



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:51 AM UTC

PDB ID : 6CFJ / pdb_00006cfj
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with histidyl-CAM and bound to mRNA and A-, P-, and E-site tRNAs at 2.8Å resolution
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.
Deposited on : 2018-02-15
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

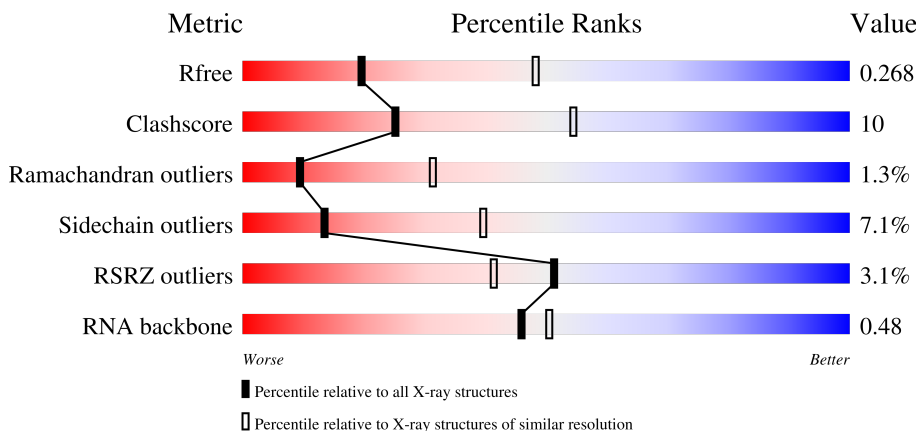
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

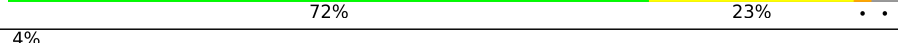
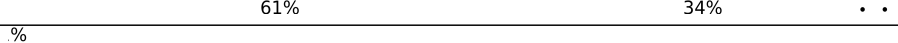
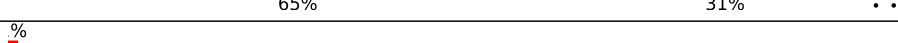
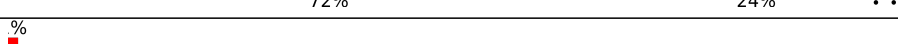
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	

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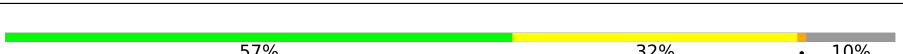
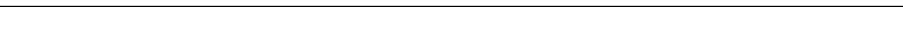
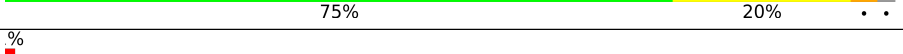
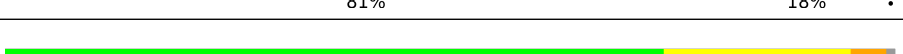
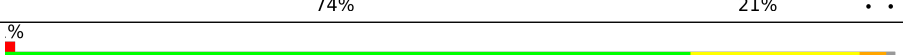
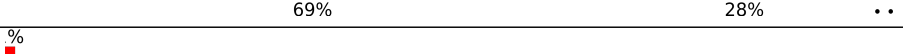
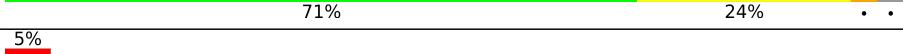
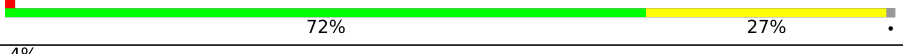
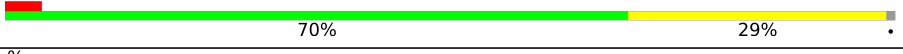
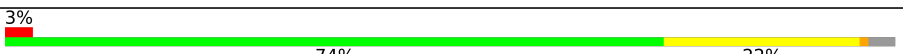
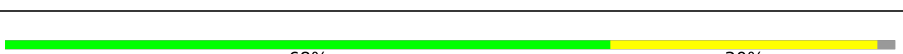
Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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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	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	2y	55	-	-	X	-
56	MG	1D	304	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 299109 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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1273	G	UNK	conflict	GB 37223181
2A	1227	G	UNK	conflict	GB 37223181

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1x	8	4SU	G	conflict	GB 205271127
2x	8	4SU	G	conflict	GB 205271127

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1063	Total	Mg	0	0
			1063	1063		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1B	38	Total 38	Mg 38	0	0
56	1D	14	Total 14	Mg 14	0	0
56	1E	13	Total 13	Mg 13	0	0
56	1F	9	Total 9	Mg 9	0	0
56	1G	5	Total 5	Mg 5	0	0
56	1I	1	Total 1	Mg 1	0	0
56	1N	5	Total 5	Mg 5	0	0
56	1O	7	Total 7	Mg 7	0	0
56	1P	3	Total 3	Mg 3	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	1R	5	Total 5	Mg 5	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	6	Total 6	Mg 6	0	0
56	1V	3	Total 3	Mg 3	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1X	6	Total 6	Mg 6	0	0
56	1Y	2	Total 2	Mg 2	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	10	5	Total 5	Mg 5	0	0
56	11	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	12	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	15	6	Total 6	Mg 6	0	0
56	16	3	Total 3	Mg 3	0	0
56	17	5	Total 5	Mg 5	0	0
56	18	3	Total 3	Mg 3	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	215	Total 215	Mg 215	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1q	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	11	Total 11	Mg 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1x	15	Total 15	Mg 15	0	0
56	1y	4	Total 4	Mg 4	0	0
56	2A	754	Total 754	Mg 754	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2D	7	Total 7	Mg 7	0	0
56	2E	10	Total 10	Mg 10	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2O	2	Total 2	Mg 2	0	0
56	2P	1	Total 1	Mg 1	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	2R	4	Total 4	Mg 4	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	6	Total 6	Mg 6	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	3	Total 3	Mg 3	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0

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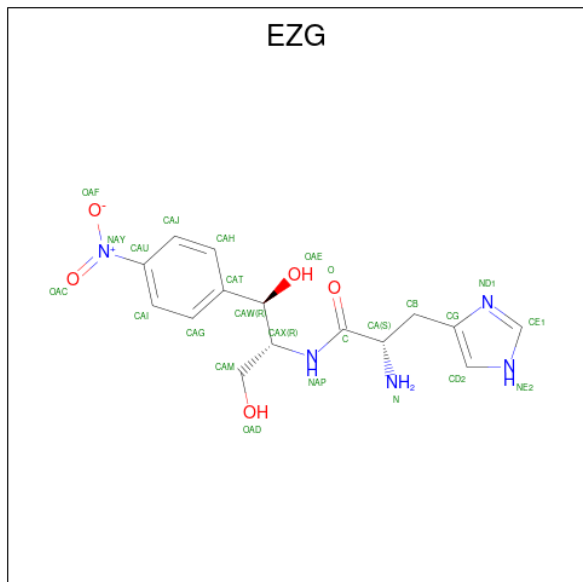
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	25	3	Total 3	Mg 3	0	0
56	27	2	Total 2	Mg 2	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	233	Total 233	Mg 233	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2q	4	Total 4	Mg 4	0	0
56	2r	2	Total 2	Mg 2	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	5	Total 5	Mg 5	0	0
56	2w	9	Total 9	Mg 9	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2y	7	Total 7	Mg 7	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	2	Total 2	K 2	0	0
57	2A	2	Total 2	K 2	0	0

- Molecule 58 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-histidinamide (CCD ID: EZG) (formula: C₁₅H₁₉N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			25	15	5	5		
58	2A	1	Total	C	N	O	0	0
			25	15	5	5		

