	1a	1623	1/1	0.81	0.27	58,58,58,58	0
57	MG	2A	3349	1/1	0.81	0.18	68,68,68,68	0
57	MG	2a	1748	1/1	0.81	0.14	73,73,73,73	0
57	MG	2A	3255	1/1	0.81	0.09	69,69,69,69	0
57	MG	2A	3748	1/1	0.81	0.17	59,59,59,59	0
57	MG	2G	201	1/1	0.81	0.25	56,56,56,56	0
57	MG	2a	1803	1/1	0.81	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3380	1/1	0.81	0.23	72,72,72,72	0
57	MG	1a	1642	1/1	0.81	0.16	64,64,64,64	0
57	MG	1U	210	1/1	0.81	0.22	43,43,43,43	0
57	MG	1A	3725	1/1	0.81	0.15	49,49,49,49	0
57	MG	2A	3430	1/1	0.81	0.32	60,60,60,60	0
57	MG	2A	3187	1/1	0.81	0.14	68,68,68,68	0
57	MG	2A	3304	1/1	0.81	0.14	74,74,74,74	0
57	MG	2w	104	1/1	0.81	0.14	81,81,81,81	0
57	MG	1A	3956	1/1	0.81	0.13	66,66,66,66	0
57	MG	1a	1810	1/1	0.81	0.18	63,63,63,63	0
57	MG	2A	3695	1/1	0.81	0.17	57,57,57,57	0
57	MG	2A	3275	1/1	0.82	0.22	64,64,64,64	0
57	MG	2A	3276	1/1	0.82	0.19	74,74,74,74	0
57	MG	1a	1789	1/1	0.82	0.22	69,69,69,69	0
57	MG	1A	3964	1/1	0.82	0.08	46,46,46,46	0
57	MG	2A	3301	1/1	0.82	0.20	58,58,58,58	0
57	MG	1A	3722	1/1	0.82	0.11	52,52,52,52	0
57	MG	1e	201	1/1	0.82	0.11	65,65,65,65	0
57	MG	2a	1726	1/1	0.82	0.16	58,58,58,58	0
57	MG	2A	3111	1/1	0.82	0.19	60,60,60,60	0
57	MG	2a	1744	1/1	0.82	0.14	78,78,78,78	0
57	MG	1m	3002	1/1	0.82	0.20	57,57,57,57	0
57	MG	2A	3879	1/1	0.82	0.19	57,57,57,57	0
57	MG	1B	209	1/1	0.82	0.12	60,60,60,60	0
57	MG	1A	3233	1/1	0.82	0.15	59,59,59,59	0
57	MG	2A	3354	1/1	0.82	0.16	70,70,70,70	0
57	MG	1H	201	1/1	0.82	0.12	63,63,63,63	0
57	MG	1a	1697	1/1	0.82	0.28	59,59,59,59	0
57	MG	2A	3213	1/1	0.82	0.14	56,56,56,56	0
57	MG	1A	4091	1/1	0.82	0.09	71,71,71,71	0
57	MG	2E	306	1/1	0.82	0.20	49,49,49,49	0
57	MG	2A	3705	1/1	0.82	0.23	60,60,60,60	0
57	MG	2A	3709	1/1	0.82	0.09	71,71,71,71	0
57	MG	2A	3008	1/1	0.82	0.21	59,59,59,59	0
57	MG	2A	3031	1/1	0.82	0.22	67,67,67,67	0
57	MG	1a	1753	1/1	0.82	0.18	58,58,58,58	0
57	MG	2A	3101	1/1	0.82	0.20	66,66,66,66	0
57	MG	1A	4029	1/1	0.83	0.11	52,52,52,52	0
57	MG	10	107	1/1	0.83	0.16	60,60,60,60	0
57	MG	1A	3664	1/1	0.83	0.09	27,27,27,27	0
57	MG	1A	3775	1/1	0.83	0.07	12,12,12,12	0
57	MG	1A	4071	1/1	0.83	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3980	1/1	0.83	0.10	58,58,58,58	0
57	MG	2A	3488	1/1	0.83	0.16	61,61,61,61	0
57	MG	2A	3090	1/1	0.83	0.16	50,50,50,50	0
57	MG	2a	1656	1/1	0.83	0.23	72,72,72,72	0
57	MG	1A	3623	1/1	0.83	0.12	57,57,57,57	0
57	MG	1A	3996	1/1	0.83	0.11	54,54,54,54	0
57	MG	2A	3292	1/1	0.83	0.14	77,77,77,77	0
57	MG	1a	1749	1/1	0.83	0.16	54,54,54,54	0
57	MG	1A	3312	1/1	0.83	0.11	52,52,52,52	0
57	MG	2A	3587	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3854	1/1	0.83	0.28	63,63,63,63	0
57	MG	1a	1768	1/1	0.83	0.08	48,48,48,48	0
57	MG	1A	3952	1/1	0.83	0.12	57,57,57,57	0
57	MG	1B	228	1/1	0.83	0.10	68,68,68,68	0
57	MG	2a	1809	1/1	0.83	0.16	64,64,64,64	0
57	MG	1B	229	1/1	0.83	0.20	60,60,60,60	0
57	MG	1A	3713	1/1	0.83	0.13	50,50,50,50	0
57	MG	2A	3654	1/1	0.83	0.18	60,60,60,60	0
57	MG	2A	3658	1/1	0.83	0.18	54,54,54,54	0
57	MG	1A	3866	1/1	0.83	0.21	32,32,32,32	0
57	MG	2A	3363	1/1	0.83	0.17	61,61,61,61	0
57	MG	2w	101	1/1	0.83	0.23	59,59,59,59	0
57	MG	2A	3366	1/1	0.83	0.13	50,50,50,50	0
57	MG	1A	3250	1/1	0.83	0.18	60,60,60,60	0
57	MG	1Z	3702	1/1	0.83	0.11	63,63,63,63	0
57	MG	2A	3701	1/1	0.83	0.12	63,63,63,63	0
57	MG	2a	1601	1/1	0.83	0.17	59,59,59,59	0
57	MG	2A	3558	1/1	0.84	0.12	48,48,48,48	0
57	MG	2A	3759	1/1	0.84	0.17	54,54,54,54	0
57	MG	2A	3068	1/1	0.84	0.16	62,62,62,62	0
57	MG	2A	3072	1/1	0.84	0.12	57,57,57,57	0
57	MG	2A	3219	1/1	0.84	0.14	60,60,60,60	0
57	MG	1S	203	1/1	0.84	0.13	61,61,61,61	0
57	MG	2a	1665	1/1	0.84	0.13	57,57,57,57	0
57	MG	1A	3511	1/1	0.84	0.14	65,65,65,65	0
57	MG	1A	3730	1/1	0.84	0.17	64,64,64,64	0
57	MG	10	102	1/1	0.84	0.36	63,63,63,63	0
57	MG	2A	3611	1/1	0.84	0.17	51,51,51,51	0
57	MG	2A	3266	1/1	0.84	0.18	52,52,52,52	0
57	MG	2A	3882	1/1	0.84	0.16	65,65,65,65	0
57	MG	2A	3372	1/1	0.84	0.11	67,67,67,67	0
57	MG	2A	3376	1/1	0.84	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3738	1/1	0.84	0.12	52,52,52,52	0
57	MG	2A	3387	1/1	0.84	0.13	60,60,60,60	0
57	MG	1A	3060	1/1	0.84	0.13	58,58,58,58	0
57	MG	1x	102	1/1	0.84	0.15	62,62,62,62	0
57	MG	2B	217	1/1	0.84	0.14	54,54,54,54	0
57	MG	1a	1785	1/1	0.84	0.15	53,53,53,53	0
57	MG	2a	1829	1/1	0.84	0.12	57,57,57,57	0
57	MG	1A	3979	1/1	0.84	0.09	30,30,30,30	0
57	MG	2l	203	1/1	0.84	0.14	62,62,62,62	0
57	MG	2A	3291	1/1	0.84	0.20	67,67,67,67	0
57	MG	2A	3171	1/1	0.84	0.17	62,62,62,62	0
57	MG	2V	202	1/1	0.84	0.15	59,59,59,59	0
57	MG	2A	3295	1/1	0.84	0.31	65,65,65,65	0
57	MG	2A	3176	1/1	0.84	0.11	49,49,49,49	0
57	MG	1A	3679	1/1	0.84	0.09	19,19,19,19	0
57	MG	2A	3316	1/1	0.84	0.26	58,58,58,58	0
57	MG	2y	104	1/1	0.84	0.09	71,71,71,71	0
57	MG	1A	4024	1/1	0.84	0.20	50,50,50,50	0
57	MG	1l	104	1/1	0.85	0.11	50,50,50,50	0
57	MG	2A	3320	1/1	0.85	0.15	55,55,55,55	0
57	MG	2E	301	1/1	0.85	0.11	58,58,58,58	0
57	MG	2A	3122	1/1	0.85	0.14	58,58,58,58	0
57	MG	1w	103	1/1	0.85	0.09	55,55,55,55	0
57	MG	1A	3487	1/1	0.85	0.13	62,62,62,62	0
57	MG	2A	3178	1/1	0.85	0.17	61,61,61,61	0
57	MG	27	101	1/1	0.85	0.26	58,58,58,58	0
57	MG	2A	3184	1/1	0.85	0.21	56,56,56,56	0
57	MG	1w	106	1/1	0.85	0.10	42,42,42,42	0
57	MG	2A	3684	1/1	0.85	0.10	62,62,62,62	0
57	MG	1A	3596	1/1	0.85	0.16	60,60,60,60	0
57	MG	1A	3492	1/1	0.85	0.18	50,50,50,50	0
57	MG	2A	3206	1/1	0.85	0.18	62,62,62,62	0
57	MG	2A	3211	1/1	0.85	0.10	64,64,64,64	0
57	MG	1x	112	1/1	0.85	0.11	54,54,54,54	0
57	MG	2A	3707	1/1	0.85	0.12	57,57,57,57	0
57	MG	1a	1649	1/1	0.85	0.12	57,57,57,57	0
57	MG	2A	3382	1/1	0.85	0.16	47,47,47,47	0
57	MG	1A	3752	1/1	0.85	0.23	57,57,57,57	0
57	MG	2A	3399	1/1	0.85	0.14	64,64,64,64	0
57	MG	2A	3406	1/1	0.85	0.16	65,65,65,65	0
57	MG	2a	1714	1/1	0.85	0.17	62,62,62,62	0
57	MG	1A	3204	1/1	0.85	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4001	1/1	0.85	0.08	24,24,24,24	0
57	MG	1A	3947	1/1	0.85	0.10	23,23,23,23	0
57	MG	1A	3122	1/1	0.85	0.13	35,35,35,35	0
57	MG	2a	1756	1/1	0.85	0.15	64,64,64,64	0
57	MG	2A	3075	1/1	0.85	0.13	63,63,63,63	0
57	MG	2A	3776	1/1	0.85	0.11	65,65,65,65	0
57	MG	1A	3718	1/1	0.85	0.09	58,58,58,58	0
57	MG	2A	3094	1/1	0.85	0.18	38,38,38,38	0
57	MG	1A	3844	1/1	0.85	0.12	42,42,42,42	0
57	MG	2a	1812	1/1	0.85	0.13	70,70,70,70	0
57	MG	2A	3285	1/1	0.85	0.13	53,53,53,53	0
57	MG	2A	3839	1/1	0.85	0.09	28,28,28,28	0
57	MG	2A	3847	1/1	0.85	0.19	70,70,70,70	0
57	MG	1A	3352	1/1	0.85	0.12	45,45,45,45	0
57	MG	2a	1833	1/1	0.85	0.14	62,62,62,62	0
57	MG	1A	3958	1/1	0.85	0.13	54,54,54,54	0
57	MG	1A	3864	1/1	0.85	0.22	31,31,31,31	0
57	MG	2A	3294	1/1	0.85	0.11	55,55,55,55	0
57	MG	2A	3564	1/1	0.85	0.13	47,47,47,47	0
57	MG	1A	4047	1/1	0.85	0.14	31,31,31,31	0
57	MG	2A	3583	1/1	0.85	0.14	44,44,44,44	0
57	MG	2B	209	1/1	0.85	0.23	56,56,56,56	0
57	MG	1A	3865	1/1	0.85	0.12	50,50,50,50	0
57	MG	1A	3966	1/1	0.85	0.18	48,48,48,48	0
57	MG	2B	215	1/1	0.85	0.10	47,47,47,47	0
57	MG	2A	3310	1/1	0.85	0.25	64,64,64,64	0
57	MG	2a	1639	1/1	0.86	0.15	65,65,65,65	0
57	MG	1O	205	1/1	0.86	0.18	56,56,56,56	0
57	MG	1a	1731	1/1	0.86	0.10	39,39,39,39	0
57	MG	2A	3273	1/1	0.86	0.14	65,65,65,65	0
57	MG	2A	3851	1/1	0.86	0.12	59,59,59,59	0
57	MG	2A	3853	1/1	0.86	0.11	32,32,32,32	0
57	MG	2a	1706	1/1	0.86	0.11	53,53,53,53	0
57	MG	1A	3193	1/1	0.86	0.11	47,47,47,47	0
57	MG	1A	3962	1/1	0.86	0.10	42,42,42,42	0
57	MG	2a	1717	1/1	0.86	0.17	70,70,70,70	0
57	MG	2a	1720	1/1	0.86	0.22	66,66,66,66	0
57	MG	1x	111	1/1	0.86	0.13	55,55,55,55	0
57	MG	2a	1731	1/1	0.86	0.16	64,64,64,64	0
57	MG	1A	3721	1/1	0.86	0.15	43,43,43,43	0
57	MG	2A	3409	1/1	0.86	0.16	64,64,64,64	0
57	MG	2A	3682	1/1	0.86	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3003	1/1	0.86	0.13	47,47,47,47	0
57	MG	2A	3175	1/1	0.86	0.18	57,57,57,57	0
57	MG	1a	1760	1/1	0.86	0.11	60,60,60,60	0
57	MG	1A	3510	1/1	0.86	0.10	55,55,55,55	0
57	MG	2B	213	1/1	0.86	0.21	58,58,58,58	0
57	MG	2a	1804	1/1	0.86	0.17	64,64,64,64	0
57	MG	1A	3843	1/1	0.86	0.14	56,56,56,56	0
57	MG	1A	4095	1/1	0.86	0.10	37,37,37,37	0
57	MG	2A	3189	1/1	0.86	0.19	68,68,68,68	0
57	MG	1a	1798	1/1	0.86	0.15	81,81,81,81	0
57	MG	2A	3502	1/1	0.86	0.09	61,61,61,61	0
57	MG	2a	1823	1/1	0.86	0.19	59,59,59,59	0
57	MG	2a	1826	1/1	0.86	0.14	62,62,62,62	0
57	MG	2A	3195	1/1	0.86	0.24	53,53,53,53	0
57	MG	1A	3469	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3204	1/1	0.86	0.13	45,45,45,45	0
57	MG	2A	3555	1/1	0.86	0.11	42,42,42,42	0
57	MG	15	109	1/1	0.86	0.11	45,45,45,45	0
57	MG	1A	3712	1/1	0.86	0.13	34,34,34,34	0
57	MG	2A	3091	1/1	0.86	0.14	66,66,66,66	0
57	MG	1A	3737	1/1	0.86	0.15	65,65,65,65	0
57	MG	2A	3097	1/1	0.86	0.15	58,58,58,58	0
57	MG	1A	4036	1/1	0.86	0.11	45,45,45,45	0
57	MG	2A	3791	1/1	0.86	0.10	49,49,49,49	0
57	MG	1A	3210	1/1	0.86	0.12	64,64,64,64	0
57	MG	1A	3716	1/1	0.86	0.15	45,45,45,45	0
57	MG	2A	3440	1/1	0.87	0.19	53,53,53,53	0
57	MG	1a	1755	1/1	0.87	0.09	47,47,47,47	0
57	MG	2A	3449	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3735	1/1	0.87	0.14	51,51,51,51	0
57	MG	2A	3740	1/1	0.87	0.11	50,50,50,50	0
57	MG	1A	3382	1/1	0.87	0.09	61,61,61,61	0
57	MG	2a	1638	1/1	0.87	0.30	54,54,54,54	0
57	MG	2A	3299	1/1	0.87	0.16	56,56,56,56	0
57	MG	1A	3038	1/1	0.87	0.14	56,56,56,56	0
57	MG	1a	1774	1/1	0.87	0.11	70,70,70,70	0
57	MG	2a	1649	1/1	0.87	0.24	61,61,61,61	0
57	MG	2a	1653	1/1	0.87	0.22	57,57,57,57	0
57	MG	1A	3989	1/1	0.87	0.09	30,30,30,30	0
57	MG	2A	3762	1/1	0.87	0.17	37,37,37,37	0
57	MG	2A	3514	1/1	0.87	0.13	56,56,56,56	0
57	MG	2a	1701	1/1	0.87	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3198	1/1	0.87	0.23	55,55,55,55	0
57	MG	2a	1708	1/1	0.87	0.16	54,54,54,54	0
57	MG	2A	3083	1/1	0.87	0.10	37,37,37,37	0
57	MG	1A	3535	1/1	0.87	0.25	53,53,53,53	0
57	MG	2A	3323	1/1	0.87	0.19	52,52,52,52	0
57	MG	1A	3341	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3814	1/1	0.87	0.12	49,49,49,49	0
57	MG	2a	1727	1/1	0.87	0.18	66,66,66,66	0
57	MG	1A	3860	1/1	0.87	0.09	21,21,21,21	0
57	MG	2A	3838	1/1	0.87	0.12	68,68,68,68	0
57	MG	2A	3565	1/1	0.87	0.18	42,42,42,42	0
57	MG	1A	3545	1/1	0.87	0.19	50,50,50,50	0
57	MG	2A	3222	1/1	0.87	0.16	57,57,57,57	0
57	MG	2a	1766	1/1	0.87	0.14	54,54,54,54	0
57	MG	2A	3224	1/1	0.87	0.10	50,50,50,50	0
57	MG	2A	3357	1/1	0.87	0.12	62,62,62,62	0
57	MG	17	105	1/1	0.87	0.30	48,48,48,48	0
57	MG	1A	3493	1/1	0.87	0.11	51,51,51,51	0
57	MG	2A	3367	1/1	0.87	0.25	62,62,62,62	0
57	MG	1A	3561	1/1	0.87	0.14	55,55,55,55	0
57	MG	2A	3612	1/1	0.87	0.13	63,63,63,63	0
57	MG	1a	1628	1/1	0.87	0.25	60,60,60,60	0
57	MG	2B	207	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3623	1/1	0.87	0.13	42,42,42,42	0
57	MG	1a	1634	1/1	0.87	0.09	46,46,46,46	0
57	MG	1B	214	1/1	0.87	0.10	44,44,44,44	0
57	MG	1B	225	1/1	0.87	0.11	49,49,49,49	0
57	MG	2A	3274	1/1	0.87	0.12	61,61,61,61	0
57	MG	2a	1834	1/1	0.87	0.21	63,63,63,63	0
57	MG	2e	201	1/1	0.87	0.10	59,59,59,59	0
57	MG	2A	3677	1/1	0.87	0.18	56,56,56,56	0
57	MG	2l	202	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3391	1/1	0.87	0.15	63,63,63,63	0
57	MG	2A	3397	1/1	0.87	0.14	58,58,58,58	0
57	MG	1A	3562	1/1	0.87	0.12	52,52,52,52	0
57	MG	1A	3710	1/1	0.87	0.11	21,21,21,21	0
57	MG	1A	3972	1/1	0.87	0.12	62,62,62,62	0
57	MG	1a	1739	1/1	0.87	0.16	64,64,64,64	0
57	MG	1A	3591	1/1	0.87	0.29	45,45,45,45	0
57	MG	2w	109	1/1	0.87	0.20	65,65,65,65	0
57	MG	1A	4038	1/1	0.87	0.08	26,26,26,26	0
57	MG	1A	3265	1/1	0.87	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3710	1/1	0.87	0.11	60,60,60,60	0
57	MG	2A	3359	1/1	0.88	0.10	50,50,50,50	0
57	MG	2A	3778	1/1	0.88	0.10	56,56,56,56	0
57	MG	1A	3649	1/1	0.88	0.12	47,47,47,47	0
57	MG	2A	3098	1/1	0.88	0.17	61,61,61,61	0
57	MG	2A	3799	1/1	0.88	0.16	58,58,58,58	0
57	MG	1A	3470	1/1	0.88	0.10	41,41,41,41	0
57	MG	1A	3405	1/1	0.88	0.16	50,50,50,50	0
57	MG	2A	3811	1/1	0.88	0.08	43,43,43,43	0
57	MG	1A	3277	1/1	0.88	0.07	48,48,48,48	0
57	MG	1A	3821	1/1	0.88	0.12	49,49,49,49	0
57	MG	18	102	1/1	0.88	0.15	50,50,50,50	0
57	MG	1B	203	1/1	0.88	0.19	55,55,55,55	0
57	MG	1A	3064	1/1	0.88	0.11	50,50,50,50	0
57	MG	1A	3891	1/1	0.88	0.12	35,35,35,35	0
57	MG	2a	1719	1/1	0.88	0.15	65,65,65,65	0
57	MG	1B	217	1/1	0.88	0.09	40,40,40,40	0
57	MG	2a	1721	1/1	0.88	0.18	54,54,54,54	0
57	MG	2A	3137	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3401	1/1	0.88	0.19	65,65,65,65	0
57	MG	1B	223	1/1	0.88	0.13	59,59,59,59	0
57	MG	2a	1741	1/1	0.88	0.10	44,44,44,44	0
57	MG	1a	1643	1/1	0.88	0.18	53,53,53,53	0
57	MG	2A	3679	1/1	0.88	0.18	51,51,51,51	0
57	MG	1A	3897	1/1	0.88	0.07	23,23,23,23	0
57	MG	1a	1658	1/1	0.88	0.20	45,45,45,45	0
57	MG	2a	1758	1/1	0.88	0.08	49,49,49,49	0
57	MG	2a	1761	1/1	0.88	0.09	54,54,54,54	0
57	MG	2B	203	1/1	0.88	0.18	61,61,61,61	0
57	MG	1a	1663	1/1	0.88	0.18	61,61,61,61	0
57	MG	2a	1785	1/1	0.88	0.16	54,54,54,54	0
57	MG	2B	208	1/1	0.88	0.11	51,51,51,51	0
57	MG	1A	3196	1/1	0.88	0.25	33,33,33,33	0
57	MG	2B	210	1/1	0.88	0.16	67,67,67,67	0
57	MG	1A	3727	1/1	0.88	0.16	49,49,49,49	0
57	MG	2A	3698	1/1	0.88	0.08	34,34,34,34	0
57	MG	1a	1711	1/1	0.88	0.17	56,56,56,56	0
57	MG	1a	1724	1/1	0.88	0.14	62,62,62,62	0
57	MG	2A	3311	1/1	0.88	0.24	63,63,63,63	0
57	MG	2A	3464	1/1	0.88	0.20	49,49,49,49	0
57	MG	1A	4039	1/1	0.88	0.08	38,38,38,38	0
57	MG	2D	307	1/1	0.88	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1D	312	1/1	0.88	0.16	39,39,39,39	0
57	MG	1A	4040	1/1	0.88	0.11	28,28,28,28	0
57	MG	2A	3729	1/1	0.88	0.08	39,39,39,39	0
57	MG	1A	3855	1/1	0.88	0.23	56,56,56,56	0
57	MG	1A	3644	1/1	0.88	0.09	19,19,19,19	0
57	MG	2A	3736	1/1	0.88	0.12	69,69,69,69	0
57	MG	2A	3522	1/1	0.88	0.17	50,50,50,50	0
57	MG	2A	3338	1/1	0.88	0.19	55,55,55,55	0
57	MG	2a	1609	1/1	0.88	0.15	62,62,62,62	0
57	MG	1A	3395	1/1	0.88	0.13	56,56,56,56	0
57	MG	1Y	202	1/1	0.88	0.09	53,53,53,53	0
57	MG	1A	4068	1/1	0.88	0.10	38,38,38,38	0
57	MG	2a	1623	1/1	0.88	0.26	58,58,58,58	0
57	MG	1A	4000	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3355	1/1	0.88	0.09	37,37,37,37	0
57	MG	2A	3767	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3228	1/1	0.88	0.15	53,53,53,53	0
57	MG	1A	3434	1/1	0.89	0.17	51,51,51,51	0
57	MG	2A	3622	1/1	0.89	0.12	40,40,40,40	0
57	MG	1a	1772	1/1	0.89	0.09	47,47,47,47	0
57	MG	2A	3639	1/1	0.89	0.08	44,44,44,44	0
57	MG	1Z	3700	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3656	1/1	0.89	0.26	61,61,61,61	0
57	MG	2R	202	1/1	0.89	0.18	45,45,45,45	0
57	MG	2R	203	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3436	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3351	1/1	0.89	0.08	73,73,73,73	0
57	MG	23	101	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3236	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3675	1/1	0.89	0.18	52,52,52,52	0
57	MG	1A	3653	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3356	1/1	0.89	0.21	40,40,40,40	0
57	MG	1A	4060	1/1	0.89	0.10	45,45,45,45	0
57	MG	1a	1809	1/1	0.89	0.14	61,61,61,61	0
57	MG	2A	3360	1/1	0.89	0.11	60,60,60,60	0
57	MG	2A	3191	1/1	0.89	0.07	50,50,50,50	0
57	MG	1A	3468	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3194	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3173	1/1	0.89	0.09	34,34,34,34	0
57	MG	1A	3026	1/1	0.89	0.09	49,49,49,49	0
57	MG	1A	4081	1/1	0.89	0.09	29,29,29,29	0
57	MG	2a	1640	1/1	0.89	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3377	1/1	0.89	0.13	67,67,67,67	0
57	MG	1A	3990	1/1	0.89	0.10	33,33,33,33	0
57	MG	2a	1648	1/1	0.89	0.10	50,50,50,50	0
57	MG	1A	3795	1/1	0.89	0.11	67,67,67,67	0
57	MG	1A	3917	1/1	0.89	0.24	38,38,38,38	0
57	MG	2a	1655	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3723	1/1	0.89	0.08	42,42,42,42	0
57	MG	2A	3724	1/1	0.89	0.10	56,56,56,56	0
57	MG	2a	1675	1/1	0.89	0.28	54,54,54,54	0
57	MG	2a	1679	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3933	1/1	0.89	0.08	31,31,31,31	0
57	MG	2a	1699	1/1	0.89	0.11	65,65,65,65	0
57	MG	2a	1700	1/1	0.89	0.18	56,56,56,56	0
57	MG	2A	3217	1/1	0.89	0.11	51,51,51,51	0
57	MG	1A	3479	1/1	0.89	0.17	38,38,38,38	0
57	MG	1B	208	1/1	0.89	0.09	58,58,58,58	0
57	MG	2a	1710	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3814	1/1	0.89	0.41	50,50,50,50	0
57	MG	1a	1651	1/1	0.89	0.16	50,50,50,50	0
57	MG	2A	3241	1/1	0.89	0.23	52,52,52,52	0
57	MG	2A	3749	1/1	0.89	0.09	66,66,66,66	0
57	MG	1A	4016	1/1	0.89	0.08	33,33,33,33	0
57	MG	2A	3752	1/1	0.89	0.14	44,44,44,44	0
57	MG	1a	1659	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3417	1/1	0.89	0.10	64,64,64,64	0
57	MG	2A	3418	1/1	0.89	0.18	66,66,66,66	0