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

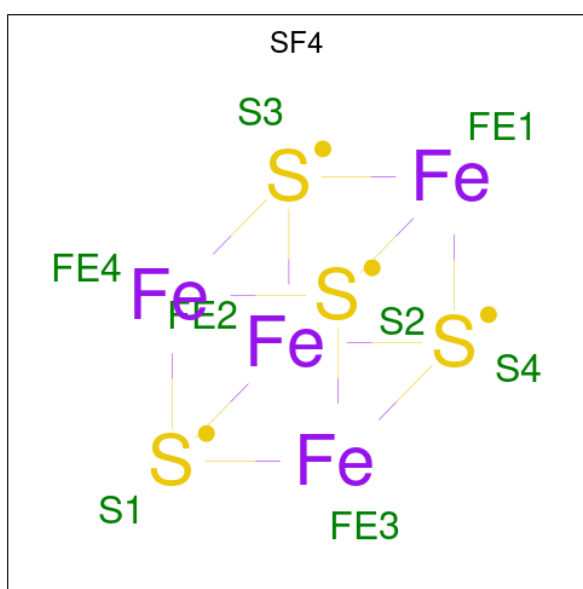
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1433	Total	O	0	0
			1433	1433		
61	1B	65	Total	O	0	0
			65	65		
61	1D	24	Total	O	0	0
			24	24		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	30	Total 30	O 30	0	0
61	1F	10	Total 10	O 10	0	0
61	1G	8	Total 8	O 8	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	6	Total 6	O 6	0	0
61	1O	8	Total 8	O 8	0	0
61	1P	18	Total 18	O 18	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	9	Total 9	O 9	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	8	Total 8	O 8	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	7	Total 7	O 7	0	0
61	12	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	4	Total 4	O 4	0	0
61	15	5	Total 5	O 5	0	0
61	16	2	Total 2	O 2	0	0
61	17	9	Total 9	O 9	0	0
61	18	7	Total 7	O 7	0	0
61	1a	315	Total 315	O 315	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	20	Total 20	O 20	0	0
61	1x	14	Total 14	O 14	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	885	Total 885	O 885	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2B	26	Total 26	O 26	0	0
61	2D	18	Total 18	O 18	0	0
61	2E	14	Total 14	O 14	0	0
61	2F	18	Total 18	O 18	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2P	12	Total 12	O 12	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0
61	21	8	Total 8	O 8	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	26	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	258	Total 258	O 258	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	5	Total 5	O 5	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	6	Total 6	O 6	0	0

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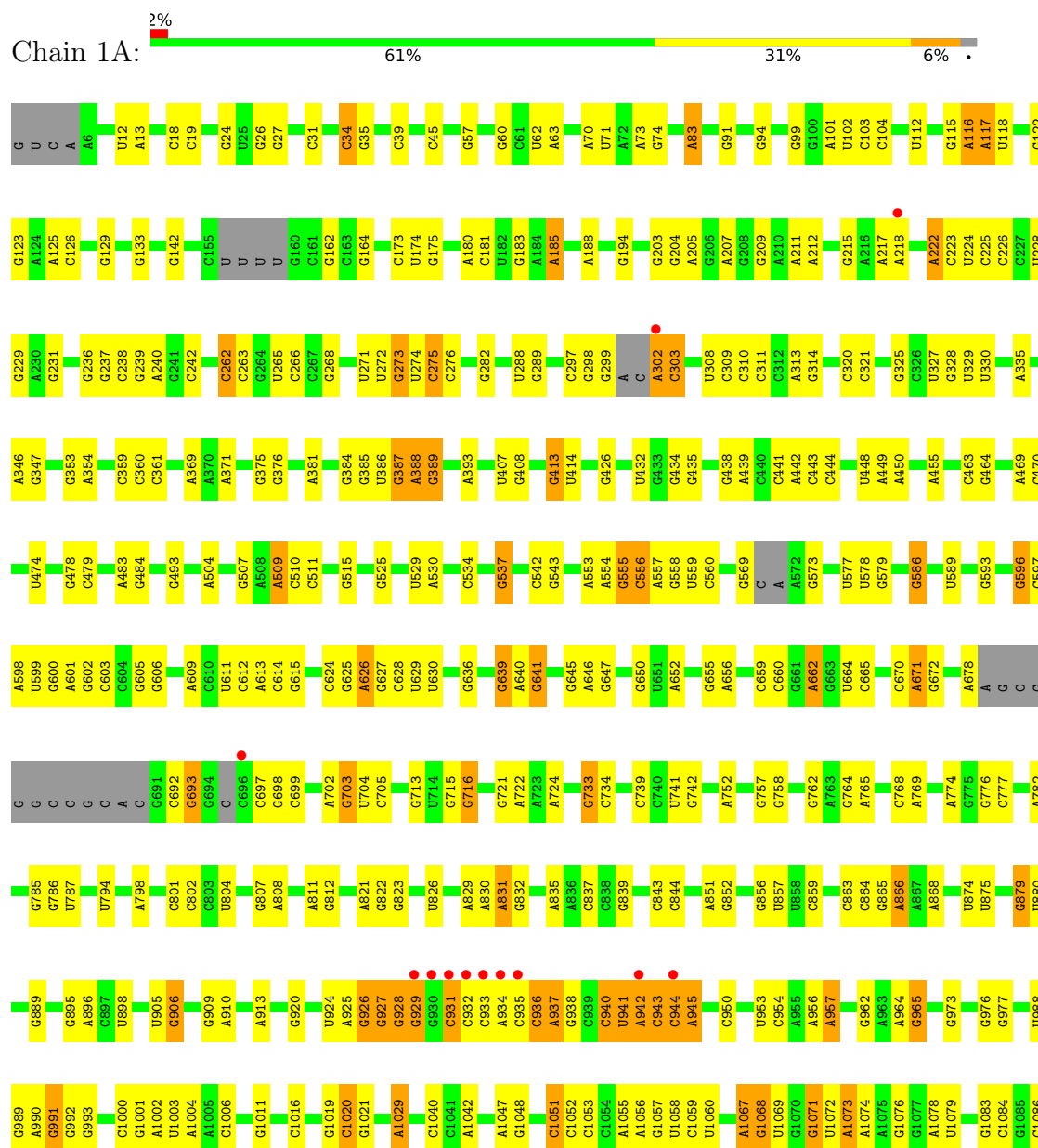
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	18	Total	O	0	0
			18	18		

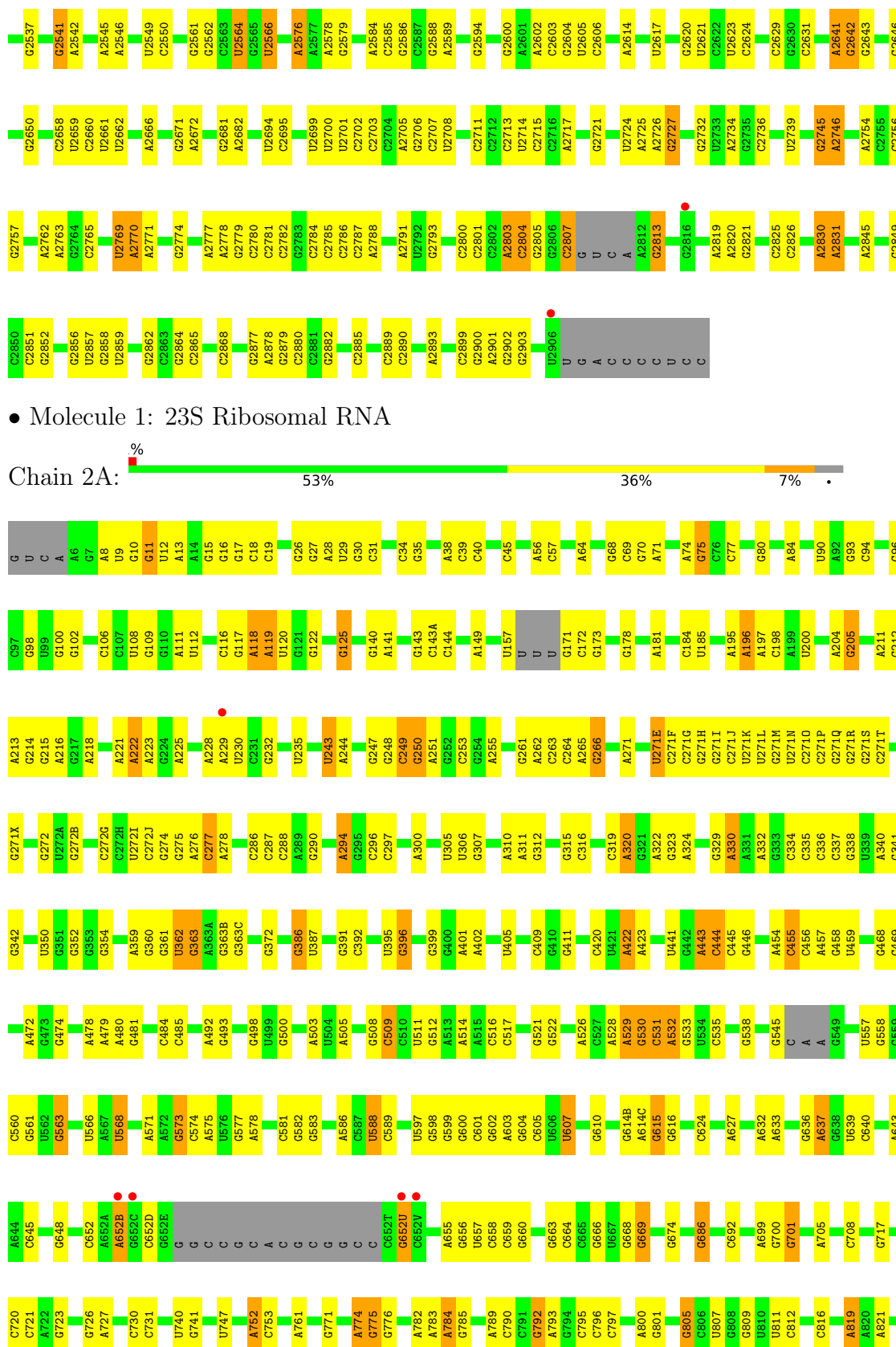
3 Residue-property plots

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

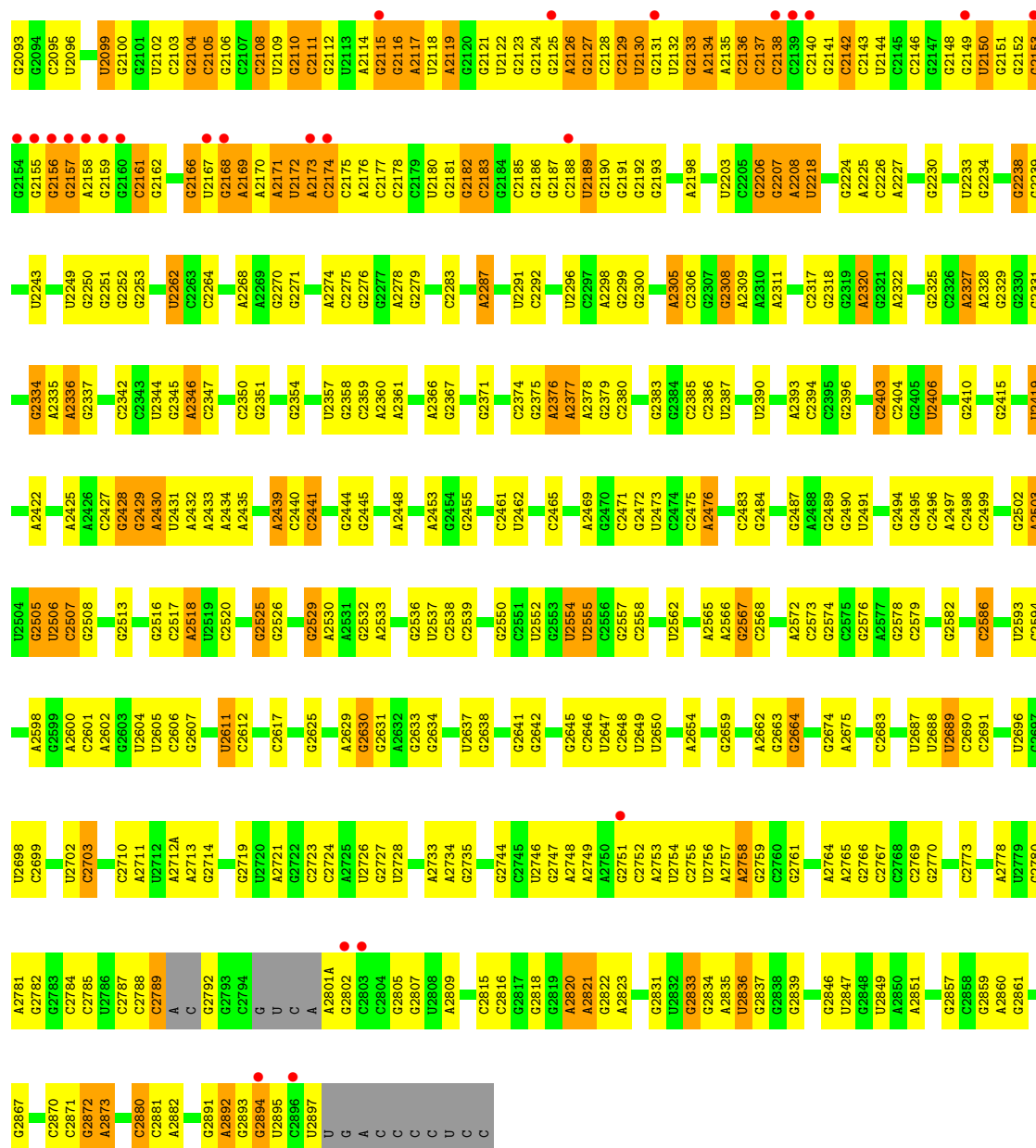


A2434	G2337	G2236	G2163	U1973	U1740	A1826	G1530	A1400	C1245	A1149	C1087
A2437	C2338	A2237	C2164	A1974	G1743	A1827	A1536	G1401	C1246	G1150	G1088
G2441	A2239	G2083	G2165	A1975	A1846	G2084	A1537	A1405	U1151	U1151	G1089
A2442	G2340	C2085	U2166	G1976	G1847	G1977	C1539	A1406	G1152	G1152	G1090
U2443	G2341	G2086	C2167	U1977	A1848	U1978	A1540	A1407	U1153	U1153	A1091
A2447	G2342	G2087	G2168	A1978	U1849	A1849	A1541	G1410	U1154	U1154	A1092
A2451	G2343	G2088	G2169	C1983	U1850	G1983	A1542	A1411	G1155	G1155	G1093
C2452	G2344	G2089	G2170	U1984	U1851	G1984	C1543	U1418	G1156	G1156	A1094
C2453	G2345	G2090	G2171	U1985	G1852	U1985	C1544	U1419	A1157	A1157	A1095
C2454	G2346	G2091	G2172	U1986	G1853	U1986	C1545	U1420	U1158	U1158	A1096
G2455	G2347	G2092	U2096	A1987	U1756	U1987	C1546	U1421	U1159	U1159	G1097
G2456	A2347	U2097	U2097	G1989	C1757	G1989	C1547	C1422	G1160	G1160	C1098
A2460	A2348	U2101	U2101	G1990	U1760	G1990	C1548	A1423	U1161	U1161	A1099
G2466	C2359	A2104	A2104	A1991	G1761	A1991	C1549	A1424	C1162	C1162	A1100
C2483	C2362	G2178	G2178	A1992	G1762	A1992	A1553	G1425	G1163	G1163	G1101
A2488	G2365	G2179	G2179	A1993	G1763	A1993	A1554	G1426	U1164	U1164	U1102
C2489	G2366	A2180	A2180	A1994	A1767	A1994	A1555	A1430	G1165	G1165	A1103
A2490	G2367	G2181	G2181	G1997	A1770	G1997	A1556	C1432	G1168	G1168	G1104
G2494	C2381	G2182	G2182	G1998	C1775	G1998	U1580	C1433	G1171	G1171	G1105
C2495	G2382	C2116	C2116	G2006	G1776	G2006	C1561	U1440	U1176	U1176	U1106
A2500	G2383	G2117	G2117	U2013	G1777	U2013	G1567	A1441	G1180	G1180	U
G2501	A2372	G2118	G2118	G2014	G1778	G2014	U1568	U1442	G1181	G1181	G1108
U2503	A2373	U2120	U2120	U2015	A1783	U2015	G1569	C1445	G1182	G1182	G1109