57	MG	2A	3764	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3428	1/1	0.89	0.14	39,39,39,39	0
57	MG	2A	3253	1/1	0.89	0.22	63,63,63,63	0
57	MG	2A	3005	1/1	0.89	0.11	52,52,52,52	0
57	MG	1A	3323	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3028	1/1	0.89	0.31	43,43,43,43	0
57	MG	2a	1760	1/1	0.89	0.10	68,68,68,68	0
57	MG	1A	3408	1/1	0.89	0.10	54,54,54,54	0
57	MG	2A	3035	1/1	0.89	0.11	53,53,53,53	0
57	MG	2A	3053	1/1	0.89	0.18	55,55,55,55	0
57	MG	1a	1677	1/1	0.89	0.13	53,53,53,53	0
57	MG	1a	1679	1/1	0.89	0.20	45,45,45,45	0
57	MG	2A	3279	1/1	0.89	0.11	53,53,53,53	0
57	MG	2a	1799	1/1	0.89	0.09	55,55,55,55	0
57	MG	1a	1681	1/1	0.89	0.11	58,58,58,58	0
57	MG	2A	3823	1/1	0.89	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1806	1/1	0.89	0.09	58,58,58,58	0
57	MG	2A	3826	1/1	0.89	0.10	49,49,49,49	0
57	MG	2A	3515	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3520	1/1	0.89	0.13	38,38,38,38	0
57	MG	2a	1819	1/1	0.89	0.10	52,52,52,52	0
57	MG	1A	3604	1/1	0.89	0.13	44,44,44,44	0
57	MG	2A	3536	1/1	0.89	0.09	40,40,40,40	0
57	MG	1a	1702	1/1	0.89	0.17	55,55,55,55	0
57	MG	2A	3550	1/1	0.89	0.10	44,44,44,44	0
57	MG	1a	1708	1/1	0.89	0.12	50,50,50,50	0
57	MG	2a	1831	1/1	0.89	0.11	61,61,61,61	0
57	MG	1A	3413	1/1	0.89	0.10	47,47,47,47	0
57	MG	1a	1718	1/1	0.89	0.20	45,45,45,45	0
57	MG	2d	302	1/1	0.89	0.09	65,65,65,65	0
57	MG	1a	1720	1/1	0.89	0.11	64,64,64,64	0
57	MG	1A	4028	1/1	0.89	0.10	61,61,61,61	0
57	MG	1A	3613	1/1	0.89	0.09	26,26,26,26	0
57	MG	1a	1738	1/1	0.89	0.07	36,36,36,36	0
57	MG	2l	204	1/1	0.89	0.08	55,55,55,55	0
57	MG	2B	204	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	4033	1/1	0.89	0.11	44,44,44,44	0
57	MG	1A	4035	1/1	0.89	0.08	41,41,41,41	0
57	MG	2w	102	1/1	0.89	0.20	73,73,73,73	0
57	MG	2A	3588	1/1	0.89	0.11	60,60,60,60	0
57	MG	1A	3340	1/1	0.89	0.20	46,46,46,46	0
57	MG	1Q	205	1/1	0.89	0.09	36,36,36,36	0
57	MG	1A	3859	1/1	0.89	0.09	55,55,55,55	0
57	MG	2x	102	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3235	1/1	0.89	0.09	31,31,31,31	0
57	MG	2y	101	1/1	0.89	0.13	71,71,71,71	0
57	MG	1a	1761	1/1	0.89	0.11	47,47,47,47	0
57	MG	2y	105	1/1	0.89	0.23	65,65,65,65	0
57	MG	2A	3337	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3481	1/1	0.90	0.09	43,43,43,43	0
57	MG	1a	1725	1/1	0.90	0.10	39,39,39,39	0
57	MG	2A	3231	1/1	0.90	0.21	42,42,42,42	0
57	MG	2a	1616	1/1	0.90	0.16	51,51,51,51	0
57	MG	1A	3848	1/1	0.90	0.08	47,47,47,47	0
57	MG	2A	3057	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	3853	1/1	0.90	0.08	40,40,40,40	0
57	MG	2A	3715	1/1	0.90	0.10	61,61,61,61	0
57	MG	2a	1625	1/1	0.90	0.29	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3717	1/1	0.90	0.09	55,55,55,55	0
57	MG	2A	3250	1/1	0.90	0.12	51,51,51,51	0
57	MG	2a	1635	1/1	0.90	0.19	51,51,51,51	0
57	MG	2A	3411	1/1	0.90	0.20	60,60,60,60	0
57	MG	2A	3067	1/1	0.90	0.08	40,40,40,40	0
57	MG	2A	3254	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3317	1/1	0.90	0.17	43,43,43,43	0
57	MG	2A	3256	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3426	1/1	0.90	0.15	47,47,47,47	0
57	MG	1a	1741	1/1	0.90	0.07	42,42,42,42	0
57	MG	2A	3745	1/1	0.90	0.12	47,47,47,47	0
57	MG	2A	3074	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3436	1/1	0.90	0.28	55,55,55,55	0
57	MG	1A	3281	1/1	0.90	0.11	47,47,47,47	0
57	MG	2a	1670	1/1	0.90	0.15	69,69,69,69	0
57	MG	2A	3080	1/1	0.90	0.09	53,53,53,53	0
57	MG	1a	1745	1/1	0.90	0.12	54,54,54,54	0
57	MG	2a	1684	1/1	0.90	0.19	50,50,50,50	0
57	MG	2a	1688	1/1	0.90	0.09	63,63,63,63	0
57	MG	2A	3086	1/1	0.90	0.17	43,43,43,43	0
57	MG	2a	1698	1/1	0.90	0.14	49,49,49,49	0
57	MG	2A	3462	1/1	0.90	0.14	42,42,42,42	0
57	MG	1A	3655	1/1	0.90	0.10	30,30,30,30	0
57	MG	2A	3486	1/1	0.90	0.18	49,49,49,49	0
57	MG	2A	3277	1/1	0.90	0.12	56,56,56,56	0
57	MG	2A	3497	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3278	1/1	0.90	0.17	45,45,45,45	0
57	MG	1A	3389	1/1	0.90	0.10	52,52,52,52	0
57	MG	13	105	1/1	0.90	0.12	46,46,46,46	0
57	MG	1a	1758	1/1	0.90	0.15	43,43,43,43	0
57	MG	2A	3792	1/1	0.90	0.10	35,35,35,35	0
57	MG	1A	3731	1/1	0.90	0.08	40,40,40,40	0
57	MG	2A	3802	1/1	0.90	0.09	56,56,56,56	0
57	MG	1A	3667	1/1	0.90	0.12	53,53,53,53	0
57	MG	1A	4088	1/1	0.90	0.16	50,50,50,50	0
57	MG	2A	3810	1/1	0.90	0.11	63,63,63,63	0
57	MG	1a	1769	1/1	0.90	0.08	69,69,69,69	0
57	MG	18	103	1/1	0.90	0.20	50,50,50,50	0
57	MG	2A	3815	1/1	0.90	0.10	50,50,50,50	0
57	MG	2a	1745	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3668	1/1	0.90	0.07	31,31,31,31	0
57	MG	1a	1780	1/1	0.90	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3873	1/1	0.90	0.10	42,42,42,42	0
57	MG	2A	3837	1/1	0.90	0.12	74,74,74,74	0
57	MG	2A	3305	1/1	0.90	0.13	53,53,53,53	0
57	MG	1A	3744	1/1	0.90	0.10	45,45,45,45	0
57	MG	2A	3118	1/1	0.90	0.13	50,50,50,50	0
57	MG	2a	1775	1/1	0.90	0.13	62,62,62,62	0
57	MG	1A	3335	1/1	0.90	0.17	36,36,36,36	0
57	MG	2A	3318	1/1	0.90	0.08	44,44,44,44	0
57	MG	2a	1789	1/1	0.90	0.09	53,53,53,53	0
57	MG	1a	1637	1/1	0.90	0.26	66,66,66,66	0
57	MG	2A	3153	1/1	0.90	0.24	55,55,55,55	0
57	MG	2A	3869	1/1	0.90	0.09	50,50,50,50	0
57	MG	2A	3870	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3162	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3590	1/1	0.90	0.08	44,44,44,44	0
57	MG	1A	4098	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3761	1/1	0.90	0.13	34,34,34,34	0
57	MG	1a	1812	1/1	0.90	0.14	60,60,60,60	0
57	MG	1A	3888	1/1	0.90	0.09	13,13,13,13	0
57	MG	2A	3610	1/1	0.90	0.13	53,53,53,53	0
57	MG	2B	205	1/1	0.90	0.13	45,45,45,45	0
57	MG	1A	3769	1/1	0.90	0.10	37,37,37,37	0
57	MG	1t	201	1/1	0.90	0.19	56,56,56,56	0
57	MG	1A	4012	1/1	0.90	0.07	27,27,27,27	0
57	MG	2A	3619	1/1	0.90	0.10	65,65,65,65	0
57	MG	1A	3895	1/1	0.90	0.11	18,18,18,18	0
57	MG	1A	3770	1/1	0.90	0.08	22,22,22,22	0
57	MG	1a	1670	1/1	0.90	0.16	49,49,49,49	0
57	MG	2B	214	1/1	0.90	0.18	55,55,55,55	0
57	MG	1A	3337	1/1	0.90	0.24	47,47,47,47	0
57	MG	1A	3338	1/1	0.90	0.08	39,39,39,39	0
57	MG	1A	3532	1/1	0.90	0.09	45,45,45,45	0
57	MG	2A	3202	1/1	0.90	0.11	46,46,46,46	0
57	MG	2q	202	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3946	1/1	0.90	0.08	21,21,21,21	0
57	MG	2v	103	1/1	0.90	0.23	56,56,56,56	0
57	MG	1A	3272	1/1	0.90	0.11	36,36,36,36	0
57	MG	2A	3209	1/1	0.90	0.11	44,44,44,44	0
57	MG	2F	306	1/1	0.90	0.16	53,53,53,53	0
57	MG	2A	3371	1/1	0.90	0.18	61,61,61,61	0
57	MG	1A	3476	1/1	0.90	0.13	39,39,39,39	0
57	MG	1A	3822	1/1	0.90	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3830	1/1	0.90	0.11	40,40,40,40	0
57	MG	1A	3100	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3220	1/1	0.90	0.14	56,56,56,56	0
57	MG	25	103	1/1	0.90	0.22	47,47,47,47	0
57	MG	2A	3696	1/1	0.90	0.11	54,54,54,54	0
57	MG	1A	3647	1/1	0.90	0.09	52,52,52,52	0
59	A1C9N	2A	3885	74/74	0.90	0.15	27,48,58,59	0
57	MG	1A	3232	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3366	1/1	0.91	0.11	28,28,28,28	0
57	MG	1E	314	1/1	0.91	0.06	34,34,34,34	0
57	MG	2D	303	1/1	0.91	0.21	57,57,57,57	0
57	MG	1A	4007	1/1	0.91	0.07	40,40,40,40	0
57	MG	1A	3615	1/1	0.91	0.09	30,30,30,30	0
57	MG	2E	302	1/1	0.91	0.09	41,41,41,41	0
57	MG	2A	3334	1/1	0.91	0.16	56,56,56,56	0
57	MG	2F	302	1/1	0.91	0.08	39,39,39,39	0
57	MG	1A	3170	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3139	1/1	0.91	0.10	44,44,44,44	0
57	MG	2A	3340	1/1	0.91	0.09	43,43,43,43	0
57	MG	2A	3146	1/1	0.91	0.14	55,55,55,55	0
57	MG	2T	202	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3345	1/1	0.91	0.11	64,64,64,64	0
57	MG	1R	202	1/1	0.91	0.18	56,56,56,56	0
57	MG	2Z	301	1/1	0.91	0.13	57,57,57,57	0
57	MG	2I	101	1/1	0.91	0.17	33,33,33,33	0
57	MG	2A	3632	1/1	0.91	0.14	61,61,61,61	0
57	MG	1a	1767	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3644	1/1	0.91	0.08	40,40,40,40	0
57	MG	28	102	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3653	1/1	0.91	0.08	41,41,41,41	0
57	MG	2A	3350	1/1	0.91	0.11	61,61,61,61	0
57	MG	2a	1603	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	1606	1/1	0.91	0.14	52,52,52,52	0
57	MG	2a	1607	1/1	0.91	0.26	54,54,54,54	0
57	MG	1A	3875	1/1	0.91	0.10	27,27,27,27	0
57	MG	2A	3353	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	4015	1/1	0.91	0.09	28,28,28,28	0
57	MG	2A	3668	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3878	1/1	0.91	0.24	27,27,27,27	0
57	MG	1A	3733	1/1	0.91	0.09	37,37,37,37	0
57	MG	1A	3885	1/1	0.91	0.08	29,29,29,29	0
57	MG	2A	3358	1/1	0.91	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1626	1/1	0.91	0.10	46,46,46,46	0
57	MG	1a	1783	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3641	1/1	0.91	0.14	53,53,53,53	0
57	MG	2a	1632	1/1	0.91	0.07	73,73,73,73	0
57	MG	2A	3685	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3362	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3098	1/1	0.91	0.08	50,50,50,50	0
57	MG	1a	1791	1/1	0.91	0.08	41,41,41,41	0
57	MG	1a	1792	1/1	0.91	0.08	68,68,68,68	0
57	MG	2a	1642	1/1	0.91	0.31	69,69,69,69	0
57	MG	1A	3186	1/1	0.91	0.06	28,28,28,28	0
57	MG	2A	3700	1/1	0.91	0.19	46,46,46,46	0
57	MG	1A	3751	1/1	0.91	0.08	46,46,46,46	0
57	MG	1A	3896	1/1	0.91	0.07	12,12,12,12	0
57	MG	1A	3047	1/1	0.91	0.06	12,12,12,12	0
57	MG	1A	3910	1/1	0.91	0.17	18,18,18,18	0
57	MG	2a	1659	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3378	1/1	0.91	0.15	56,56,56,56	0
57	MG	2a	1666	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3711	1/1	0.91	0.07	39,39,39,39	0
57	MG	2a	1673	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	3914	1/1	0.91	0.08	32,32,32,32	0
57	MG	2a	1678	1/1	0.91	0.31	66,66,66,66	0
57	MG	1l	201	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	3407	1/1	0.91	0.15	53,53,53,53	0
57	MG	18	105	1/1	0.91	0.20	54,54,54,54	0
57	MG	1a	1608	1/1	0.91	0.15	48,48,48,48	0
57	MG	1A	3923	1/1	0.91	0.13	50,50,50,50	0
57	MG	2A	3400	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3929	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3731	1/1	0.91	0.10	34,34,34,34	0
57	MG	1A	3494	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	4050	1/1	0.91	0.07	41,41,41,41	0
57	MG	1a	1636	1/1	0.91	0.17	50,50,50,50	0
57	MG	1A	4055	1/1	0.91	0.17	62,62,62,62	0
57	MG	1a	1640	1/1	0.91	0.15	46,46,46,46	0
57	MG	2a	1715	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3413	1/1	0.91	0.09	58,58,58,58	0
57	MG	1A	3322	1/1	0.91	0.08	34,34,34,34	0
57	MG	1A	4058	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3409	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3753	1/1	0.91	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3784	1/1	0.91	0.09	32,32,32,32	0
57	MG	2A	3760	1/1	0.91	0.11	32,32,32,32	0
57	MG	2a	1733	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3785	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3017	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3763	1/1	0.91	0.11	39,39,39,39	0
57	MG	1A	3659	1/1	0.91	0.09	33,33,33,33	0
57	MG	2A	3765	1/1	0.91	0.10	49,49,49,49	0
57	MG	2a	1753	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3438	1/1	0.91	0.26	56,56,56,56	0
57	MG	2a	1757	1/1	0.91	0.07	72,72,72,72	0
57	MG	2A	3257	1/1	0.91	0.16	55,55,55,55	0
57	MG	2a	1759	1/1	0.91	0.11	63,63,63,63	0
57	MG	2A	3441	1/1	0.91	0.11	53,53,53,53	0
57	MG	2A	3777	1/1	0.91	0.09	52,52,52,52	0
57	MG	2A	3261	1/1	0.91	0.10	47,47,47,47	0
57	MG	2A	3447	1/1	0.91	0.21	54,54,54,54	0
57	MG	2a	1773	1/1	0.91	0.08	64,64,64,64	0
57	MG	1a	1660	1/1	0.91	0.11	59,59,59,59	0
57	MG	2a	1777	1/1	0.91	0.18	47,47,47,47	0
57	MG	2a	1778	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3450	1/1	0.91	0.19	56,56,56,56	0
57	MG	2a	1787	1/1	0.91	0.09	65,65,65,65	0
57	MG	2A	3795	1/1	0.91	0.20	58,58,58,58	0
57	MG	2A	3452	1/1	0.91	0.08	46,46,46,46	0
57	MG	2A	3457	1/1	0.91	0.15	46,46,46,46	0
57	MG	1A	3258	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3271	1/1	0.91	0.31	61,61,61,61	0
57	MG	1a	1665	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3465	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3470	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3327	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3330	1/1	0.91	0.08	39,39,39,39	0
57	MG	1A	4093	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3264	1/1	0.91	0.17	59,59,59,59	0
57	MG	2A	3827	1/1	0.91	0.09	41,41,41,41	0
57	MG	1A	3073	1/1	0.91	0.22	66,66,66,66	0
57	MG	2A	3503	1/1	0.91	0.07	18,18,18,18	0
57	MG	2A	3505	1/1	0.91	0.12	38,38,38,38	0
57	MG	2a	1830	1/1	0.91	0.17	50,50,50,50	0
57	MG	1a	1689	1/1	0.91	0.13	69,69,69,69	0
57	MG	2A	3508	1/1	0.91	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3512	1/1	0.91	0.07	47,47,47,47	0
57	MG	2d	301	1/1	0.91	0.20	54,54,54,54	0
57	MG	2A	3513	1/1	0.91	0.10	64,64,64,64	0
57	MG	2A	3856	1/1	0.91	0.09	40,40,40,40	0
57	MG	2A	3864	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3686	1/1	0.91	0.12	46,46,46,46	0
57	MG	2A	3281	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3517	1/1	0.91	0.18	55,55,55,55	0
57	MG	2A	3518	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3078	1/1	0.91	0.09	39,39,39,39	0
57	MG	1A	3450	1/1	0.91	0.07	47,47,47,47	0
57	MG	1a	1707	1/1	0.91	0.10	61,61,61,61	0
57	MG	2A	3290	1/1	0.91	0.12	65,65,65,65	0
57	MG	1A	3457	1/1	0.91	0.25	34,34,34,34	0
57	MG	1A	3466	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3570	1/1	0.91	0.13	54,54,54,54	0
57	MG	1B	210	1/1	0.91	0.10	45,45,45,45	0
57	MG	2w	107	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3131	1/1	0.91	0.19	47,47,47,47	0
57	MG	1A	3271	1/1	0.91	0.07	25,25,25,25	0
57	MG	2x	103	1/1	0.91	0.13	64,64,64,64	0
57	MG	1A	3598	1/1	0.91	0.31	60,60,60,60	0
57	MG	1B	224	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3577	1/1	0.91	0.07	33,33,33,33	0
57	MG	1A	3158	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	3723	1/1	0.91	0.07	36,36,36,36	0
57	MG	1A	3997	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3460	1/1	0.92	0.06	34,34,34,34	0
57	MG	1A	3572	1/1	0.92	0.08	42,42,42,42	0
57	MG	1A	3870	1/1	0.92	0.12	34,34,34,34	0
57	MG	1a	1799	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3872	1/1	0.92	0.23	40,40,40,40	0
57	MG	1A	3359	1/1	0.92	0.15	46,46,46,46	0
57	MG	1A	3057	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3527	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3529	1/1	0.92	0.14	45,45,45,45	0
57	MG	1A	3058	1/1	0.92	0.09	29,29,29,29	0
57	MG	1a	1813	1/1	0.92	0.07	56,56,56,56	0
57	MG	2A	3547	1/1	0.92	0.10	49,49,49,49	0
57	MG	1b	301	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3385	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3269	1/1	0.92	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3605	1/1	0.92	0.11	47,47,47,47	0
57	MG	2E	304	1/1	0.92	0.11	35,35,35,35	0
57	MG	15	103	1/1	0.92	0.19	29,29,29,29	0
57	MG	2F	301	1/1	0.92	0.31	40,40,40,40	0
57	MG	1n	102	1/1	0.92	0.14	38,38,38,38	0
57	MG	15	106	1/1	0.92	0.19	35,35,35,35	0
57	MG	1A	4026	1/1	0.92	0.08	37,37,37,37	0
57	MG	2P	202	1/1	0.92	0.17	47,47,47,47	0
57	MG	2P	203	1/1	0.92	0.07	52,52,52,52	0
57	MG	2A	3575	1/1	0.92	0.07	29,29,29,29	0
57	MG	1A	3729	1/1	0.92	0.09	37,37,37,37	0
57	MG	2A	3581	1/1	0.92	0.16	64,64,64,64	0
57	MG	2A	3582	1/1	0.92	0.10	33,33,33,33	0
57	MG	1A	3326	1/1	0.92	0.11	25,25,25,25	0
57	MG	1A	3391	1/1	0.92	0.24	39,39,39,39	0
57	MG	20	101	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3392	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3589	1/1	0.92	0.12	27,27,27,27	0
57	MG	1a	1604	1/1	0.92	0.16	53,53,53,53	0
57	MG	1a	1606	1/1	0.92	0.12	57,57,57,57	0
57	MG	28	101	1/1	0.92	0.10	54,54,54,54	0
57	MG	1x	108	1/1	0.92	0.23	58,58,58,58	0
57	MG	2A	3287	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3892	1/1	0.92	0.07	29,29,29,29	0
57	MG	2A	3609	1/1	0.92	0.17	51,51,51,51	0
57	MG	1A	3197	1/1	0.92	0.19	39,39,39,39	0
57	MG	1y	101	1/1	0.92	0.08	58,58,58,58	0
57	MG	2a	1608	1/1	0.92	0.20	58,58,58,58	0
57	MG	1a	1614	1/1	0.92	0.07	57,57,57,57	0
57	MG	2A	3293	1/1	0.92	0.14	54,54,54,54	0
57	MG	2a	1611	1/1	0.92	0.14	45,45,45,45	0
57	MG	1a	1615	1/1	0.92	0.14	54,54,54,54	0
57	MG	2A	3621	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3484	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3297	1/1	0.92	0.18	53,53,53,53	0
57	MG	2A	3625	1/1	0.92	0.07	47,47,47,47	0
57	MG	1A	3328	1/1	0.92	0.13	39,39,39,39	0
57	MG	2A	3300	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	4042	1/1	0.92	0.08	25,25,25,25	0
57	MG	2A	3652	1/1	0.92	0.07	43,43,43,43	0
57	MG	2A	3303	1/1	0.92	0.10	63,63,63,63	0