U2504	C2376	U2121	U2121	G2019	G1793	G2019	G1570	U1451	G1183	G1183	G1110
U2505	G2377	G2122	G2122	G2020	G1794	G2020	G1571	U1452	G1184	G1184	U1111
G2506	G2378	G2123	G2123	C2021	G1795	C2021	G1572	C1453	G1185	G1185	U1112
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A2515	C2384	C2130	C2130	A2035	A1811	A2035	G1577	G1467	G1197	G1197	G1116
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C2524	C2390	G2137	G2137	G2041	A1817	G2041	G1583	U1211	U1211	U1211	U1126
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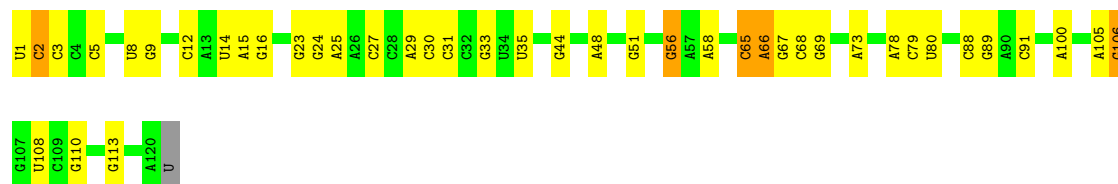
• Molecule 1: 23S Ribosomal RNA

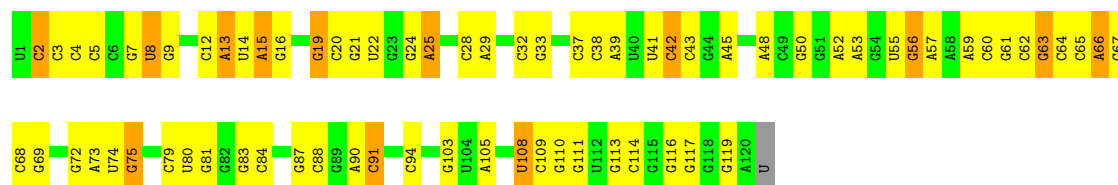
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G2012	A1912	C1797	G1682	C1408	A1284	G1200	G1115	G	C982	C902	U827
A2013	C1914	U1798	C1683	C1409	U1292	C1201	G1116	A	A983	C903	U828
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C2021	A1803	C1804	U1590	G1413	C1297	C1208	A1126	U	C991	C840	U839
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A2060	A1847	C1640	C1543	U1460	A1365	U1249	G1170	C	A1027	U877	U877
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G2069	G1877	A1654	C1558	A1469	U1372	U1255	A	C	C1038	C883	C883
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G2087	A1786	G1674	U1578	U1481	C1399	G1270	U1187	U	A	G972	G972
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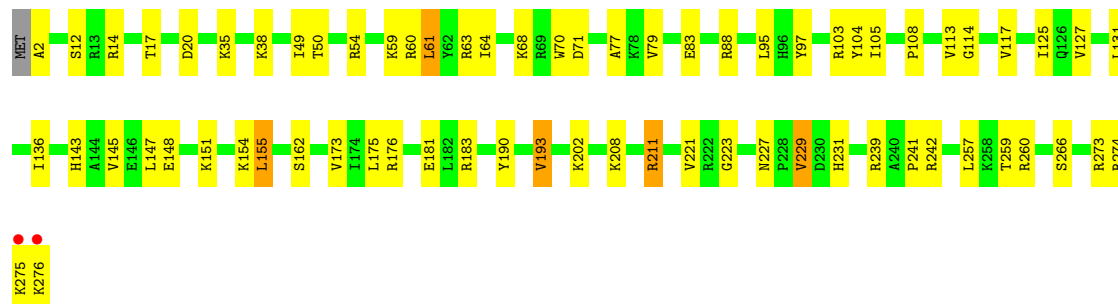
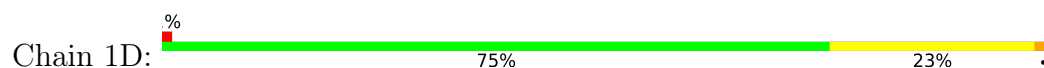
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 31% . .

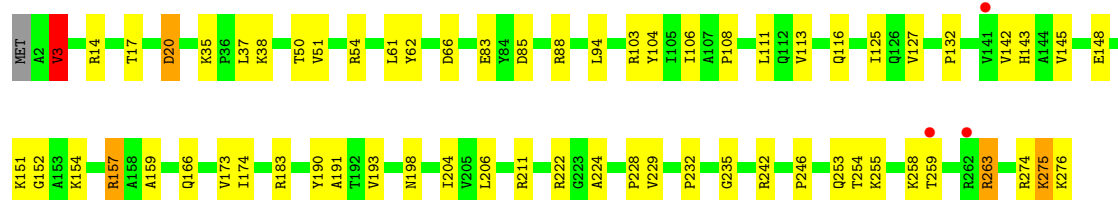
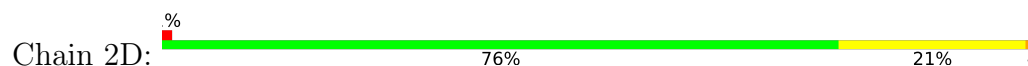




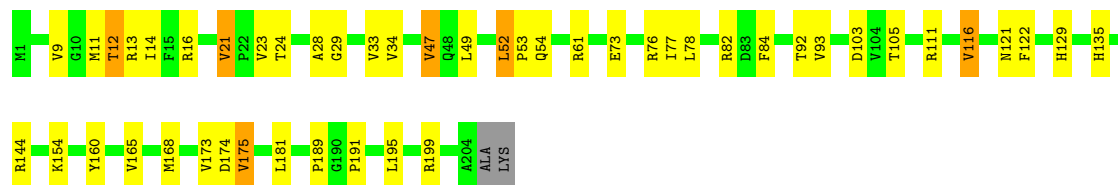
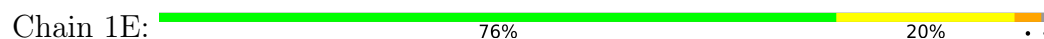
• Molecule 3: 50S ribosomal protein L2



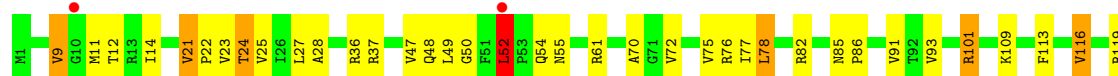
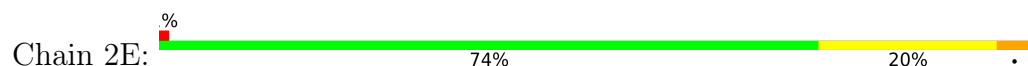
• Molecule 3: 50S ribosomal protein L2