57	MG	1a	1635	1/1	0.92	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1636	1/1	0.92	0.22	52,52,52,52	0
57	MG	2A	3029	1/1	0.92	0.15	61,61,61,61	0
57	MG	2A	3307	1/1	0.92	0.16	49,49,49,49	0
57	MG	2A	3308	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3667	1/1	0.92	0.17	50,50,50,50	0
57	MG	2A	3030	1/1	0.92	0.14	43,43,43,43	0
57	MG	1A	4043	1/1	0.92	0.14	40,40,40,40	0
57	MG	2A	3672	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3674	1/1	0.92	0.09	40,40,40,40	0
57	MG	2a	1650	1/1	0.92	0.13	61,61,61,61	0
57	MG	2a	1652	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	4044	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3043	1/1	0.92	0.25	45,45,45,45	0
57	MG	2A	3319	1/1	0.92	0.17	62,62,62,62	0
57	MG	2a	1658	1/1	0.92	0.08	48,48,48,48	0
57	MG	2A	3046	1/1	0.92	0.24	58,58,58,58	0
57	MG	2a	1663	1/1	0.92	0.16	57,57,57,57	0
57	MG	2A	3048	1/1	0.92	0.09	41,41,41,41	0
57	MG	2A	3052	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3686	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3906	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3055	1/1	0.92	0.12	47,47,47,47	0
57	MG	1A	3909	1/1	0.92	0.13	24,24,24,24	0
57	MG	1A	3750	1/1	0.92	0.13	56,56,56,56	0
57	MG	1a	1645	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3699	1/1	0.92	0.09	52,52,52,52	0
57	MG	2a	1691	1/1	0.92	0.27	56,56,56,56	0
57	MG	1a	1646	1/1	0.92	0.18	49,49,49,49	0
57	MG	1A	3248	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	3332	1/1	0.92	0.07	37,37,37,37	0
57	MG	1A	3757	1/1	0.92	0.17	43,43,43,43	0
57	MG	1A	3928	1/1	0.92	0.09	53,53,53,53	0
57	MG	2a	1702	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3129	1/1	0.92	0.09	34,34,34,34	0
57	MG	1A	3495	1/1	0.92	0.11	39,39,39,39	0
57	MG	1A	3940	1/1	0.92	0.07	45,45,45,45	0
57	MG	1a	1668	1/1	0.92	0.12	49,49,49,49	0
57	MG	2a	1712	1/1	0.92	0.17	56,56,56,56	0
57	MG	2a	1713	1/1	0.92	0.11	48,48,48,48	0
57	MG	1a	1669	1/1	0.92	0.22	44,44,44,44	0
57	MG	1A	3410	1/1	0.92	0.07	34,34,34,34	0
57	MG	1A	3183	1/1	0.92	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3658	1/1	0.92	0.05	18,18,18,18	0
57	MG	1A	3415	1/1	0.92	0.30	59,59,59,59	0
57	MG	1A	3662	1/1	0.92	0.07	37,37,37,37	0
57	MG	1a	1683	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3105	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1684	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3804	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	1737	1/1	0.92	0.13	55,55,55,55	0
57	MG	2a	1740	1/1	0.92	0.08	51,51,51,51	0
57	MG	1a	1692	1/1	0.92	0.24	43,43,43,43	0
57	MG	2A	3112	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3374	1/1	0.92	0.16	33,33,33,33	0
57	MG	2A	3114	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3525	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3416	1/1	0.92	0.09	39,39,39,39	0
57	MG	2a	1754	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3818	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3534	1/1	0.92	0.10	33,33,33,33	0
57	MG	2A	3129	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3670	1/1	0.92	0.15	33,33,33,33	0
57	MG	1A	3296	1/1	0.92	0.17	50,50,50,50	0
57	MG	2A	3143	1/1	0.92	0.19	41,41,41,41	0
57	MG	1a	1719	1/1	0.92	0.31	54,54,54,54	0
57	MG	2a	1770	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3147	1/1	0.92	0.21	59,59,59,59	0
57	MG	1B	213	1/1	0.92	0.20	63,63,63,63	0
57	MG	2A	3159	1/1	0.92	0.27	51,51,51,51	0
57	MG	2A	3771	1/1	0.92	0.16	57,57,57,57	0
57	MG	2A	3775	1/1	0.92	0.15	48,48,48,48	0
57	MG	2a	1783	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3970	1/1	0.92	0.07	24,24,24,24	0
57	MG	2A	3164	1/1	0.92	0.14	53,53,53,53	0
57	MG	1B	215	1/1	0.92	0.08	45,45,45,45	0
57	MG	1A	3540	1/1	0.92	0.15	30,30,30,30	0
57	MG	2a	1791	1/1	0.92	0.11	66,66,66,66	0
57	MG	2a	1796	1/1	0.92	0.08	43,43,43,43	0
57	MG	1a	1736	1/1	0.92	0.16	51,51,51,51	0
57	MG	2A	3177	1/1	0.92	0.10	44,44,44,44	0
57	MG	2a	1802	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3793	1/1	0.92	0.10	58,58,58,58	0
57	MG	1a	1737	1/1	0.92	0.10	45,45,45,45	0
57	MG	1B	218	1/1	0.92	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1808	1/1	0.92	0.11	50,50,50,50	0
57	MG	2A	3801	1/1	0.92	0.09	52,52,52,52	0
57	MG	2a	1810	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3681	1/1	0.92	0.10	16,16,16,16	0
57	MG	2a	1816	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3804	1/1	0.92	0.09	36,36,36,36	0
57	MG	2A	3806	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3339	1/1	0.92	0.08	40,40,40,40	0
57	MG	2A	3432	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3298	1/1	0.92	0.08	38,38,38,38	0
57	MG	1A	3981	1/1	0.92	0.08	73,73,73,73	0
57	MG	1A	3851	1/1	0.92	0.10	43,43,43,43	0
57	MG	1a	1752	1/1	0.92	0.08	41,41,41,41	0
57	MG	1A	3987	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3197	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3448	1/1	0.92	0.13	38,38,38,38	0
57	MG	1D	306	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3828	1/1	0.92	0.08	33,33,33,33	0
57	MG	2A	3835	1/1	0.92	0.10	43,43,43,43	0
57	MG	2i	201	1/1	0.92	0.17	66,66,66,66	0
57	MG	1A	3852	1/1	0.92	0.12	42,42,42,42	0
57	MG	2l	201	1/1	0.92	0.08	59,59,59,59	0
57	MG	1E	310	1/1	0.92	0.08	24,24,24,24	0
57	MG	2A	3453	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3455	1/1	0.92	0.10	49,49,49,49	0
57	MG	1E	313	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3208	1/1	0.92	0.08	53,53,53,53	0
57	MG	1a	1765	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3702	1/1	0.92	0.11	28,28,28,28	0
57	MG	2A	3857	1/1	0.92	0.08	39,39,39,39	0
57	MG	1A	3706	1/1	0.92	0.10	17,17,17,17	0
57	MG	2A	3867	1/1	0.92	0.16	45,45,45,45	0
57	MG	2A	3214	1/1	0.92	0.18	45,45,45,45	0
57	MG	2A	3215	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3708	1/1	0.92	0.15	49,49,49,49	0
57	MG	2A	3871	1/1	0.92	0.10	50,50,50,50	0
57	MG	1Q	204	1/1	0.92	0.08	58,58,58,58	0
57	MG	1A	3220	1/1	0.92	0.08	39,39,39,39	0
57	MG	1a	1775	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3345	1/1	0.92	0.13	50,50,50,50	0
57	MG	2y	103	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3027	1/1	0.92	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1T	203	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3237	1/1	0.92	0.10	50,50,50,50	0
57	MG	1U	203	1/1	0.92	0.09	47,47,47,47	0
57	MG	2A	3042	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3300	1/1	0.93	0.17	49,49,49,49	0
57	MG	2A	3044	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3453	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3346	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	3302	1/1	0.93	0.17	34,34,34,34	0
57	MG	1A	3357	1/1	0.93	0.14	54,54,54,54	0
57	MG	2N	201	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3924	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3925	1/1	0.93	0.06	39,39,39,39	0
57	MG	2A	3604	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3058	1/1	0.93	0.17	46,46,46,46	0
57	MG	1A	4096	1/1	0.93	0.14	54,54,54,54	0
57	MG	1a	1678	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3739	1/1	0.93	0.09	35,35,35,35	0
57	MG	2W	201	1/1	0.93	0.14	57,57,57,57	0
57	MG	2W	203	1/1	0.93	0.09	35,35,35,35	0
57	MG	2A	3069	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3610	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3073	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3617	1/1	0.93	0.08	57,57,57,57	0
57	MG	25	101	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3930	1/1	0.93	0.09	28,28,28,28	0
57	MG	1A	3358	1/1	0.93	0.08	53,53,53,53	0
57	MG	1a	1686	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3310	1/1	0.93	0.22	39,39,39,39	0
57	MG	2A	3082	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3627	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3311	1/1	0.93	0.09	45,45,45,45	0
57	MG	2a	1605	1/1	0.93	0.24	56,56,56,56	0
57	MG	2A	3636	1/1	0.93	0.07	25,25,25,25	0
57	MG	2A	3638	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3321	1/1	0.93	0.13	46,46,46,46	0
57	MG	2A	3642	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3619	1/1	0.93	0.08	21,21,21,21	0
57	MG	2A	3650	1/1	0.93	0.13	38,38,38,38	0
57	MG	1a	1698	1/1	0.93	0.09	40,40,40,40	0
57	MG	2a	1617	1/1	0.93	0.06	41,41,41,41	0
57	MG	1a	1699	1/1	0.93	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3092	1/1	0.93	0.11	47,47,47,47	0
57	MG	2A	3655	1/1	0.93	0.07	42,42,42,42	0
57	MG	1a	1701	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3759	1/1	0.93	0.06	31,31,31,31	0
57	MG	1A	3053	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3949	1/1	0.93	0.15	51,51,51,51	0
57	MG	1a	1709	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3669	1/1	0.93	0.10	55,55,55,55	0
57	MG	2a	1633	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3764	1/1	0.93	0.11	33,33,33,33	0
57	MG	2A	3671	1/1	0.93	0.10	48,48,48,48	0
57	MG	2a	1637	1/1	0.93	0.14	50,50,50,50	0
57	MG	1a	1713	1/1	0.93	0.17	53,53,53,53	0
57	MG	1a	1715	1/1	0.93	0.18	48,48,48,48	0
57	MG	1A	3767	1/1	0.93	0.08	19,19,19,19	0
57	MG	1A	3062	1/1	0.93	0.27	51,51,51,51	0
57	MG	1A	3109	1/1	0.93	0.06	29,29,29,29	0
57	MG	1A	3390	1/1	0.93	0.25	31,31,31,31	0
57	MG	1A	3207	1/1	0.93	0.09	45,45,45,45	0
57	MG	1B	230	1/1	0.93	0.07	50,50,50,50	0
57	MG	1A	3485	1/1	0.93	0.09	43,43,43,43	0
57	MG	2a	1651	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3325	1/1	0.93	0.11	38,38,38,38	0
57	MG	2A	3128	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3797	1/1	0.93	0.11	51,51,51,51	0
57	MG	1E	302	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3802	1/1	0.93	0.08	13,13,13,13	0
57	MG	1A	3115	1/1	0.93	0.16	36,36,36,36	0
57	MG	2a	1660	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3368	1/1	0.93	0.17	45,45,45,45	0
57	MG	2a	1664	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3399	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3703	1/1	0.93	0.10	76,76,76,76	0
57	MG	1a	1748	1/1	0.93	0.07	51,51,51,51	0
57	MG	2a	1672	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	3401	1/1	0.93	0.08	40,40,40,40	0
57	MG	2A	3155	1/1	0.93	0.11	49,49,49,49	0
57	MG	1N	205	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3219	1/1	0.93	0.08	42,42,42,42	0
57	MG	2a	1681	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	1754	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3165	1/1	0.93	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3381	1/1	0.93	0.07	56,56,56,56	0
57	MG	2a	1693	1/1	0.93	0.12	46,46,46,46	0
57	MG	2a	1694	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3170	1/1	0.93	0.14	48,48,48,48	0
57	MG	2a	1696	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3385	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3496	1/1	0.93	0.21	36,36,36,36	0
57	MG	2A	3388	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3500	1/1	0.93	0.09	53,53,53,53	0
57	MG	1Q	206	1/1	0.93	0.15	40,40,40,40	0
57	MG	2a	1703	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3118	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3184	1/1	0.93	0.12	46,46,46,46	0
57	MG	2a	1709	1/1	0.93	0.11	61,61,61,61	0
57	MG	2A	3181	1/1	0.93	0.19	47,47,47,47	0
57	MG	2A	3744	1/1	0.93	0.06	36,36,36,36	0
57	MG	2A	3402	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3403	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3182	1/1	0.93	0.22	54,54,54,54	0
57	MG	2A	3408	1/1	0.93	0.08	58,58,58,58	0
57	MG	1T	202	1/1	0.93	0.08	57,57,57,57	0
57	MG	2a	1718	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3991	1/1	0.93	0.05	23,23,23,23	0
57	MG	1A	3993	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3757	1/1	0.93	0.08	35,35,35,35	0
57	MG	1A	3994	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3006	1/1	0.93	0.07	27,27,27,27	0
57	MG	2a	1728	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3673	1/1	0.93	0.10	23,23,23,23	0
57	MG	1A	3845	1/1	0.93	0.06	26,26,26,26	0
57	MG	2a	1735	1/1	0.93	0.15	42,42,42,42	0
57	MG	2a	1736	1/1	0.93	0.10	54,54,54,54	0
57	MG	1Z	3703	1/1	0.93	0.07	32,32,32,32	0
57	MG	2a	1738	1/1	0.93	0.18	50,50,50,50	0
57	MG	2A	3423	1/1	0.93	0.19	43,43,43,43	0
57	MG	1A	3523	1/1	0.93	0.08	62,62,62,62	0
57	MG	10	105	1/1	0.93	0.13	62,62,62,62	0
57	MG	1a	1790	1/1	0.93	0.06	47,47,47,47	0
57	MG	2A	3769	1/1	0.93	0.11	64,64,64,64	0
57	MG	1A	3850	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3524	1/1	0.93	0.18	53,53,53,53	0
57	MG	1A	3334	1/1	0.93	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3189	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3210	1/1	0.93	0.06	37,37,37,37	0
57	MG	2A	3442	1/1	0.93	0.35	60,60,60,60	0
57	MG	2A	3782	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3443	1/1	0.93	0.15	48,48,48,48	0
57	MG	2A	3444	1/1	0.93	0.14	58,58,58,58	0
57	MG	1a	1802	1/1	0.93	0.10	52,52,52,52	0
57	MG	2a	1769	1/1	0.93	0.12	40,40,40,40	0
57	MG	1a	1803	1/1	0.93	0.08	67,67,67,67	0
57	MG	2A	3797	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3688	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3690	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3694	1/1	0.93	0.08	24,24,24,24	0
57	MG	1A	3533	1/1	0.93	0.11	39,39,39,39	0
57	MG	17	107	1/1	0.93	0.11	39,39,39,39	0
57	MG	2A	3221	1/1	0.93	0.13	41,41,41,41	0
57	MG	2A	3808	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3863	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3223	1/1	0.93	0.21	49,49,49,49	0
57	MG	1d	301	1/1	0.93	0.16	50,50,50,50	0
57	MG	2a	1794	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3701	1/1	0.93	0.10	26,26,26,26	0
57	MG	2A	3230	1/1	0.93	0.17	40,40,40,40	0
57	MG	2A	3816	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	1801	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3466	1/1	0.93	0.06	44,44,44,44	0
57	MG	1A	3288	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3471	1/1	0.93	0.08	46,46,46,46	0
57	MG	2A	3475	1/1	0.93	0.10	62,62,62,62	0
57	MG	2A	3483	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3232	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3233	1/1	0.93	0.24	52,52,52,52	0
57	MG	2A	3495	1/1	0.93	0.09	59,59,59,59	0
57	MG	2a	1813	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3016	1/1	0.93	0.09	50,50,50,50	0
57	MG	2A	3842	1/1	0.93	0.08	54,54,54,54	0
57	MG	2A	3240	1/1	0.93	0.10	32,32,32,32	0
57	MG	2a	1820	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3417	1/1	0.93	0.12	36,36,36,36	0
57	MG	2A	3852	1/1	0.93	0.08	60,60,60,60	0
57	MG	1A	3295	1/1	0.93	0.10	42,42,42,42	0
57	MG	2a	1825	1/1	0.93	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1611	1/1	0.93	0.11	51,51,51,51	0
57	MG	2A	3248	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3421	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3550	1/1	0.93	0.11	51,51,51,51	0
57	MG	2a	1832	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3715	1/1	0.93	0.10	65,65,65,65	0
57	MG	1a	1621	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3876	1/1	0.93	0.06	25,25,25,25	0
57	MG	2A	3516	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	3427	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3872	1/1	0.93	0.15	56,56,56,56	0
57	MG	2j	201	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3875	1/1	0.93	0.22	52,52,52,52	0
57	MG	1x	104	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3881	1/1	0.93	0.09	51,51,51,51	0
57	MG	1a	1629	1/1	0.93	0.15	44,44,44,44	0
57	MG	1A	3560	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	3719	1/1	0.93	0.05	10,10,10,10	0
57	MG	2q	201	1/1	0.93	0.19	59,59,59,59	0
57	MG	1A	3886	1/1	0.93	0.07	31,31,31,31	0
57	MG	2r	102	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	4045	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	3720	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3541	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3241	1/1	0.93	0.07	30,30,30,30	0
57	MG	1A	3245	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3565	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3023	1/1	0.93	0.17	63,63,63,63	0
57	MG	2w	106	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3566	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3726	1/1	0.93	0.07	23,23,23,23	0
57	MG	2A	3563	1/1	0.93	0.11	40,40,40,40	0
57	MG	1A	3344	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3900	1/1	0.93	0.20	58,58,58,58	0
57	MG	2A	3566	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3284	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3572	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3439	1/1	0.93	0.26	49,49,49,49	0
57	MG	2A	3037	1/1	0.93	0.08	37,37,37,37	0
59	A1C9N	1A	4101	74/74	0.93	0.12	13,37,50,51	0
57	MG	2A	3579	1/1	0.93	0.09	54,54,54,54	0
57	MG	2A	3238	1/1	0.94	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3580	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3458	1/1	0.94	0.11	46,46,46,46	0
57	MG	2A	3242	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3305	1/1	0.94	0.12	36,36,36,36	0
57	MG	2A	3525	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	4030	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3528	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3247	1/1	0.94	0.09	52,52,52,52	0
57	MG	1m	3001	1/1	0.94	0.08	36,36,36,36	0
57	MG	17	106	1/1	0.94	0.07	35,35,35,35	0
57	MG	2A	3251	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3544	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3546	1/1	0.94	0.16	41,41,41,41	0
57	MG	1n	101	1/1	0.94	0.17	40,40,40,40	0
57	MG	1A	3728	1/1	0.94	0.13	42,42,42,42	0
57	MG	2A	3552	1/1	0.94	0.07	32,32,32,32	0
57	MG	2F	304	1/1	0.94	0.17	39,39,39,39	0
57	MG	1A	3375	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3377	1/1	0.94	0.14	39,39,39,39	0
57	MG	18	104	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3234	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3028	1/1	0.94	0.10	42,42,42,42	0
57	MG	2Q	201	1/1	0.94	0.15	52,52,52,52	0
57	MG	2Q	202	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3178	1/1	0.94	0.05	23,23,23,23	0
57	MG	1w	107	1/1	0.94	0.06	56,56,56,56	0
57	MG	1a	1607	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3893	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3571	1/1	0.94	0.06	37,37,37,37	0
57	MG	1a	1609	1/1	0.94	0.07	44,44,44,44	0
57	MG	2W	202	1/1	0.94	0.08	40,40,40,40	0
57	MG	1x	106	1/1	0.94	0.23	51,51,51,51	0
57	MG	2X	101	1/1	0.94	0.07	60,60,60,60	0
57	MG	1A	3180	1/1	0.94	0.06	34,34,34,34	0
57	MG	1A	3112	1/1	0.94	0.13	27,27,27,27	0
57	MG	20	102	1/1	0.94	0.18	50,50,50,50	0
57	MG	1A	3740	1/1	0.94	0.08	55,55,55,55	0
57	MG	1x	114	1/1	0.94	0.10	36,36,36,36	0
57	MG	1A	3743	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3280	1/1	0.94	0.11	37,37,37,37	0
57	MG	2A	3002	1/1	0.94	0.22	44,44,44,44	0
57	MG	27	102	1/1	0.94	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1619	1/1	0.94	0.08	37,37,37,37	0
57	MG	1A	3903	1/1	0.94	0.09	31,31,31,31	0
57	MG	1A	3618	1/1	0.94	0.05	20,20,20,20	0
57	MG	2A	3006	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	3054	1/1	0.94	0.10	24,24,24,24	0
57	MG	2a	1604	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3605	1/1	0.94	0.08	40,40,40,40	0
57	MG	1A	3324	1/1	0.94	0.15	43,43,43,43	0
57	MG	2A	3018	1/1	0.94	0.18	48,48,48,48	0
57	MG	2A	3022	1/1	0.94	0.16	41,41,41,41	0
57	MG	1a	1631	1/1	0.94	0.14	39,39,39,39	0
57	MG	1a	1633	1/1	0.94	0.24	55,55,55,55	0
57	MG	1A	3912	1/1	0.94	0.07	36,36,36,36	0
57	MG	2a	1614	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	4059	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3637	1/1	0.94	0.14	43,43,43,43	0
57	MG	2A	3032	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	4065	1/1	0.94	0.05	34,34,34,34	0
57	MG	2a	1621	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3302	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	4066	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3397	1/1	0.94	0.06	27,27,27,27	0
57	MG	1A	3920	1/1	0.94	0.05	24,24,24,24	0
57	MG	2a	1628	1/1	0.94	0.22	52,52,52,52	0
57	MG	2A	3629	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3643	1/1	0.94	0.06	34,34,34,34	0
57	MG	2A	3633	1/1	0.94	0.17	48,48,48,48	0
57	MG	1A	4078	1/1	0.94	0.07	30,30,30,30	0
57	MG	1A	4080	1/1	0.94	0.08	44,44,44,44	0
57	MG	1a	1650	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3185	1/1	0.94	0.10	56,56,56,56	0
57	MG	1a	1655	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3648	1/1	0.94	0.13	44,44,44,44	0
57	MG	1a	1656	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3488	1/1	0.94	0.10	36,36,36,36	0
57	MG	1A	3007	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	4092	1/1	0.94	0.10	44,44,44,44	0
57	MG	2a	1645	1/1	0.94	0.09	44,44,44,44	0
57	MG	2a	1647	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3402	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3325	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3263	1/1	0.94	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3660	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3332	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3665	1/1	0.94	0.06	49,49,49,49	0
57	MG	2A	3333	1/1	0.94	0.34	54,54,54,54	0
57	MG	1A	3771	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3336	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3406	1/1	0.94	0.25	28,28,28,28	0
57	MG	1A	3187	1/1	0.94	0.10	28,28,28,28	0
57	MG	2A	3339	1/1	0.94	0.09	57,57,57,57	0
57	MG	2A	3673	1/1	0.94	0.07	27,27,27,27	0
57	MG	1a	1671	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3341	1/1	0.94	0.08	48,48,48,48	0
57	MG	2a	1669	1/1	0.94	0.07	47,47,47,47	0
57	MG	1a	1674	1/1	0.94	0.06	44,44,44,44	0
57	MG	1a	1675	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3680	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3346	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3081	1/1	0.94	0.20	28,28,28,28	0
57	MG	1A	3793	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3503	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3796	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3088	1/1	0.94	0.07	33,33,33,33	0
57	MG	2a	1689	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	1690	1/1	0.94	0.08	49,49,49,49	0
57	MG	1B	212	1/1	0.94	0.05	44,44,44,44	0
57	MG	1A	3333	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3697	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3195	1/1	0.94	0.09	25,25,25,25	0
57	MG	1a	1688	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3093	1/1	0.94	0.06	44,44,44,44	0
57	MG	1A	3961	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3275	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3145	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3674	1/1	0.94	0.06	32,32,32,32	0
57	MG	2A	3107	1/1	0.94	0.13	42,42,42,42	0
57	MG	2a	1704	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1705	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3528	1/1	0.94	0.28	52,52,52,52	0
57	MG	2a	1707	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3149	1/1	0.94	0.17	30,30,30,30	0
57	MG	2A	3369	1/1	0.94	0.10	57,57,57,57	0
57	MG	1a	1705	1/1	0.94	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3832	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3835	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3373	1/1	0.94	0.07	48,48,48,48	0
57	MG	1B	231	1/1	0.94	0.19	42,42,42,42	0
57	MG	1B	232	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3836	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3127	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3734	1/1	0.94	0.06	23,23,23,23	0
57	MG	2A	3379	1/1	0.94	0.20	48,48,48,48	0
57	MG	1D	303	1/1	0.94	0.10	34,34,34,34	0
57	MG	2a	1724	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3738	1/1	0.94	0.09	60,60,60,60	0
57	MG	1a	1716	1/1	0.94	0.16	41,41,41,41	0
57	MG	2A	3743	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3132	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3134	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3386	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3419	1/1	0.94	0.07	44,44,44,44	0
57	MG	1A	3151	1/1	0.94	0.07	20,20,20,20	0
57	MG	1A	3984	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3751	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3393	1/1	0.94	0.10	47,47,47,47	0
57	MG	2a	1742	1/1	0.94	0.20	60,60,60,60	0
57	MG	1E	303	1/1	0.94	0.10	41,41,41,41	0
57	MG	1E	307	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3148	1/1	0.94	0.21	49,49,49,49	0
57	MG	2A	3151	1/1	0.94	0.07	57,57,57,57	0
57	MG	2a	1752	1/1	0.94	0.07	55,55,55,55	0
57	MG	1E	308	1/1	0.94	0.10	35,35,35,35	0
57	MG	1A	3985	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3687	1/1	0.94	0.05	15,15,15,15	0
57	MG	2A	3161	1/1	0.94	0.08	40,40,40,40	0
57	MG	1A	3290	1/1	0.94	0.11	46,46,46,46	0
57	MG	1F	311	1/1	0.94	0.07	34,34,34,34	0
57	MG	1F	312	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3169	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3770	1/1	0.94	0.11	48,48,48,48	0
57	MG	1G	203	1/1	0.94	0.07	60,60,60,60	0
57	MG	2A	3774	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3153	1/1	0.94	0.10	34,34,34,34	0
57	MG	1a	1747	1/1	0.94	0.07	48,48,48,48	0
57	MG	1N	202	1/1	0.94	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3419	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3421	1/1	0.94	0.20	41,41,41,41	0
57	MG	1N	204	1/1	0.94	0.23	43,43,43,43	0
57	MG	2A	3790	1/1	0.94	0.10	49,49,49,49	0
57	MG	1a	1751	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3542	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3429	1/1	0.94	0.06	27,27,27,27	0
57	MG	2a	1790	1/1	0.94	0.07	41,41,41,41	0
57	MG	1P	203	1/1	0.94	0.21	32,32,32,32	0
57	MG	2A	3796	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3433	1/1	0.94	0.14	42,42,42,42	0
57	MG	2A	3798	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3434	1/1	0.94	0.26	52,52,52,52	0
57	MG	2a	1800	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3800	1/1	0.94	0.10	52,52,52,52	0
57	MG	1Q	201	1/1	0.94	0.22	32,32,32,32	0
57	MG	2A	3437	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3803	1/1	0.94	0.11	44,44,44,44	0
57	MG	2a	1805	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3188	1/1	0.94	0.08	46,46,46,46	0
57	MG	2a	1807	1/1	0.94	0.24	52,52,52,52	0
57	MG	2A	3439	1/1	0.94	0.24	51,51,51,51	0
57	MG	1A	3431	1/1	0.94	0.09	37,37,37,37	0
57	MG	1a	1759	1/1	0.94	0.13	47,47,47,47	0
57	MG	1A	3548	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3995	1/1	0.94	0.47	35,35,35,35	0
57	MG	2a	1814	1/1	0.94	0.10	56,56,56,56	0
57	MG	1a	1763	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3294	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3435	1/1	0.94	0.12	38,38,38,38	0
57	MG	1T	201	1/1	0.94	0.15	42,42,42,42	0
57	MG	2A	3819	1/1	0.94	0.06	57,57,57,57	0
57	MG	2A	3199	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3201	1/1	0.94	0.08	43,43,43,43	0
57	MG	2A	3451	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3999	1/1	0.94	0.08	42,42,42,42	0
57	MG	2a	1828	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3203	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3830	1/1	0.94	0.06	35,35,35,35	0
57	MG	2A	3831	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3552	1/1	0.94	0.10	31,31,31,31	0
57	MG	1A	3217	1/1	0.94	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3207	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3042	1/1	0.94	0.14	23,23,23,23	0
57	MG	1a	1779	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3843	1/1	0.94	0.08	39,39,39,39	0
57	MG	1W	206	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3848	1/1	0.94	0.09	58,58,58,58	0
57	MG	1X	107	1/1	0.94	0.06	44,44,44,44	0
57	MG	2A	3467	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3468	1/1	0.94	0.09	54,54,54,54	0
57	MG	1Y	201	1/1	0.94	0.06	40,40,40,40	0
57	MG	2A	3855	1/1	0.94	0.08	54,54,54,54	0
57	MG	2m	201	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3448	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3563	1/1	0.94	0.11	35,35,35,35	0
57	MG	2A	3860	1/1	0.94	0.16	46,46,46,46	0
57	MG	2r	101	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3482	1/1	0.94	0.08	58,58,58,58	0
57	MG	2t	201	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3159	1/1	0.94	0.06	47,47,47,47	0
57	MG	2A	3484	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	4013	1/1	0.94	0.08	27,27,27,27	0
57	MG	1A	3869	1/1	0.94	0.05	39,39,39,39	0
57	MG	2A	3490	1/1	0.94	0.13	52,52,52,52	0
57	MG	2A	3494	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3168	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3454	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3880	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3025	1/1	0.94	0.09	34,34,34,34	0
57	MG	10	108	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3225	1/1	0.94	0.22	54,54,54,54	0
57	MG	1a	1807	1/1	0.94	0.07	36,36,36,36	0
57	MG	2x	105	1/1	0.94	0.16	39,39,39,39	0
57	MG	1a	1808	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3507	1/1	0.94	0.08	63,63,63,63	0
57	MG	1A	3576	1/1	0.94	0.15	35,35,35,35	0
57	MG	12	101	1/1	0.94	0.07	38,38,38,38	0
57	MG	13	103	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3236	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3577	1/1	0.94	0.17	36,36,36,36	0
57	MG	1A	3932	1/1	0.95	0.07	44,44,44,44	0
57	MG	1a	1722	1/1	0.95	0.14	41,41,41,41	0
57	MG	1D	308	1/1	0.95	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3070	1/1	0.95	0.07	26,26,26,26	0
57	MG	2A	3186	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3474	1/1	0.95	0.08	47,47,47,47	0
57	MG	1a	1727	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3476	1/1	0.95	0.09	32,32,32,32	0
57	MG	2A	3874	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3479	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3876	1/1	0.95	0.14	44,44,44,44	0
57	MG	2A	3877	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3480	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3481	1/1	0.95	0.11	30,30,30,30	0
57	MG	1a	1728	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3579	1/1	0.95	0.09	39,39,39,39	0
57	MG	1a	1733	1/1	0.95	0.07	31,31,31,31	0
57	MG	1a	1734	1/1	0.95	0.06	30,30,30,30	0
57	MG	1a	1735	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3941	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3492	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3742	1/1	0.95	0.07	54,54,54,54	0
57	MG	2B	206	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3182	1/1	0.95	0.05	28,28,28,28	0
57	MG	2A	3496	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3583	1/1	0.95	0.04	22,22,22,22	0
57	MG	2A	3499	1/1	0.95	0.05	49,49,49,49	0
57	MG	1E	312	1/1	0.95	0.06	51,51,51,51	0
57	MG	1a	1742	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3749	1/1	0.95	0.06	9,9,9,9	0
57	MG	1A	3584	1/1	0.95	0.06	32,32,32,32	0
57	MG	1F	305	1/1	0.95	0.04	39,39,39,39	0
57	MG	1F	310	1/1	0.95	0.19	29,29,29,29	0
57	MG	1A	3587	1/1	0.95	0.05	39,39,39,39	0
57	MG	2B	218	1/1	0.95	0.09	60,60,60,60	0
57	MG	2B	219	1/1	0.95	0.16	55,55,55,55	0
57	MG	2A	3510	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3954	1/1	0.95	0.06	45,45,45,45	0
57	MG	2D	305	1/1	0.95	0.05	20,20,20,20	0
57	MG	1G	202	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3462	1/1	0.95	0.07	44,44,44,44	0
57	MG	1G	204	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3593	1/1	0.95	0.05	23,23,23,23	0
57	MG	1A	3957	1/1	0.95	0.12	47,47,47,47	0
57	MG	2E	307	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3465	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3519	1/1	0.95	0.08	25,25,25,25	0
57	MG	2F	303	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3959	1/1	0.95	0.13	37,37,37,37	0
57	MG	2A	3521	1/1	0.95	0.07	17,17,17,17	0
57	MG	1N	206	1/1	0.95	0.22	28,28,28,28	0
57	MG	2A	3523	1/1	0.95	0.06	39,39,39,39	0
57	MG	1a	1762	1/1	0.95	0.16	49,49,49,49	0
57	MG	1A	3597	1/1	0.95	0.24	39,39,39,39	0
57	MG	1A	3762	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3301	1/1	0.95	0.08	34,34,34,34	0
57	MG	2A	3532	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3120	1/1	0.95	0.14	33,33,33,33	0
57	MG	2T	201	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3383	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3227	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3002	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3545	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3971	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3388	1/1	0.95	0.12	15,15,15,15	0
57	MG	1a	1776	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3772	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3773	1/1	0.95	0.09	25,25,25,25	0
57	MG	1A	3471	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3780	1/1	0.95	0.06	52,52,52,52	0
57	MG	1U	209	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3473	1/1	0.95	0.10	39,39,39,39	0
57	MG	1V	204	1/1	0.95	0.20	36,36,36,36	0
57	MG	25	104	1/1	0.95	0.11	45,45,45,45	0
57	MG	1V	208	1/1	0.95	0.11	44,44,44,44	0