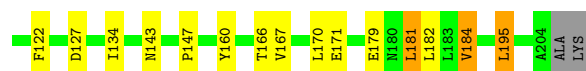


• Molecule 4: 50S ribosomal protein L3



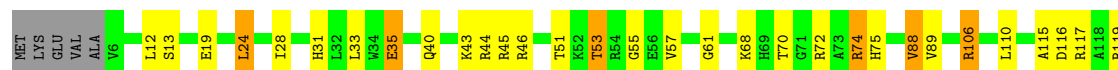
• Molecule 4: 50S ribosomal protein L3





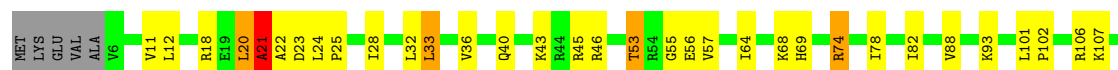
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 68% 24%



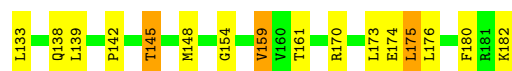
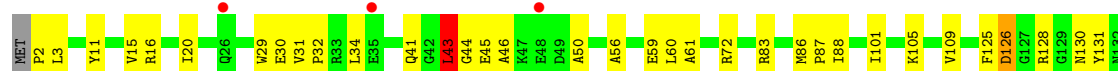
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 62% 30%