57	MG	2A	3244	1/1	0.95	0.09	58,58,58,58	0
57	MG	1W	204	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3306	1/1	0.95	0.13	32,32,32,32	0
57	MG	1X	101	1/1	0.95	0.12	48,48,48,48	0
57	MG	1X	102	1/1	0.95	0.13	27,27,27,27	0
57	MG	2a	1602	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3788	1/1	0.95	0.06	43,43,43,43	0
57	MG	2A	3252	1/1	0.95	0.10	59,59,59,59	0
57	MG	1a	1806	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3478	1/1	0.95	0.11	25,25,25,25	0
57	MG	1A	3622	1/1	0.95	0.08	23,23,23,23	0
57	MG	2A	3586	1/1	0.95	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3307	1/1	0.95	0.09	27,27,27,27	0
57	MG	1Z	3701	1/1	0.95	0.05	31,31,31,31	0
57	MG	1A	3624	1/1	0.95	0.05	20,20,20,20	0
57	MG	2a	1612	1/1	0.95	0.07	52,52,52,52	0
57	MG	2a	1613	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3800	1/1	0.95	0.06	16,16,16,16	0
57	MG	2A	3592	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3265	1/1	0.95	0.12	38,38,38,38	0
57	MG	2A	3598	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3629	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	3803	1/1	0.95	0.06	35,35,35,35	0
57	MG	1A	3633	1/1	0.95	0.05	29,29,29,29	0
57	MG	1e	202	1/1	0.95	0.22	48,48,48,48	0
57	MG	1A	3238	1/1	0.95	0.18	19,19,19,19	0
57	MG	1A	3998	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3808	1/1	0.95	0.06	22,22,22,22	0
57	MG	1A	3640	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3815	1/1	0.95	0.08	26,26,26,26	0
57	MG	2a	1631	1/1	0.95	0.21	51,51,51,51	0
57	MG	2A	3613	1/1	0.95	0.13	52,52,52,52	0
57	MG	1n	103	1/1	0.95	0.18	44,44,44,44	0
57	MG	2a	1634	1/1	0.95	0.08	59,59,59,59	0
57	MG	1A	3074	1/1	0.95	0.08	27,27,27,27	0
57	MG	14	101	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3620	1/1	0.95	0.05	26,26,26,26	0
57	MG	1A	3819	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3393	1/1	0.95	0.07	52,52,52,52	0
57	MG	1w	104	1/1	0.95	0.20	64,64,64,64	0
57	MG	1A	3394	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3626	1/1	0.95	0.14	53,53,53,53	0
57	MG	16	101	1/1	0.95	0.06	39,39,39,39	0
57	MG	17	103	1/1	0.95	0.10	29,29,29,29	0
57	MG	17	104	1/1	0.95	0.12	42,42,42,42	0
57	MG	1A	3243	1/1	0.95	0.21	27,27,27,27	0
57	MG	2A	3635	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3313	1/1	0.95	0.06	30,30,30,30	0
57	MG	1x	105	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3833	1/1	0.95	0.11	42,42,42,42	0
57	MG	1x	107	1/1	0.95	0.06	42,42,42,42	0
57	MG	2a	1654	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3079	1/1	0.95	0.08	44,44,44,44	0
57	MG	2A	3646	1/1	0.95	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1657	1/1	0.95	0.12	56,56,56,56	0
57	MG	2A	3647	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3321	1/1	0.95	0.13	25,25,25,25	0
57	MG	2A	3649	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3837	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3246	1/1	0.95	0.11	50,50,50,50	0
57	MG	1a	1601	1/1	0.95	0.06	42,42,42,42	0
57	MG	2A	3001	1/1	0.95	0.19	41,41,41,41	0
57	MG	2a	1667	1/1	0.95	0.18	55,55,55,55	0
57	MG	1A	3840	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3842	1/1	0.95	0.06	39,39,39,39	0
57	MG	1A	3247	1/1	0.95	0.23	49,49,49,49	0
57	MG	2A	3659	1/1	0.95	0.14	54,54,54,54	0
57	MG	1A	3656	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3661	1/1	0.95	0.15	40,40,40,40	0
57	MG	2A	3662	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3309	1/1	0.95	0.07	45,45,45,45	0
57	MG	2a	1683	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3052	1/1	0.95	0.06	40,40,40,40	0
57	MG	2a	1686	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3666	1/1	0.95	0.07	53,53,53,53	0
57	MG	1a	1610	1/1	0.95	0.15	42,42,42,42	0
57	MG	2A	3312	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3314	1/1	0.95	0.09	53,53,53,53	0
57	MG	2a	1692	1/1	0.95	0.16	46,46,46,46	0
57	MG	2A	3016	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3501	1/1	0.95	0.06	36,36,36,36	0
57	MG	1a	1612	1/1	0.95	0.12	29,29,29,29	0
57	MG	1A	3661	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3188	1/1	0.95	0.16	25,25,25,25	0
57	MG	2A	3025	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	3504	1/1	0.95	0.07	27,27,27,27	0
57	MG	1A	3506	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3257	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3330	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3856	1/1	0.95	0.07	13,13,13,13	0
57	MG	1a	1624	1/1	0.95	0.09	47,47,47,47	0
57	MG	1a	1625	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3335	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3688	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	1626	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3691	1/1	0.95	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3692	1/1	0.95	0.11	55,55,55,55	0
57	MG	2A	3693	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3040	1/1	0.95	0.21	50,50,50,50	0
57	MG	2A	3041	1/1	0.95	0.10	48,48,48,48	0
57	MG	1a	1627	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3085	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3191	1/1	0.95	0.12	25,25,25,25	0
57	MG	2A	3045	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	4046	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3047	1/1	0.95	0.07	56,56,56,56	0
57	MG	2a	1722	1/1	0.95	0.19	54,54,54,54	0
57	MG	2A	3704	1/1	0.95	0.05	48,48,48,48	0
57	MG	2a	1725	1/1	0.95	0.06	39,39,39,39	0
57	MG	1a	1632	1/1	0.95	0.23	50,50,50,50	0
57	MG	2A	3049	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3708	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3050	1/1	0.95	0.16	31,31,31,31	0
57	MG	2a	1732	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3051	1/1	0.95	0.20	49,49,49,49	0
57	MG	2a	1734	1/1	0.95	0.18	41,41,41,41	0
57	MG	2A	3352	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3712	1/1	0.95	0.10	61,61,61,61	0
57	MG	1A	3017	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3862	1/1	0.95	0.08	33,33,33,33	0
57	MG	2a	1739	1/1	0.95	0.27	53,53,53,53	0
57	MG	1A	3414	1/1	0.95	0.05	26,26,26,26	0
57	MG	1A	4054	1/1	0.95	0.11	38,38,38,38	0
57	MG	2A	3722	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3194	1/1	0.95	0.12	21,21,21,21	0
57	MG	1a	1639	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3726	1/1	0.95	0.07	51,51,51,51	0
57	MG	2a	1747	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3727	1/1	0.95	0.07	48,48,48,48	0
57	MG	2a	1749	1/1	0.95	0.17	72,72,72,72	0
57	MG	2A	3061	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3526	1/1	0.95	0.05	36,36,36,36	0
57	MG	2A	3361	1/1	0.95	0.14	53,53,53,53	0
57	MG	1A	3683	1/1	0.95	0.08	52,52,52,52	0
57	MG	1A	3527	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3364	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3071	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3092	1/1	0.95	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3741	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3742	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3157	1/1	0.95	0.50	22,22,22,22	0
57	MG	1a	1647	1/1	0.95	0.13	36,36,36,36	0
57	MG	1A	3018	1/1	0.95	0.11	22,22,22,22	0
57	MG	2a	1772	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3693	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3336	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3274	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3538	1/1	0.95	0.10	38,38,38,38	0
57	MG	2a	1782	1/1	0.95	0.21	48,48,48,48	0
57	MG	2A	3084	1/1	0.95	0.06	35,35,35,35	0
57	MG	2a	1784	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3881	1/1	0.95	0.15	35,35,35,35	0
57	MG	2a	1786	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3089	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3755	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3882	1/1	0.95	0.08	22,22,22,22	0
57	MG	1A	4086	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	4087	1/1	0.95	0.11	48,48,48,48	0
57	MG	2a	1792	1/1	0.95	0.18	55,55,55,55	0
57	MG	1a	1664	1/1	0.95	0.04	38,38,38,38	0
57	MG	2A	3384	1/1	0.95	0.10	35,35,35,35	0
57	MG	2a	1797	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3095	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3539	1/1	0.95	0.27	54,54,54,54	0
57	MG	1a	1666	1/1	0.95	0.13	42,42,42,42	0
57	MG	2A	3766	1/1	0.95	0.10	66,66,66,66	0
57	MG	2A	3100	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3705	1/1	0.95	0.07	25,25,25,25	0
57	MG	2A	3392	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3426	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3395	1/1	0.95	0.19	52,52,52,52	0
57	MG	2A	3773	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3396	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3541	1/1	0.95	0.04	18,18,18,18	0
57	MG	1A	3019	1/1	0.95	0.13	32,32,32,32	0
57	MG	2a	1811	1/1	0.95	0.16	50,50,50,50	0
57	MG	1a	1673	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3276	1/1	0.95	0.21	38,38,38,38	0
57	MG	1A	3164	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3714	1/1	0.95	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3789	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3404	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3547	1/1	0.95	0.05	36,36,36,36	0
57	MG	2A	3407	1/1	0.95	0.12	60,60,60,60	0
57	MG	2A	3113	1/1	0.95	0.17	48,48,48,48	0
57	MG	1A	3209	1/1	0.95	0.09	33,33,33,33	0
57	MG	1B	205	1/1	0.95	0.13	48,48,48,48	0
57	MG	1a	1680	1/1	0.95	0.16	34,34,34,34	0
57	MG	2a	1827	1/1	0.95	0.20	42,42,42,42	0
57	MG	1B	206	1/1	0.95	0.07	36,36,36,36	0
57	MG	1a	1682	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3342	1/1	0.95	0.27	31,31,31,31	0
57	MG	2A	3415	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3032	1/1	0.95	0.22	25,25,25,25	0
57	MG	1a	1685	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3131	1/1	0.95	0.22	50,50,50,50	0
57	MG	1A	3901	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3422	1/1	0.95	0.14	33,33,33,33	0
57	MG	1A	3169	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3135	1/1	0.95	0.06	33,33,33,33	0
57	MG	2A	3136	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	3555	1/1	0.95	0.20	34,34,34,34	0
57	MG	2k	201	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3813	1/1	0.95	0.06	54,54,54,54	0
57	MG	1a	1690	1/1	0.95	0.09	37,37,37,37	0
57	MG	1a	1691	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3145	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3818	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3556	1/1	0.95	0.07	26,26,26,26	0
57	MG	1a	1696	1/1	0.95	0.20	43,43,43,43	0
57	MG	1A	3559	1/1	0.95	0.08	36,36,36,36	0
57	MG	2A	3824	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3825	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3149	1/1	0.95	0.18	42,42,42,42	0
57	MG	1A	3437	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3020	1/1	0.95	0.09	40,40,40,40	0
57	MG	2A	3829	1/1	0.95	0.09	40,40,40,40	0
57	MG	2A	3154	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3441	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3834	1/1	0.95	0.06	43,43,43,43	0
57	MG	2A	3156	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3350	1/1	0.95	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3160	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3922	1/1	0.95	0.10	30,30,30,30	0
57	MG	1B	227	1/1	0.95	0.04	23,23,23,23	0
57	MG	1A	3039	1/1	0.95	0.06	22,22,22,22	0
57	MG	1A	3223	1/1	0.95	0.10	20,20,20,20	0
57	MG	1A	3024	1/1	0.95	0.16	44,44,44,44	0
57	MG	2x	106	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3927	1/1	0.95	0.06	27,27,27,27	0
57	MG	2y	102	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3456	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3172	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3174	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3574	1/1	0.95	0.09	41,41,41,41	0
57	MG	1D	302	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3297	1/1	0.95	0.09	41,41,41,41	0
57	MG	2A	3849	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3850	1/1	0.96	0.07	19,19,19,19	0
57	MG	1a	1657	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3639	1/1	0.96	0.04	10,10,10,10	0
57	MG	2A	3120	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3480	1/1	0.96	0.08	40,40,40,40	0
57	MG	2A	3124	1/1	0.96	0.21	56,56,56,56	0
57	MG	2A	3125	1/1	0.96	0.22	44,44,44,44	0
57	MG	2A	3126	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3289	1/1	0.96	0.07	19,19,19,19	0
57	MG	1A	3642	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3482	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	4061	1/1	0.96	0.24	40,40,40,40	0
57	MG	2A	3460	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	4064	1/1	0.96	0.04	14,14,14,14	0
57	MG	1a	1667	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3463	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3483	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3203	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	4067	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3138	1/1	0.96	0.17	32,32,32,32	0
57	MG	2A	3878	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3379	1/1	0.96	0.04	37,37,37,37	0
57	MG	2A	3469	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3140	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	4069	1/1	0.96	0.10	16,16,16,16	0
57	MG	2A	3883	1/1	0.96	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3473	1/1	0.96	0.14	17,17,17,17	0
57	MG	1A	3648	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3846	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	4074	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3478	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	4077	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3486	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3381	1/1	0.96	0.10	28,28,28,28	0
57	MG	1A	3138	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	4085	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3654	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3485	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3142	1/1	0.96	0.10	10,10,10,10	0
57	MG	2A	3157	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3158	1/1	0.96	0.05	26,26,26,26	0
57	MG	1A	3854	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3208	1/1	0.96	0.08	27,27,27,27	0
57	MG	1A	3657	1/1	0.96	0.08	30,30,30,30	0
57	MG	1a	1687	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3857	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3498	1/1	0.96	0.11	45,45,45,45	0
57	MG	2D	302	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3087	1/1	0.96	0.06	37,37,37,37	0
57	MG	2D	304	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3500	1/1	0.96	0.13	48,48,48,48	0
57	MG	2D	306	1/1	0.96	0.24	35,35,35,35	0
57	MG	2A	3166	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3168	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3009	1/1	0.96	0.06	26,26,26,26	0
57	MG	2E	303	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3660	1/1	0.96	0.05	30,30,30,30	0
57	MG	2E	305	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3211	1/1	0.96	0.08	41,41,41,41	0
57	MG	1a	1695	1/1	0.96	0.22	41,41,41,41	0
57	MG	2A	3173	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3497	1/1	0.96	0.08	23,23,23,23	0
57	MG	1B	201	1/1	0.96	0.06	30,30,30,30	0
57	MG	1B	202	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3663	1/1	0.96	0.07	35,35,35,35	0
57	MG	1a	1700	1/1	0.96	0.14	42,42,42,42	0
57	MG	1A	3498	1/1	0.96	0.17	36,36,36,36	0
57	MG	2O	201	1/1	0.96	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3666	1/1	0.96	0.05	15,15,15,15	0
57	MG	1a	1703	1/1	0.96	0.17	49,49,49,49	0
57	MG	2A	3185	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	1704	1/1	0.96	0.09	49,49,49,49	0
57	MG	2Q	203	1/1	0.96	0.10	48,48,48,48	0
57	MG	2R	201	1/1	0.96	0.06	32,32,32,32	0
57	MG	1B	207	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3868	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	3499	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3524	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3190	1/1	0.96	0.09	46,46,46,46	0
57	MG	2V	201	1/1	0.96	0.16	51,51,51,51	0
57	MG	2A	3526	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3216	1/1	0.96	0.06	37,37,37,37	0
57	MG	1B	211	1/1	0.96	0.10	43,43,43,43	0
57	MG	1a	1712	1/1	0.96	0.04	35,35,35,35	0
57	MG	2A	3530	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3089	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3534	1/1	0.96	0.04	36,36,36,36	0
57	MG	2A	3535	1/1	0.96	0.09	28,28,28,28	0
57	MG	1a	1714	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3538	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3672	1/1	0.96	0.04	15,15,15,15	0
57	MG	1A	3090	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3543	1/1	0.96	0.13	42,42,42,42	0
57	MG	1a	1717	1/1	0.96	0.11	44,44,44,44	0
57	MG	2A	3200	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3155	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3221	1/1	0.96	0.06	27,27,27,27	0
57	MG	28	104	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3548	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3549	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3877	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3396	1/1	0.96	0.17	28,28,28,28	0
57	MG	1a	1723	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3222	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3398	1/1	0.96	0.13	16,16,16,16	0
57	MG	2A	3559	1/1	0.96	0.05	20,20,20,20	0
57	MG	2A	3561	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	1726	1/1	0.96	0.20	57,57,57,57	0
57	MG	1A	3518	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3522	1/1	0.96	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3309	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3400	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3091	1/1	0.96	0.09	21,21,21,21	0
57	MG	2a	1615	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3216	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3225	1/1	0.96	0.18	37,37,37,37	0
57	MG	2A	3573	1/1	0.96	0.05	37,37,37,37	0
57	MG	2a	1619	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3404	1/1	0.96	0.10	27,27,27,27	0
57	MG	1B	235	1/1	0.96	0.06	39,39,39,39	0
57	MG	2a	1622	1/1	0.96	0.17	57,57,57,57	0
57	MG	2A	3578	1/1	0.96	0.17	38,38,38,38	0
57	MG	1A	3697	1/1	0.96	0.13	59,59,59,59	0
57	MG	2A	3580	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3699	1/1	0.96	0.07	33,33,33,33	0
57	MG	1D	304	1/1	0.96	0.09	30,30,30,30	0
57	MG	1D	305	1/1	0.96	0.04	16,16,16,16	0
57	MG	1A	3227	1/1	0.96	0.17	39,39,39,39	0
57	MG	2A	3226	1/1	0.96	0.31	40,40,40,40	0
57	MG	1A	3228	1/1	0.96	0.10	36,36,36,36	0
57	MG	1a	1746	1/1	0.96	0.04	48,48,48,48	0
57	MG	2A	3229	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3591	1/1	0.96	0.12	49,49,49,49	0
57	MG	1D	311	1/1	0.96	0.24	23,23,23,23	0
57	MG	1A	3703	1/1	0.96	0.05	10,10,10,10	0
57	MG	1E	301	1/1	0.96	0.05	21,21,21,21	0
57	MG	1A	3314	1/1	0.96	0.13	33,33,33,33	0
57	MG	2A	3600	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3235	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3902	1/1	0.96	0.11	29,29,29,29	0
57	MG	2a	1643	1/1	0.96	0.22	54,54,54,54	0
57	MG	1A	3316	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3230	1/1	0.96	0.09	20,20,20,20	0
57	MG	1A	3907	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3908	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3536	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3537	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3911	1/1	0.96	0.11	41,41,41,41	0
57	MG	2A	3245	1/1	0.96	0.09	47,47,47,47	0
57	MG	1F	308	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3618	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3319	1/1	0.96	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3411	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3249	1/1	0.96	0.07	51,51,51,51	0
57	MG	1a	1766	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3915	1/1	0.96	0.07	34,34,34,34	0
57	MG	1G	201	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3916	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3065	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3918	1/1	0.96	0.04	31,31,31,31	0
57	MG	1A	3066	1/1	0.96	0.05	19,19,19,19	0
57	MG	1I	201	1/1	0.96	0.08	49,49,49,49	0
57	MG	2a	1668	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3260	1/1	0.96	0.08	39,39,39,39	0
57	MG	1a	1777	1/1	0.96	0.06	49,49,49,49	0
57	MG	2a	1671	1/1	0.96	0.10	45,45,45,45	0
57	MG	1a	1778	1/1	0.96	0.08	36,36,36,36	0
57	MG	1N	201	1/1	0.96	0.12	42,42,42,42	0
57	MG	2a	1674	1/1	0.96	0.05	42,42,42,42	0
57	MG	1A	3094	1/1	0.96	0.12	31,31,31,31	0
57	MG	2a	1676	1/1	0.96	0.10	51,51,51,51	0
57	MG	2A	3643	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3004	1/1	0.96	0.06	19,19,19,19	0
57	MG	2a	1680	1/1	0.96	0.10	64,64,64,64	0
57	MG	1a	1784	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3099	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3546	1/1	0.96	0.11	36,36,36,36	0
57	MG	1O	201	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	1687	1/1	0.96	0.10	43,43,43,43	0
57	MG	1O	202	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3926	1/1	0.96	0.09	34,34,34,34	0
57	MG	1a	1795	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3033	1/1	0.96	0.04	29,29,29,29	0
57	MG	1A	3102	1/1	0.96	0.07	16,16,16,16	0
57	MG	1a	1800	1/1	0.96	0.08	56,56,56,56	0
57	MG	1Q	202	1/1	0.96	0.06	30,30,30,30	0
57	MG	1Q	203	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3724	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3420	1/1	0.96	0.05	29,29,29,29	0
57	MG	2A	3286	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3931	1/1	0.96	0.04	31,31,31,31	0
57	MG	1Q	207	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3104	1/1	0.96	0.07	24,24,24,24	0
57	MG	1R	203	1/1	0.96	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1R	204	1/1	0.96	0.07	16,16,16,16	0
57	MG	1A	3425	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3936	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3939	1/1	0.96	0.04	34,34,34,34	0
57	MG	1A	3329	1/1	0.96	0.15	44,44,44,44	0
57	MG	2A	3298	1/1	0.96	0.06	36,36,36,36	0
57	MG	1U	202	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3045	1/1	0.96	0.07	17,17,17,17	0
57	MG	2A	3676	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3111	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3945	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3075	1/1	0.96	0.08	27,27,27,27	0
57	MG	2a	1716	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3681	1/1	0.96	0.10	44,44,44,44	0
57	MG	1V	205	1/1	0.96	0.07	24,24,24,24	0
57	MG	1A	3114	1/1	0.96	0.15	30,30,30,30	0
57	MG	2A	3306	1/1	0.96	0.06	37,37,37,37	0
57	MG	1V	210	1/1	0.96	0.05	41,41,41,41	0
57	MG	1W	202	1/1	0.96	0.12	46,46,46,46	0
57	MG	1W	203	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3433	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3076	1/1	0.96	0.22	35,35,35,35	0
57	MG	1W	207	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3253	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3694	1/1	0.96	0.13	48,48,48,48	0
57	MG	2A	3315	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3034	1/1	0.96	0.08	32,32,32,32	0
57	MG	1X	103	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3741	1/1	0.96	0.12	41,41,41,41	0
57	MG	1x	103	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3119	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3261	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3702	1/1	0.96	0.08	33,33,33,33	0
57	MG	1Y	203	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3440	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3746	1/1	0.96	0.08	20,20,20,20	0
57	MG	2A	3706	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3748	1/1	0.96	0.10	23,23,23,23	0
57	MG	1A	3080	1/1	0.96	0.14	25,25,25,25	0
57	MG	10	101	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3446	1/1	0.96	0.06	27,27,27,27	0
57	MG	10	103	1/1	0.96	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3447	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3048	1/1	0.96	0.15	34,34,34,34	0
57	MG	2A	3714	1/1	0.96	0.11	20,20,20,20	0
57	MG	1A	3581	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3582	1/1	0.96	0.06	32,32,32,32	0
57	MG	11	101	1/1	0.96	0.17	32,32,32,32	0
57	MG	11	102	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3010	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3015	1/1	0.96	0.15	37,37,37,37	0
57	MG	2a	1763	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	1765	1/1	0.96	0.06	49,49,49,49	0
57	MG	11	103	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3760	1/1	0.96	0.05	50,50,50,50	0
57	MG	11	105	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3019	1/1	0.96	0.07	33,33,33,33	0
57	MG	2A	3021	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3976	1/1	0.96	0.10	53,53,53,53	0
57	MG	12	102	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3977	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3449	1/1	0.96	0.10	31,31,31,31	0
57	MG	2A	3739	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3190	1/1	0.96	0.08	32,32,32,32	0
57	MG	1A	3763	1/1	0.96	0.06	14,14,14,14	0
57	MG	1A	3585	1/1	0.96	0.07	40,40,40,40	0
57	MG	15	108	1/1	0.96	0.15	33,33,33,33	0
57	MG	2A	3034	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3766	1/1	0.96	0.07	13,13,13,13	0
57	MG	2A	3746	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3036	1/1	0.96	0.04	25,25,25,25	0
57	MG	1A	3124	1/1	0.96	0.15	28,28,28,28	0
57	MG	17	101	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3083	1/1	0.96	0.09	19,19,19,19	0
57	MG	1A	3592	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3130	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3594	1/1	0.96	0.14	36,36,36,36	0
57	MG	2A	3754	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3347	1/1	0.96	0.22	23,23,23,23	0
57	MG	1A	3992	1/1	0.96	0.03	26,26,26,26	0
57	MG	1A	3051	1/1	0.96	0.07	27,27,27,27	0
57	MG	1A	3777	1/1	0.96	0.04	18,18,18,18	0
57	MG	1A	3459	1/1	0.96	0.25	50,50,50,50	0
57	MG	2A	3375	1/1	0.96	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3781	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3782	1/1	0.96	0.06	26,26,26,26	0
57	MG	1a	1605	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3783	1/1	0.96	0.04	18,18,18,18	0
57	MG	1A	3351	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3056	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3135	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3383	1/1	0.96	0.21	56,56,56,56	0
57	MG	1A	3786	1/1	0.96	0.12	46,46,46,46	0
57	MG	2a	1815	1/1	0.96	0.04	54,54,54,54	0
57	MG	1A	4003	1/1	0.96	0.09	19,19,19,19	0
57	MG	2a	1817	1/1	0.96	0.07	59,59,59,59	0
57	MG	1A	3607	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3062	1/1	0.96	0.05	47,47,47,47	0
57	MG	2A	3063	1/1	0.96	0.17	38,38,38,38	0
57	MG	2A	3389	1/1	0.96	0.16	46,46,46,46	0
57	MG	2A	3066	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3789	1/1	0.96	0.10	42,42,42,42	0
57	MG	2a	1824	1/1	0.96	0.15	57,57,57,57	0
57	MG	2A	3780	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3790	1/1	0.96	0.05	19,19,19,19	0
57	MG	2A	3394	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3608	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3794	1/1	0.96	0.04	17,17,17,17	0
57	MG	1a	1616	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3398	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3463	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3611	1/1	0.96	0.06	15,15,15,15	0
57	MG	1A	3353	1/1	0.96	0.05	28,28,28,28	0
57	MG	2A	3076	1/1	0.96	0.21	41,41,41,41	0
57	MG	2A	3077	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3137	1/1	0.96	0.32	23,23,23,23	0
57	MG	2g	201	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	4022	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3801	1/1	0.96	0.10	20,20,20,20	0
57	MG	1A	3614	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3198	1/1	0.96	0.04	30,30,30,30	0
57	MG	2A	3085	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3616	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3087	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3088	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3200	1/1	0.96	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3806	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3416	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	3807	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3202	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3812	1/1	0.96	0.28	19,19,19,19	0
57	MG	2A	3420	1/1	0.96	0.16	48,48,48,48	0
57	MG	1A	4037	1/1	0.96	0.08	31,31,31,31	0
57	MG	1A	3368	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3822	1/1	0.96	0.05	30,30,30,30	0
57	MG	1A	3369	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3817	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	4041	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3429	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3370	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3431	1/1	0.96	0.12	40,40,40,40	0
57	MG	2w	108	1/1	0.96	0.06	58,58,58,58	0
57	MG	1a	1644	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3626	1/1	0.96	0.05	16,16,16,16	0
57	MG	1A	3628	1/1	0.96	0.13	34,34,34,34	0
57	MG	2A	3833	1/1	0.96	0.04	31,31,31,31	0
57	MG	2A	3435	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3371	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3109	1/1	0.96	0.15	31,31,31,31	0
57	MG	1a	1648	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3824	1/1	0.96	0.05	28,28,28,28	0
57	MG	2A	3840	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3373	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3831	1/1	0.96	0.05	22,22,22,22	0
57	MG	1A	3635	1/1	0.96	0.04	26,26,26,26	0
57	MG	1A	3374	1/1	0.96	0.11	32,32,32,32	0
60	ZN	24	501	1/1	0.96	0.09	105,105,105,105	0
60	ZN	2n	501	1/1	0.96	0.06	81,81,81,81	0
57	MG	1v	102	1/1	0.97	0.05	41,41,41,41	0
57	MG	1w	101	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	4032	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3841	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3171	1/1	0.97	0.08	8,8,8,8	0
57	MG	1A	3172	1/1	0.97	0.06	38,38,38,38	0
57	MG	2D	301	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3113	1/1	0.97	0.10	28,28,28,28	0
57	MG	1A	3176	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3671	1/1	0.97	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3553	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3847	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3077	1/1	0.97	0.18	29,29,29,29	0
57	MG	2D	308	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3849	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3258	1/1	0.97	0.07	53,53,53,53	0
57	MG	2A	3259	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3529	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3021	1/1	0.97	0.04	15,15,15,15	0
57	MG	1A	3181	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3263	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3264	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3676	1/1	0.97	0.08	13,13,13,13	0
57	MG	1x	109	1/1	0.97	0.07	13,13,13,13	0
57	MG	2A	3267	1/1	0.97	0.09	59,59,59,59	0
57	MG	2A	3268	1/1	0.97	0.13	44,44,44,44	0
57	MG	1x	110	1/1	0.97	0.11	46,46,46,46	0
57	MG	2A	3576	1/1	0.97	0.04	40,40,40,40	0
57	MG	2A	3270	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3677	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3117	1/1	0.97	0.05	21,21,21,21	0
57	MG	1x	113	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4049	1/1	0.97	0.04	26,26,26,26	0
57	MG	1a	1602	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3022	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	4052	1/1	0.97	0.03	25,25,25,25	0
57	MG	1A	3682	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3008	1/1	0.97	0.03	23,23,23,23	0
57	MG	1A	4056	1/1	0.97	0.06	11,11,11,11	0
57	MG	1A	3684	1/1	0.97	0.07	53,53,53,53	0
57	MG	2U	201	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3685	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3861	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3593	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3594	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3011	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3012	1/1	0.97	0.06	30,30,30,30	0
57	MG	2X	102	1/1	0.97	0.07	46,46,46,46	0
57	MG	2A	3013	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3288	1/1	0.97	0.12	36,36,36,36	0
57	MG	2A	3603	1/1	0.97	0.11	47,47,47,47	0
57	MG	2A	3014	1/1	0.97	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3037	1/1	0.97	0.14	20,20,20,20	0
57	MG	1A	3422	1/1	0.97	0.07	30,30,30,30	0
57	MG	25	102	1/1	0.97	0.19	41,41,41,41	0