• Molecule 6: 50S ribosomal protein L5

Chain 1G: 72% 25%

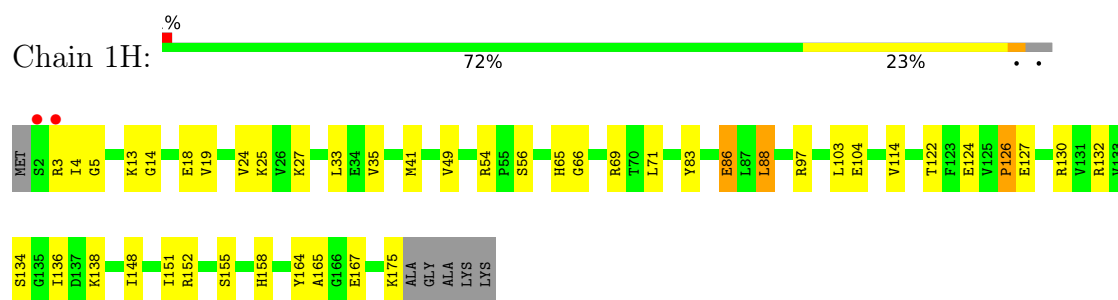


• Molecule 6: 50S ribosomal protein L5

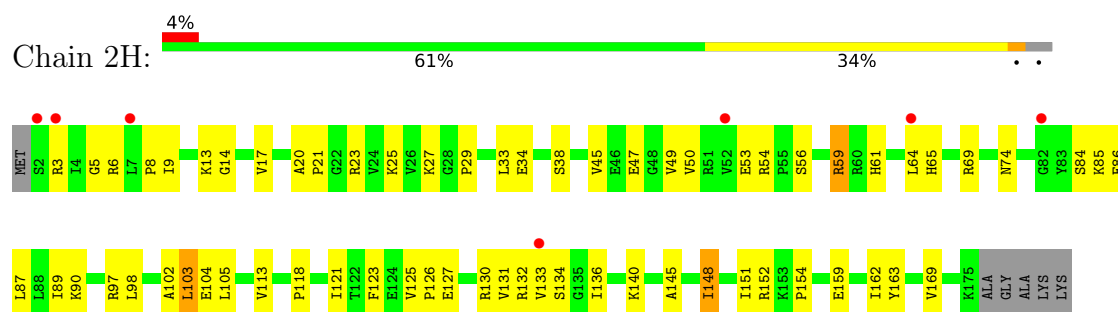
Chain 2G: 58% 39%



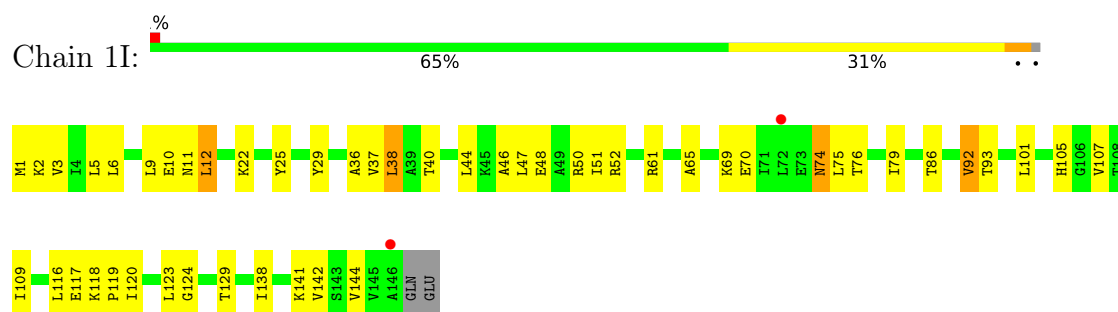
- Molecule 7: 50S ribosomal protein L6



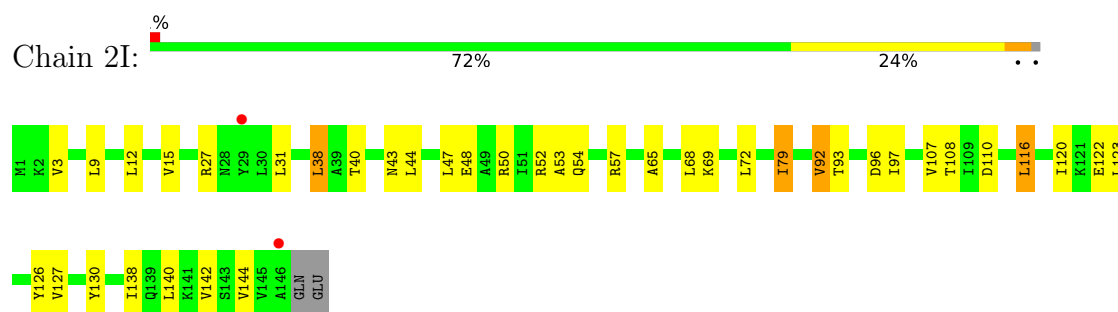
- Molecule 7: 50S ribosomal protein L6



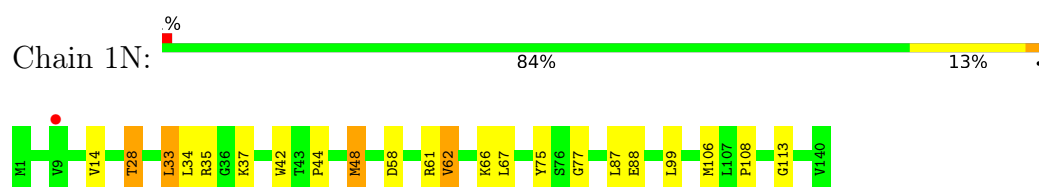
- Molecule 8: 50S ribosomal protein L9



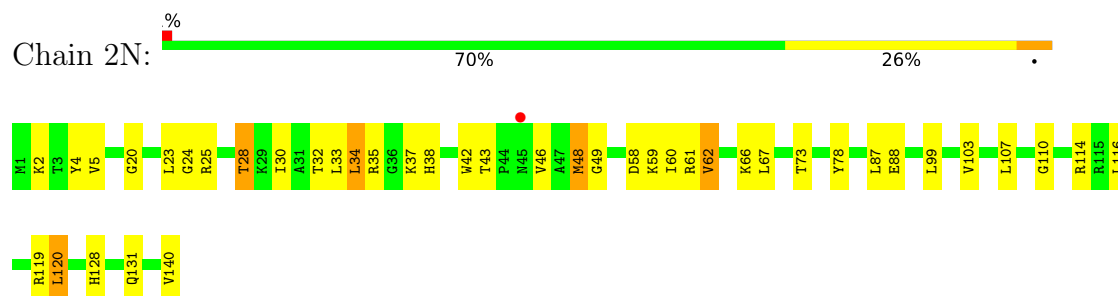
- Molecule 8: 50S ribosomal protein L9



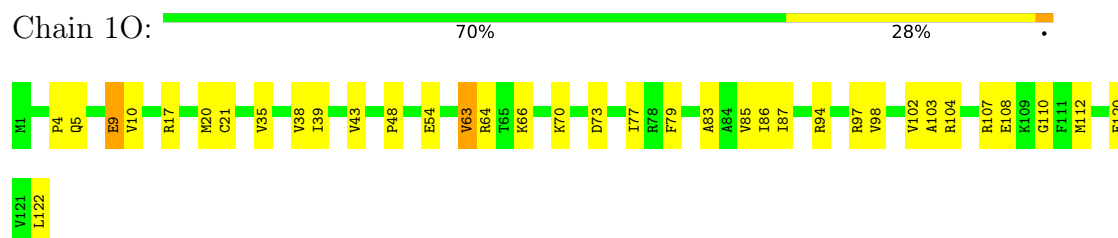
- Molecule 9: 50S ribosomal protein L13



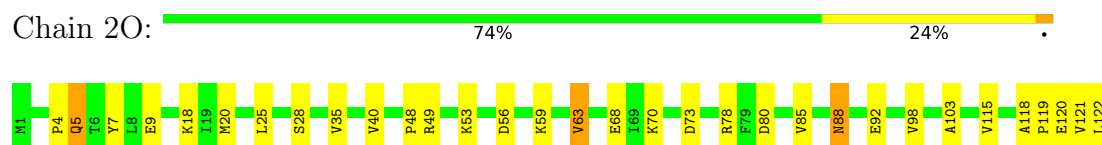
- Molecule 9: 50S ribosomal protein L13



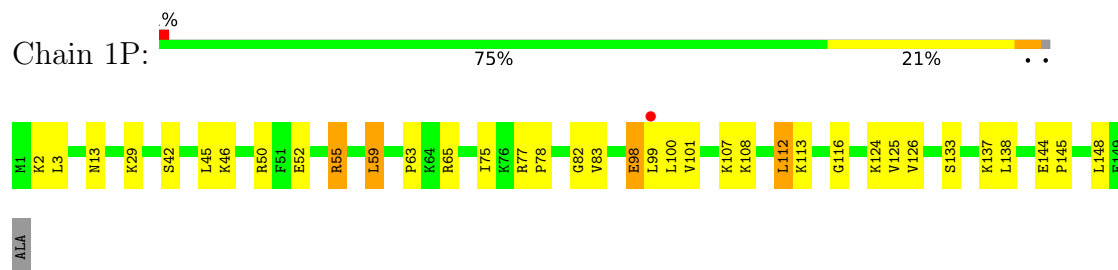
- Molecule 10: 50S ribosomal protein L14



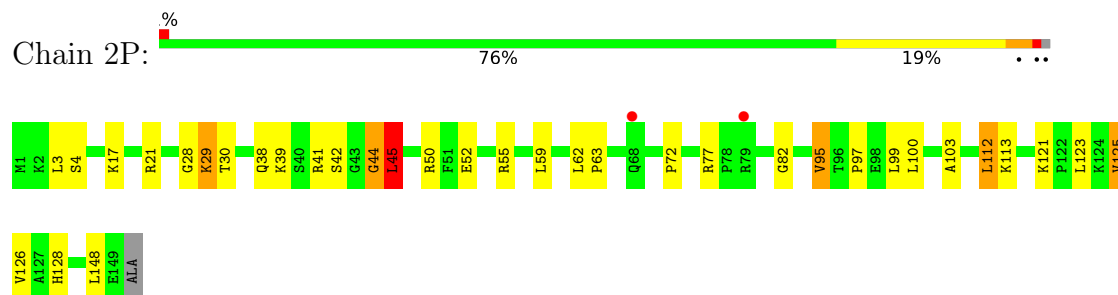
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

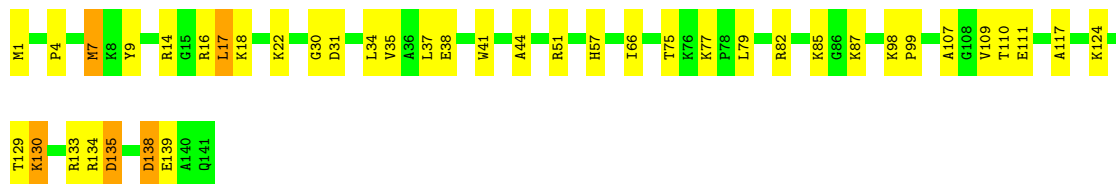


- Molecule 11: 50S ribosomal protein L15



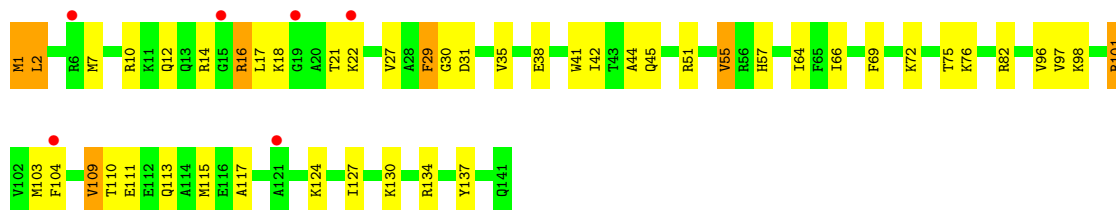
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  71% 26% .



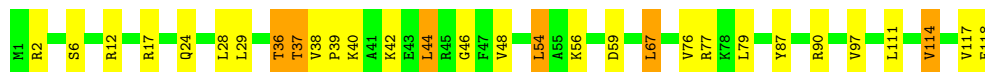
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  4% 66% 29% 5%



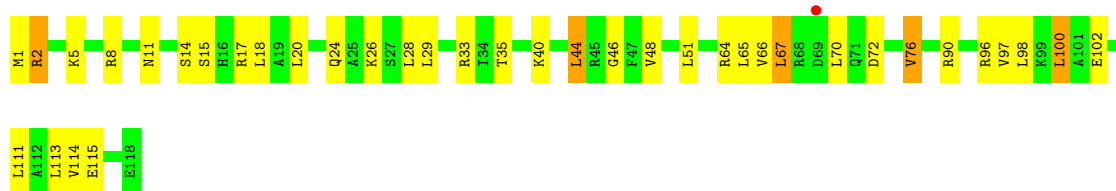
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  75% 20% 5%



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  % 68% 28% .



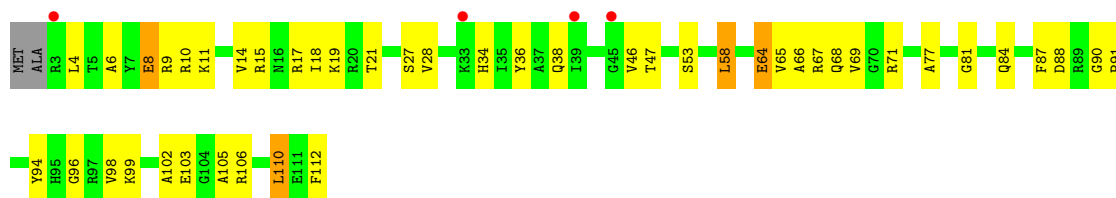
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  73% 20% 5% .