57	MG	1A	4063	1/1	0.97	0.04	27,27,27,27	0
57	MG	2A	3608	1/1	0.97	0.08	26,26,26,26	0
57	MG	25	105	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3424	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3249	1/1	0.97	0.18	28,28,28,28	0
57	MG	2A	3020	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3296	1/1	0.97	0.07	42,42,42,42	0
57	MG	28	103	1/1	0.97	0.06	44,44,44,44	0
57	MG	1a	1617	1/1	0.97	0.08	29,29,29,29	0
57	MG	1A	3121	1/1	0.97	0.13	24,24,24,24	0
57	MG	2A	3616	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3252	1/1	0.97	0.04	43,43,43,43	0
57	MG	2A	3024	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3543	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3026	1/1	0.97	0.17	40,40,40,40	0
57	MG	1A	3055	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3698	1/1	0.97	0.06	18,18,18,18	0
57	MG	1A	3254	1/1	0.97	0.04	43,43,43,43	0
57	MG	1A	3255	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3056	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3126	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	4079	1/1	0.97	0.05	25,25,25,25	0
57	MG	2A	3630	1/1	0.97	0.04	31,31,31,31	0
57	MG	1A	3704	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3549	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	4082	1/1	0.97	0.04	19,19,19,19	0
57	MG	1A	3879	1/1	0.97	0.11	30,30,30,30	0
57	MG	1A	3880	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3259	1/1	0.97	0.05	24,24,24,24	0
57	MG	2A	3640	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3641	1/1	0.97	0.04	37,37,37,37	0
57	MG	2A	3317	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3001	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3883	1/1	0.97	0.14	29,29,29,29	0
57	MG	1a	1641	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3343	1/1	0.97	0.04	43,43,43,43	0
57	MG	2a	1627	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3711	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3554	1/1	0.97	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3324	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3438	1/1	0.97	0.18	43,43,43,43	0
57	MG	1A	3010	1/1	0.97	0.04	26,26,26,26	0
57	MG	2A	3327	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3192	1/1	0.97	0.19	32,32,32,32	0
57	MG	2A	3331	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3040	1/1	0.97	0.06	25,25,25,25	0
57	MG	2A	3054	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	4100	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3442	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3894	1/1	0.97	0.08	25,25,25,25	0
57	MG	1a	1654	1/1	0.97	0.15	41,41,41,41	0
57	MG	2A	3664	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3445	1/1	0.97	0.06	40,40,40,40	0
57	MG	1B	204	1/1	0.97	0.04	22,22,22,22	0
57	MG	1A	3267	1/1	0.97	0.21	27,27,27,27	0
57	MG	2a	1646	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3348	1/1	0.97	0.08	25,25,25,25	0
57	MG	2A	3342	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3343	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3065	1/1	0.97	0.08	66,66,66,66	0
57	MG	1A	3898	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3899	1/1	0.97	0.05	11,11,11,11	0
57	MG	2A	3347	1/1	0.97	0.05	41,41,41,41	0
57	MG	1a	1662	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3349	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3567	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3568	1/1	0.97	0.13	21,21,21,21	0
57	MG	1A	3268	1/1	0.97	0.10	25,25,25,25	0
57	MG	1A	3905	1/1	0.97	0.04	31,31,31,31	0
57	MG	1A	3571	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3683	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3134	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3451	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3270	1/1	0.97	0.10	25,25,25,25	0
57	MG	1B	221	1/1	0.97	0.09	36,36,36,36	0
57	MG	2A	3081	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3061	1/1	0.97	0.12	33,33,33,33	0
57	MG	2A	3690	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3455	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3732	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3913	1/1	0.97	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3355	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3365	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3734	1/1	0.97	0.09	41,41,41,41	0
57	MG	2a	1677	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3736	1/1	0.97	0.03	9,9,9,9	0
57	MG	1A	3356	1/1	0.97	0.14	27,27,27,27	0
57	MG	1A	3041	1/1	0.97	0.10	17,17,17,17	0
57	MG	1A	3011	1/1	0.97	0.06	31,31,31,31	0
57	MG	2a	1682	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3921	1/1	0.97	0.08	20,20,20,20	0
57	MG	2A	3093	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3139	1/1	0.97	0.04	14,14,14,14	0
57	MG	1A	3461	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3586	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3360	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3099	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3361	1/1	0.97	0.07	36,36,36,36	0
57	MG	1D	307	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3745	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3464	1/1	0.97	0.15	45,45,45,45	0
57	MG	1a	1693	1/1	0.97	0.07	35,35,35,35	0
57	MG	1a	1694	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	3364	1/1	0.97	0.12	21,21,21,21	0
57	MG	2A	3108	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3365	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3595	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3719	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3721	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3140	1/1	0.97	0.09	31,31,31,31	0
57	MG	1E	306	1/1	0.97	0.08	24,24,24,24	0
57	MG	2A	3390	1/1	0.97	0.05	52,52,52,52	0
57	MG	2A	3725	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3367	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3934	1/1	0.97	0.04	30,30,30,30	0
57	MG	1E	309	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3756	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3117	1/1	0.97	0.08	38,38,38,38	0
57	MG	2A	3732	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3733	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3937	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3119	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3141	1/1	0.97	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3121	1/1	0.97	0.07	35,35,35,35	0
57	MG	1a	1706	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3600	1/1	0.97	0.17	45,45,45,45	0
57	MG	1A	3601	1/1	0.97	0.08	40,40,40,40	0
57	MG	1F	306	1/1	0.97	0.10	21,21,21,21	0
57	MG	2a	1723	1/1	0.97	0.10	52,52,52,52	0
57	MG	1a	1710	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3405	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3602	1/1	0.97	0.09	42,42,42,42	0
57	MG	1F	309	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3130	1/1	0.97	0.07	38,38,38,38	0
57	MG	2a	1730	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3603	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3278	1/1	0.97	0.09	21,21,21,21	0
57	MG	2A	3133	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3279	1/1	0.97	0.29	31,31,31,31	0
57	MG	1A	3606	1/1	0.97	0.04	18,18,18,18	0
57	MG	1A	3472	1/1	0.97	0.20	32,32,32,32	0
57	MG	1A	3951	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3043	1/1	0.97	0.07	35,35,35,35	0
57	MG	1G	205	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3758	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3953	1/1	0.97	0.06	56,56,56,56	0
57	MG	2A	3141	1/1	0.97	0.13	34,34,34,34	0
57	MG	2A	3142	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3474	1/1	0.97	0.04	27,27,27,27	0
57	MG	2A	3144	1/1	0.97	0.12	29,29,29,29	0
57	MG	2a	1746	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3285	1/1	0.97	0.04	34,34,34,34	0
57	MG	2A	3424	1/1	0.97	0.22	40,40,40,40	0
57	MG	2A	3425	1/1	0.97	0.22	48,48,48,48	0
57	MG	2a	1750	1/1	0.97	0.05	59,59,59,59	0
57	MG	2a	1751	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3477	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3427	1/1	0.97	0.12	48,48,48,48	0
57	MG	1N	203	1/1	0.97	0.11	43,43,43,43	0
57	MG	2a	1755	1/1	0.97	0.05	58,58,58,58	0
57	MG	1A	3286	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3144	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3772	1/1	0.97	0.04	36,36,36,36	0
57	MG	1a	1730	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3152	1/1	0.97	0.05	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3205	1/1	0.97	0.05	15,15,15,15	0
57	MG	1A	3378	1/1	0.97	0.04	31,31,31,31	0
57	MG	1A	3097	1/1	0.97	0.09	42,42,42,42	0
57	MG	1O	203	1/1	0.97	0.09	42,42,42,42	0
57	MG	2a	1767	1/1	0.97	0.05	53,53,53,53	0
57	MG	2a	1768	1/1	0.97	0.08	64,64,64,64	0
57	MG	1O	204	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3963	1/1	0.97	0.05	21,21,21,21	0
57	MG	2A	3781	1/1	0.97	0.13	35,35,35,35	0
57	MG	1P	202	1/1	0.97	0.15	19,19,19,19	0
57	MG	2A	3785	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3787	1/1	0.97	0.07	45,45,45,45	0
57	MG	2a	1776	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3146	1/1	0.97	0.33	29,29,29,29	0
57	MG	1A	3620	1/1	0.97	0.09	7,7,7,7	0
57	MG	2a	1779	1/1	0.97	0.10	35,35,35,35	0
57	MG	2a	1781	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3621	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3163	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3967	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3794	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3969	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3044	1/1	0.97	0.04	16,16,16,16	0
57	MG	2A	3167	1/1	0.97	0.25	52,52,52,52	0
57	MG	1A	3067	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	3152	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3212	1/1	0.97	0.08	37,37,37,37	0
57	MG	1a	1750	1/1	0.97	0.08	30,30,30,30	0
57	MG	2a	1793	1/1	0.97	0.19	50,50,50,50	0
57	MG	1A	3213	1/1	0.97	0.18	21,21,21,21	0
57	MG	2a	1795	1/1	0.97	0.12	47,47,47,47	0
57	MG	1A	3490	1/1	0.97	0.13	37,37,37,37	0
57	MG	2A	3456	1/1	0.97	0.13	34,34,34,34	0
57	MG	2A	3805	1/1	0.97	0.05	35,35,35,35	0
57	MG	1S	201	1/1	0.97	0.25	37,37,37,37	0
57	MG	2A	3459	1/1	0.97	0.23	45,45,45,45	0
57	MG	1S	202	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3630	1/1	0.97	0.06	19,19,19,19	0
57	MG	1a	1757	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3491	1/1	0.97	0.08	45,45,45,45	0
57	MG	2A	3179	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3180	1/1	0.97	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3299	1/1	0.97	0.21	23,23,23,23	0
57	MG	1A	3983	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3183	1/1	0.97	0.09	56,56,56,56	0
57	MG	1T	204	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3636	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3821	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3799	1/1	0.97	0.04	16,16,16,16	0
57	MG	1U	206	1/1	0.97	0.31	40,40,40,40	0
57	MG	1U	207	1/1	0.97	0.11	23,23,23,23	0
57	MG	1U	208	1/1	0.97	0.23	32,32,32,32	0
57	MG	1A	3215	1/1	0.97	0.07	32,32,32,32	0
57	MG	2A	3477	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3638	1/1	0.97	0.05	27,27,27,27	0
57	MG	1a	1770	1/1	0.97	0.04	37,37,37,37	0
57	MG	1a	1771	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3988	1/1	0.97	0.11	18,18,18,18	0
57	MG	1A	3012	1/1	0.97	0.03	19,19,19,19	0
57	MG	1V	206	1/1	0.97	0.08	28,28,28,28	0
57	MG	1A	3101	1/1	0.97	0.10	19,19,19,19	0
57	MG	1V	209	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3156	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3487	1/1	0.97	0.05	17,17,17,17	0
57	MG	1W	201	1/1	0.97	0.09	32,32,32,32	0
57	MG	1A	3071	1/1	0.97	0.11	17,17,17,17	0
57	MG	1a	1781	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3845	1/1	0.97	0.05	45,45,45,45	0
57	MG	2A	3493	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3046	1/1	0.97	0.05	20,20,20,20	0
57	MG	2A	3205	1/1	0.97	0.23	48,48,48,48	0
57	MG	1A	3308	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3107	1/1	0.97	0.12	22,22,22,22	0
57	MG	1a	1786	1/1	0.97	0.05	55,55,55,55	0
57	MG	1a	1787	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3810	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3161	1/1	0.97	0.07	26,26,26,26	0
57	MG	2A	3212	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3162	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3504	1/1	0.97	0.17	37,37,37,37	0
57	MG	2A	3861	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3862	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3863	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3226	1/1	0.97	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1X	106	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3816	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3505	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	4002	1/1	0.97	0.03	6,6,6,6	0
57	MG	1A	3652	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3029	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3509	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3110	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	4010	1/1	0.97	0.05	12,12,12,12	0
57	MG	1A	3031	1/1	0.97	0.11	11,11,11,11	0
57	MG	1A	3827	1/1	0.97	0.09	17,17,17,17	0
57	MG	1A	4014	1/1	0.97	0.06	31,31,31,31	0
57	MG	10	104	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3829	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	3515	1/1	0.97	0.16	23,23,23,23	0
57	MG	1A	3231	1/1	0.97	0.07	19,19,19,19	0
57	MG	2x	101	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	4019	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3517	1/1	0.97	0.21	30,30,30,30	0
57	MG	2A	3234	1/1	0.97	0.12	25,25,25,25	0
57	MG	1f	202	1/1	0.97	0.09	43,43,43,43	0
57	MG	1k	201	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3318	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	4023	1/1	0.97	0.10	28,28,28,28	0
57	MG	2A	3239	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3834	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3520	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3521	1/1	0.97	0.12	49,49,49,49	0
58	K	2A	3472	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3537	1/1	0.97	0.07	26,26,26,26	0
57	MG	1A	3049	1/1	0.97	0.04	10,10,10,10	0
60	ZN	14	102	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3320	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3665	1/1	0.97	0.03	20,20,20,20	0
57	MG	1A	3237	1/1	0.98	0.16	24,24,24,24	0
57	MG	1A	3108	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3578	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3239	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3787	1/1	0.98	0.08	13,13,13,13	0
57	MG	1A	3423	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3737	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3023	1/1	0.98	0.04	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1U	201	1/1	0.98	0.15	27,27,27,27	0
57	MG	2A	3489	1/1	0.98	0.14	37,37,37,37	0
57	MG	1A	3242	1/1	0.98	0.07	22,22,22,22	0
57	MG	2A	3491	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	4051	1/1	0.98	0.05	23,23,23,23	0
57	MG	2A	3060	1/1	0.98	0.05	34,34,34,34	0
57	MG	1U	204	1/1	0.98	0.12	25,25,25,25	0
57	MG	1U	205	1/1	0.98	0.16	24,24,24,24	0
57	MG	1A	3791	1/1	0.98	0.03	33,33,33,33	0
57	MG	1A	3678	1/1	0.98	0.06	14,14,14,14	0
57	MG	1A	3072	1/1	0.98	0.04	9,9,9,9	0
57	MG	1A	3244	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3362	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3282	1/1	0.98	0.04	33,33,33,33	0
57	MG	1V	201	1/1	0.98	0.16	22,22,22,22	0
57	MG	1V	203	1/1	0.98	0.27	35,35,35,35	0
57	MG	1A	3363	1/1	0.98	0.05	36,36,36,36	0
57	MG	2A	3756	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3798	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3430	1/1	0.98	0.04	29,29,29,29	0
57	MG	1V	207	1/1	0.98	0.18	23,23,23,23	0
57	MG	1A	3589	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3590	1/1	0.98	0.22	38,38,38,38	0
57	MG	2A	3511	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3502	1/1	0.98	0.07	51,51,51,51	0
57	MG	1a	1721	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3160	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3432	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3691	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3132	1/1	0.98	0.04	16,16,16,16	0
57	MG	2a	1661	1/1	0.98	0.15	54,54,54,54	0
57	MG	2a	1662	1/1	0.98	0.04	32,32,32,32	0
57	MG	1W	205	1/1	0.98	0.09	31,31,31,31	0
57	MG	1A	3199	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	4070	1/1	0.98	0.11	26,26,26,26	0
57	MG	1a	1729	1/1	0.98	0.06	46,46,46,46	0
57	MG	1W	208	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3507	1/1	0.98	0.04	13,13,13,13	0
57	MG	1a	1732	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	4072	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3696	1/1	0.98	0.02	22,22,22,22	0
57	MG	1X	104	1/1	0.98	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1X	105	1/1	0.98	0.09	24,24,24,24	0
57	MG	1A	3811	1/1	0.98	0.02	15,15,15,15	0
57	MG	1A	4076	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3508	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3783	1/1	0.98	0.10	34,34,34,34	0
57	MG	2A	3784	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3533	1/1	0.98	0.03	26,26,26,26	0
57	MG	2A	3786	1/1	0.98	0.04	47,47,47,47	0
57	MG	1a	1740	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3788	1/1	0.98	0.09	48,48,48,48	0
57	MG	1A	3813	1/1	0.98	0.05	31,31,31,31	0
57	MG	2A	3313	1/1	0.98	0.14	52,52,52,52	0
57	MG	2a	1685	1/1	0.98	0.24	45,45,45,45	0
57	MG	1A	3133	1/1	0.98	0.13	22,22,22,22	0
57	MG	1A	3201	1/1	0.98	0.07	16,16,16,16	0
57	MG	1a	1744	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3938	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3700	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	4083	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3163	1/1	0.98	0.28	23,23,23,23	0
57	MG	1A	3512	1/1	0.98	0.14	19,19,19,19	0
57	MG	1A	3942	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3943	1/1	0.98	0.03	43,43,43,43	0
57	MG	1A	4089	1/1	0.98	0.04	22,22,22,22	0
57	MG	2a	1697	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	4090	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3551	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3513	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3820	1/1	0.98	0.06	24,24,24,24	0
57	MG	2A	3328	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3082	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3556	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3165	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3823	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3372	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3812	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3950	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3826	1/1	0.98	0.03	28,28,28,28	0
57	MG	2A	3123	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	4099	1/1	0.98	0.14	40,40,40,40	0
57	MG	2A	3817	1/1	0.98	0.07	36,36,36,36	0
57	MG	13	102	1/1	0.98	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3567	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3707	1/1	0.98	0.07	10,10,10,10	0
57	MG	2A	3569	1/1	0.98	0.06	52,52,52,52	0
57	MG	2A	3570	1/1	0.98	0.07	55,55,55,55	0
57	MG	13	104	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3828	1/1	0.98	0.11	20,20,20,20	0
57	MG	1A	3315	1/1	0.98	0.03	31,31,31,31	0
57	MG	15	101	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3519	1/1	0.98	0.07	38,38,38,38	0
57	MG	15	105	1/1	0.98	0.13	28,28,28,28	0
57	MG	1a	1773	1/1	0.98	0.04	55,55,55,55	0
57	MG	1A	3166	1/1	0.98	0.13	29,29,29,29	0
57	MG	15	107	1/1	0.98	0.08	23,23,23,23	0
57	MG	1A	3444	1/1	0.98	0.10	21,21,21,21	0
57	MG	2a	1729	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3206	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3376	1/1	0.98	0.08	23,23,23,23	0
57	MG	2A	3584	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3585	1/1	0.98	0.09	29,29,29,29	0
57	MG	16	102	1/1	0.98	0.10	24,24,24,24	0
57	MG	1A	3256	1/1	0.98	0.03	16,16,16,16	0
57	MG	2A	3841	1/1	0.98	0.06	33,33,33,33	0
57	MG	17	102	1/1	0.98	0.04	17,17,17,17	0
57	MG	1a	1782	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3167	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3717	1/1	0.98	0.04	51,51,51,51	0
57	MG	1A	3096	1/1	0.98	0.05	9,9,9,9	0
57	MG	1A	3380	1/1	0.98	0.04	20,20,20,20	0
57	MG	1A	3136	1/1	0.98	0.06	33,33,33,33	0
57	MG	1a	1788	1/1	0.98	0.03	38,38,38,38	0
57	MG	2A	3597	1/1	0.98	0.08	51,51,51,51	0
57	MG	18	101	1/1	0.98	0.10	37,37,37,37	0
57	MG	2A	3150	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3452	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3602	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3968	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3858	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3859	1/1	0.98	0.09	41,41,41,41	0
57	MG	1B	216	1/1	0.98	0.04	34,34,34,34	0
57	MG	1a	1793	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3530	1/1	0.98	0.17	25,25,25,25	0
57	MG	1a	1796	1/1	0.98	0.04	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1797	1/1	0.98	0.04	60,60,60,60	0
57	MG	2A	3865	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3531	1/1	0.98	0.04	20,20,20,20	0
57	MG	1B	219	1/1	0.98	0.04	35,35,35,35	0
57	MG	1a	1603	1/1	0.98	0.11	42,42,42,42	0
57	MG	2a	1762	1/1	0.98	0.04	41,41,41,41	0
57	MG	1a	1801	1/1	0.98	0.04	49,49,49,49	0
57	MG	1B	220	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3063	1/1	0.98	0.06	27,27,27,27	0
57	MG	2A	3873	1/1	0.98	0.07	37,37,37,37	0
57	MG	2A	3615	1/1	0.98	0.08	43,43,43,43	0
57	MG	1B	222	1/1	0.98	0.03	28,28,28,28	0
57	MG	1a	1805	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3084	1/1	0.98	0.13	18,18,18,18	0
57	MG	1A	3973	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3625	1/1	0.98	0.07	25,25,25,25	0
57	MG	2a	1774	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3015	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3627	1/1	0.98	0.09	32,32,32,32	0
57	MG	1a	1811	1/1	0.98	0.03	31,31,31,31	0
57	MG	2A	3624	1/1	0.98	0.11	29,29,29,29	0
57	MG	1A	3387	1/1	0.98	0.10	22,22,22,22	0
57	MG	2a	1780	1/1	0.98	0.08	52,52,52,52	0
57	MG	1A	3116	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	3266	1/1	0.98	0.04	35,35,35,35	0
57	MG	2A	3628	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3982	1/1	0.98	0.03	30,30,30,30	0
57	MG	1A	3632	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3214	1/1	0.98	0.08	23,23,23,23	0
57	MG	1f	201	1/1	0.98	0.08	38,38,38,38	0
57	MG	2A	3634	1/1	0.98	0.05	22,22,22,22	0
57	MG	1a	1618	1/1	0.98	0.09	41,41,41,41	0
57	MG	1A	3634	1/1	0.98	0.05	11,11,11,11	0
57	MG	2A	3637	1/1	0.98	0.09	40,40,40,40	0
57	MG	1a	1620	1/1	0.98	0.05	41,41,41,41	0
57	MG	1l	202	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3735	1/1	0.98	0.03	22,22,22,22	0
57	MG	1A	3174	1/1	0.98	0.11	19,19,19,19	0
57	MG	1A	3175	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3035	1/1	0.98	0.09	16,16,16,16	0
57	MG	1A	3331	1/1	0.98	0.09	39,39,39,39	0
57	MG	1A	3218	1/1	0.98	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1D	309	1/1	0.98	0.06	34,34,34,34	0
57	MG	1D	310	1/1	0.98	0.05	29,29,29,29	0
57	MG	1a	1630	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3177	1/1	0.98	0.04	18,18,18,18	0
57	MG	2A	3651	1/1	0.98	0.13	44,44,44,44	0
57	MG	2A	3193	1/1	0.98	0.16	43,43,43,43	0
57	MG	1A	3059	1/1	0.98	0.05	26,26,26,26	0
57	MG	1D	313	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3143	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3003	1/1	0.98	0.04	20,20,20,20	0
57	MG	2A	3657	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3103	1/1	0.98	0.05	40,40,40,40	0
57	MG	1w	108	1/1	0.98	0.06	48,48,48,48	0
57	MG	1E	304	1/1	0.98	0.07	27,27,27,27	0
57	MG	1a	1638	1/1	0.98	0.14	37,37,37,37	0
57	MG	1E	305	1/1	0.98	0.11	23,23,23,23	0
57	MG	1A	3867	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3645	1/1	0.98	0.10	10,10,10,10	0
57	MG	1A	3747	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3224	1/1	0.98	0.09	31,31,31,31	0
57	MG	2F	305	1/1	0.98	0.17	40,40,40,40	0
57	MG	1A	3078	1/1	0.98	0.06	22,22,22,22	0
57	MG	1E	311	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3403	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3147	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	4004	1/1	0.98	0.13	14,14,14,14	0
57	MG	1F	301	1/1	0.98	0.04	22,22,22,22	0
57	MG	1F	304	1/1	0.98	0.06	21,21,21,21	0
57	MG	1A	4005	1/1	0.98	0.04	25,25,25,25	0
57	MG	1a	1652	1/1	0.98	0.07	31,31,31,31	0
57	MG	1a	1653	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	4006	1/1	0.98	0.04	32,32,32,32	0
57	MG	2A	3218	1/1	0.98	0.11	42,42,42,42	0
57	MG	1F	307	1/1	0.98	0.08	25,25,25,25	0
57	MG	1A	3650	1/1	0.98	0.03	19,19,19,19	0
57	MG	1A	3753	1/1	0.98	0.05	25,25,25,25	0
57	MG	2A	3007	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3754	1/1	0.98	0.05	33,33,33,33	0
57	MG	2f	201	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3755	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	4011	1/1	0.98	0.03	16,16,16,16	0
57	MG	1a	1661	1/1	0.98	0.03	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3282	1/1	0.98	0.12	18,18,18,18	0
57	MG	1A	3475	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	3284	1/1	0.98	0.15	22,22,22,22	0
57	MG	1A	3557	1/1	0.98	0.31	30,30,30,30	0
57	MG	1A	3558	1/1	0.98	0.08	23,23,23,23	0
57	MG	2A	3445	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3148	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	4018	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3105	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	4020	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3229	1/1	0.98	0.05	18,18,18,18	0
57	MG	1a	1672	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3150	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3123	1/1	0.98	0.11	25,25,25,25	0
57	MG	2v	102	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3454	1/1	0.98	0.09	40,40,40,40	0
57	MG	1A	3889	1/1	0.98	0.06	18,18,18,18	0
57	MG	2A	3027	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3890	1/1	0.98	0.06	32,32,32,32	0
57	MG	2A	3458	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3768	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	4027	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3412	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3106	1/1	0.98	0.09	23,23,23,23	0
57	MG	2A	3033	1/1	0.98	0.03	35,35,35,35	0
57	MG	1P	201	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3293	1/1	0.98	0.11	25,25,25,25	0
57	MG	1A	4031	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3125	1/1	0.98	0.16	24,24,24,24	0
57	MG	2A	3716	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3038	1/1	0.98	0.03	32,32,32,32	0
57	MG	2A	3039	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3569	1/1	0.98	0.09	18,18,18,18	0
57	MG	2A	3720	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3774	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3154	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3050	1/1	0.98	0.15	28,28,28,28	0
58	K	1A	3564	1/1	0.98	0.03	17,17,17,17	0
57	MG	1A	3778	1/1	0.98	0.04	19,19,19,19	0
57	MG	1A	3127	1/1	0.98	0.13	32,32,32,32	0
57	MG	1R	201	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3669	1/1	0.98	0.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	2Y	501	1/1	0.98	0.05	87,87,87,87	0
57	MG	1A	3354	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3904	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3689	1/1	0.99	0.05	25,25,25,25	0
57	MG	1A	3251	1/1	0.99	0.05	34,34,34,34	0
57	MG	2A	3678	1/1	0.99	0.04	26,26,26,26	0
57	MG	1A	3588	1/1	0.99	0.09	25,25,25,25	0
57	MG	2A	3866	1/1	0.99	0.12	29,29,29,29	0
57	MG	1A	4062	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3692	1/1	0.99	0.02	21,21,21,21	0
57	MG	1A	3386	1/1	0.99	0.10	20,20,20,20	0
57	MG	1A	3240	1/1	0.99	0.04	15,15,15,15	0
57	MG	2A	3509	1/1	0.99	0.03	55,55,55,55	0
57	MG	2A	3595	1/1	0.99	0.05	35,35,35,35	0
57	MG	1A	3283	1/1	0.99	0.05	30,30,30,30	0
57	MG	1A	3960	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3303	1/1	0.99	0.07	21,21,21,21	0
57	MG	1a	1756	1/1	0.99	0.03	33,33,33,33	0
57	MG	1B	226	1/1	0.99	0.03	27,27,27,27	0
57	MG	2A	3601	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3304	1/1	0.99	0.06	16,16,16,16	0
57	MG	1a	1622	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	3776	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3086	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3068	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3779	1/1	0.99	0.02	33,33,33,33	0
57	MG	1a	1764	1/1	0.99	0.07	35,35,35,35	0
57	MG	1A	3095	1/1	0.99	0.02	12,12,12,12	0
57	MG	1A	4075	1/1	0.99	0.06	30,30,30,30	0
57	MG	1B	234	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3871	1/1	0.99	0.06	10,10,10,10	0
57	MG	1B	236	1/1	0.99	0.03	22,22,22,22	0
57	MG	1D	301	1/1	0.99	0.09	17,17,17,17	0
57	MG	1A	3919	1/1	0.99	0.01	18,18,18,18	0
57	MG	1A	3825	1/1	0.99	0.03	10,10,10,10	0
57	MG	1A	3287	1/1	0.99	0.05	25,25,25,25	0
57	MG	2A	3531	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3064	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	3631	1/1	0.99	0.05	30,30,30,30	0
57	MG	1A	3514	1/1	0.99	0.07	25,25,25,25	0
57	MG	1A	3974	1/1	0.99	0.04	44,44,44,44	0
57	MG	1A	3975	1/1	0.99	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	101	1/1	0.99	0.06	23,23,23,23	0
57	MG	2A	3070	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	4084	1/1	0.99	0.04	29,29,29,29	0
57	MG	2A	3540	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3599	1/1	0.99	0.10	41,41,41,41	0
57	MG	2A	3542	1/1	0.99	0.12	33,33,33,33	0
57	MG	1A	3489	1/1	0.99	0.14	30,30,30,30	0
57	MG	2A	3631	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3128	1/1	0.99	0.08	37,37,37,37	0
57	MG	1A	3069	1/1	0.99	0.06	9,9,9,9	0
57	MG	1A	3443	1/1	0.99	0.07	20,20,20,20	0
57	MG	15	102	1/1	0.99	0.06	23,23,23,23	0
57	MG	1A	3709	1/1	0.99	0.03	21,21,21,21	0
57	MG	2A	3079	1/1	0.99	0.10	21,21,21,21	0
57	MG	2A	3728	1/1	0.99	0.06	40,40,40,40	0
57	MG	15	104	1/1	0.99	0.20	24,24,24,24	0
57	MG	1A	4034	1/1	0.99	0.05	19,19,19,19	0
57	MG	1A	3573	1/1	0.99	0.12	21,21,21,21	0
57	MG	1A	3005	1/1	0.99	0.07	27,27,27,27	0
57	MG	2A	3009	1/1	0.99	0.08	29,29,29,29	0
57	MG	1A	3792	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3575	1/1	0.99	0.09	30,30,30,30	0
57	MG	2A	3645	1/1	0.99	0.04	27,27,27,27	0
57	MG	2A	3557	1/1	0.99	0.05	36,36,36,36	0
57	MG	1A	3839	1/1	0.99	0.05	29,29,29,29	0
57	MG	1a	1794	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3560	1/1	0.99	0.06	30,30,30,30	0
57	MG	2A	3832	1/1	0.99	0.03	23,23,23,23	0
57	MG	2P	201	1/1	0.99	0.07	52,52,52,52	0
57	MG	1A	3935	1/1	0.99	0.02	4,4,4,4	0
57	MG	1A	3291	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3273	1/1	0.99	0.05	39,39,39,39	0
57	MG	2A	3836	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3609	1/1	0.99	0.10	15,15,15,15	0
57	MG	2a	1764	1/1	0.99	0.08	54,54,54,54	0
57	MG	1A	3013	1/1	0.99	0.08	11,11,11,11	0
57	MG	1V	202	1/1	0.99	0.13	18,18,18,18	0
57	MG	1A	3260	1/1	0.99	0.03	29,29,29,29	0
57	MG	2A	3096	1/1	0.99	0.06	30,30,30,30	0
57	MG	1A	3680	1/1	0.99	0.04	15,15,15,15	0
57	MG	2A	3329	1/1	0.99	0.11	26,26,26,26	0
57	MG	2A	3844	1/1	0.99	0.03	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	302	1/1	0.99	0.04	28,28,28,28	0
57	MG	2A	3846	1/1	0.99	0.04	45,45,45,45	0
57	MG	1F	303	1/1	0.99	0.15	23,23,23,23	0
57	MG	1A	3014	1/1	0.99	0.09	19,19,19,19	0
57	MG	2A	3574	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3758	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3262	1/1	0.99	0.05	36,36,36,36	0
57	MG	1A	3030	1/1	0.99	0.07	16,16,16,16	0
57	MG	2A	3104	1/1	0.99	0.08	22,22,22,22	0
57	MG	1A	3553	1/1	0.99	0.12	22,22,22,22	0
57	MG	1A	3179	1/1	0.99	0.02	10,10,10,10	0
57	MG	1A	4053	1/1	0.99	0.02	22,22,22,22	0
57	MG	1A	3617	1/1	0.99	0.11	31,31,31,31	0
60	ZN	1Y	204	1/1	0.99	0.03	59,59,59,59	0
57	MG	1A	3280	1/1	0.99	0.16	23,23,23,23	0
60	ZN	15	110	1/1	0.99	0.05	35,35,35,35	0
60	ZN	16	103	1/1	0.99	0.03	34,34,34,34	0
60	ZN	1n	104	1/1	0.99	0.03	48,48,48,48	0
57	MG	1A	3765	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3809	1/1	0.99	0.05	17,17,17,17	0
60	ZN	25	106	1/1	0.99	0.04	52,52,52,52	0
60	ZN	26	501	1/1	0.99	0.03	47,47,47,47	0
60	ZN	29	102	1/1	0.99	0.04	59,59,59,59	0
57	MG	1A	3384	1/1	0.99	0.04	34,34,34,34	0
61	SF4	1d	302	8/8	0.99	0.05	43,47,53,61	0
61	SF4	2d	303	8/8	0.99	0.04	42,45,50,53	0
60	ZN	19	501	1/1	1.00	0.03	34,34,34,34	0
57	MG	1A	3036	1/1	1.00	0.07	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.