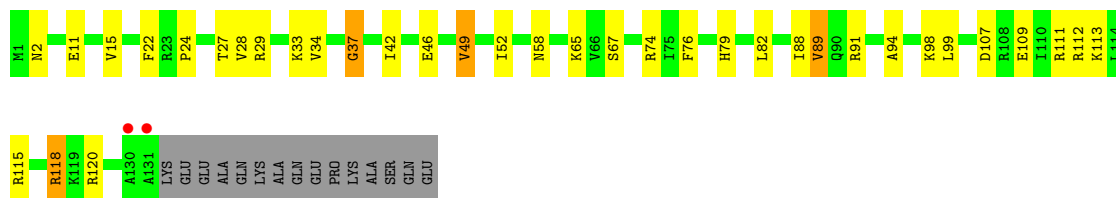


- Molecule 14: 50S ribosomal protein L18

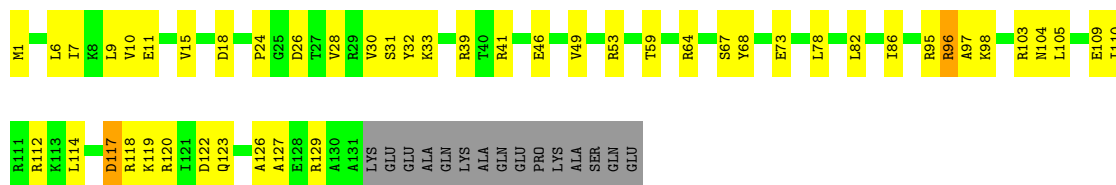
Chain 2S:  4% 58% 37% . .



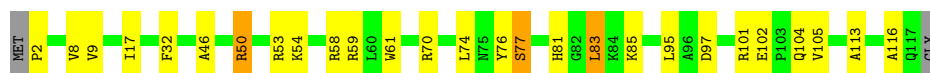
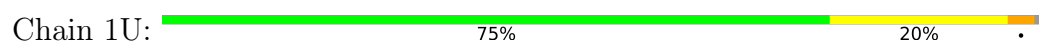
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



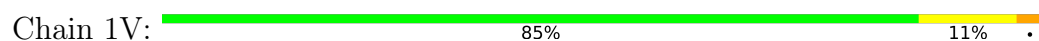
- Molecule 16: 50S ribosomal protein L20

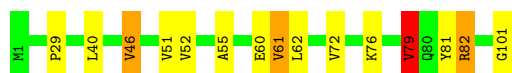


- Molecule 16: 50S ribosomal protein L20

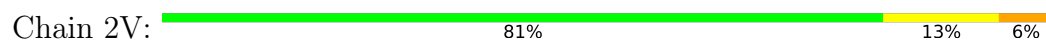


- Molecule 17: 50S ribosomal protein L21

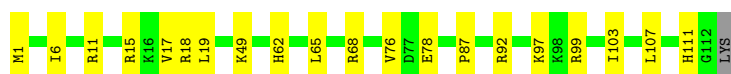
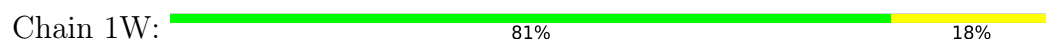




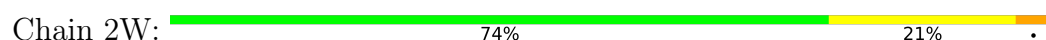
- Molecule 17: 50S ribosomal protein L21



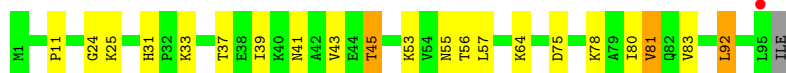
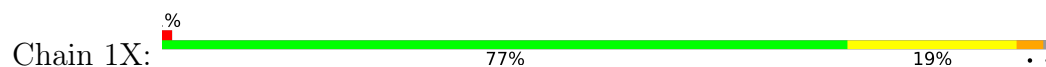
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



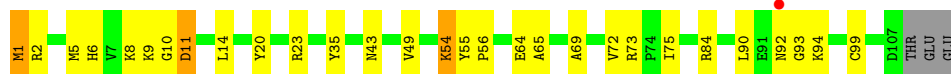
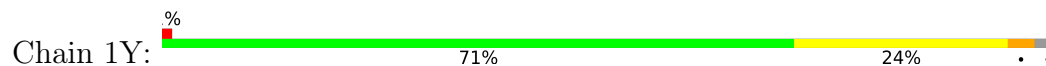
- Molecule 19: 50S ribosomal protein L23



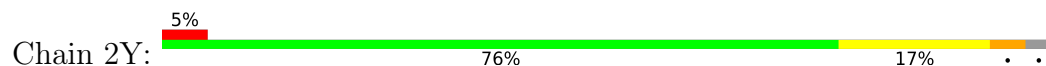
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

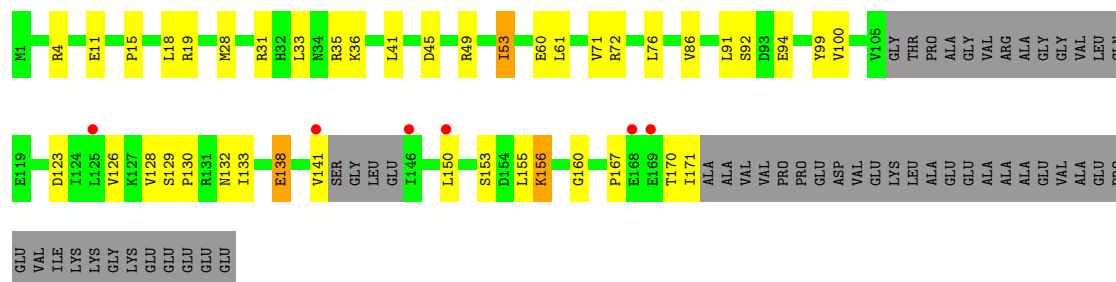


- Molecule 20: 50S ribosomal protein L24

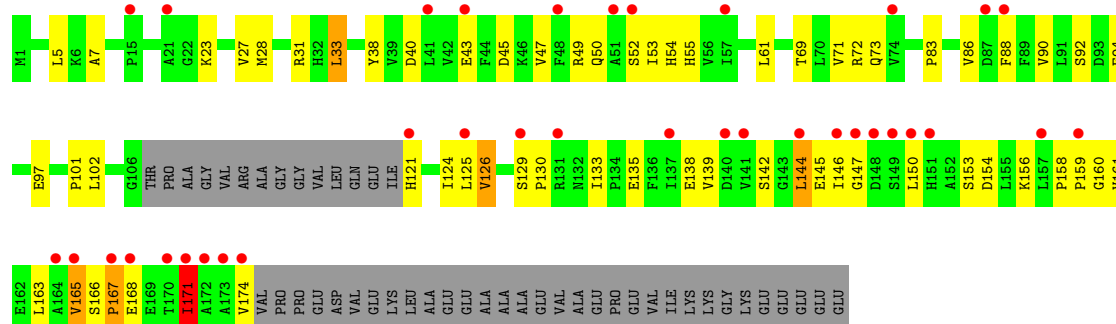




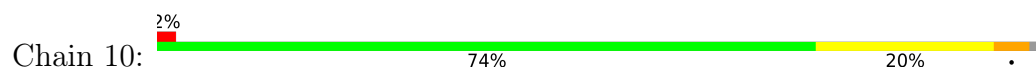
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



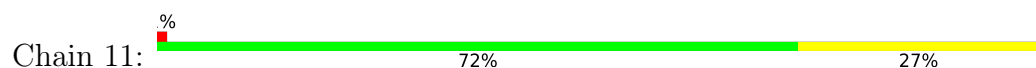
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28





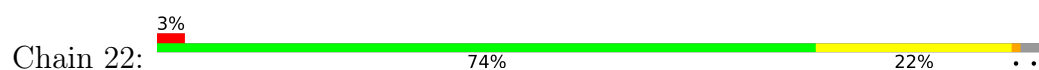
- Molecule 23: 50S ribosomal protein L28



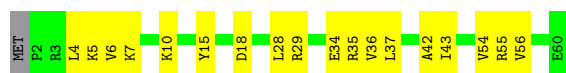
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



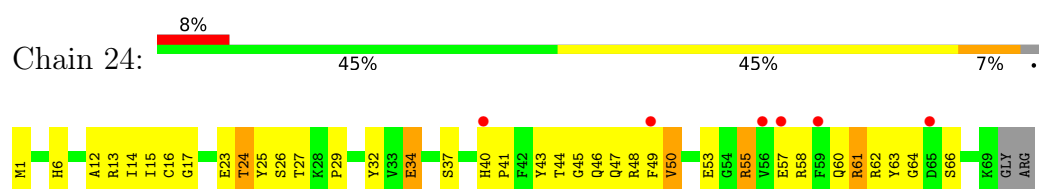
- Molecule 25: 50S ribosomal protein L30



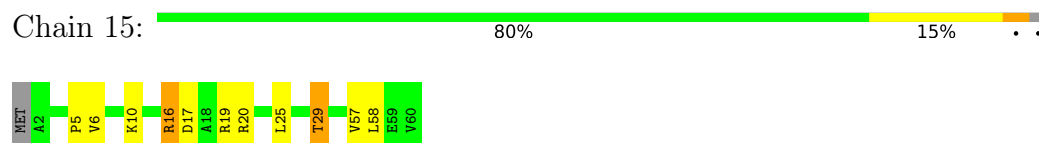
- Molecule 26: 50S ribosomal protein L31



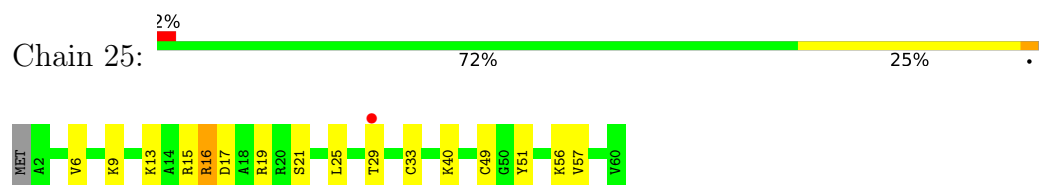
- Molecule 26: 50S ribosomal protein L31



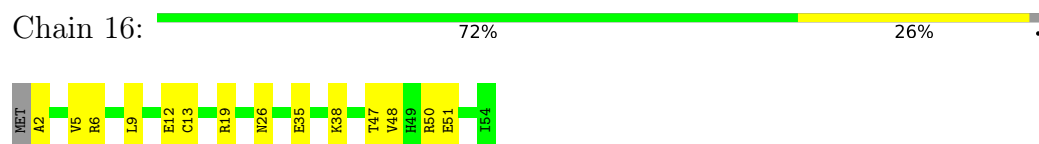
- Molecule 27: 50S ribosomal protein L32



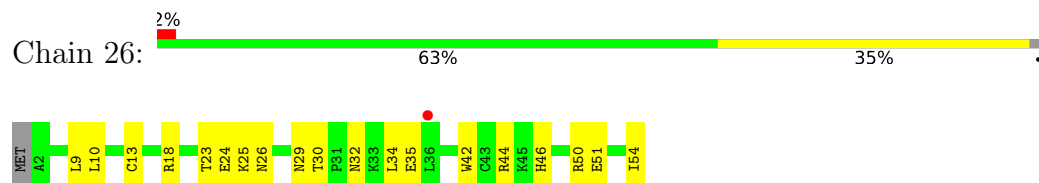
- Molecule 27: 50S ribosomal protein L32



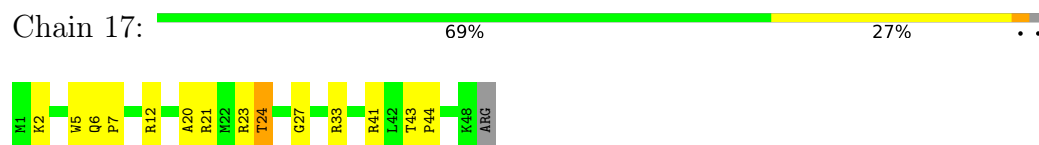
- Molecule 28: 50S ribosomal protein L33



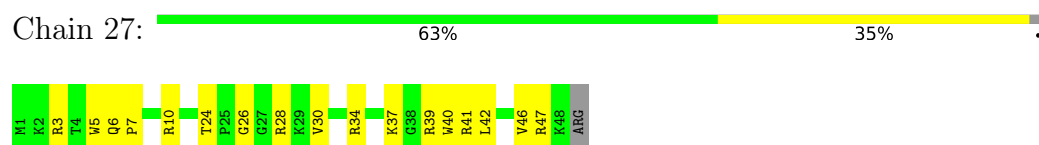
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



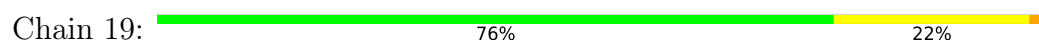
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



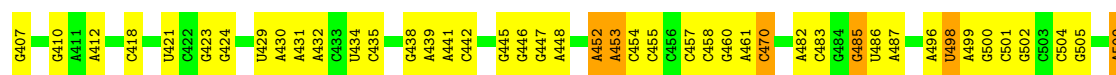
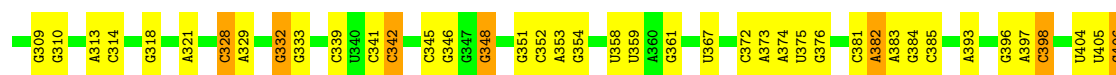
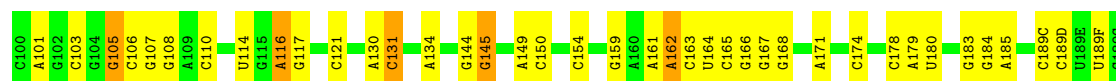
- Molecule 31: 50S ribosomal protein L36

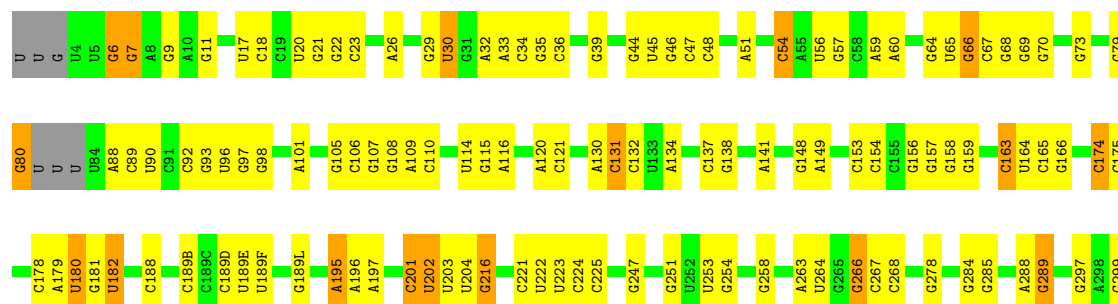


- Molecule 31: 50S ribosomal protein L36

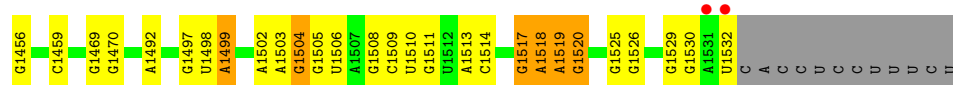


- Molecule 32: 16S Ribosomal RNA

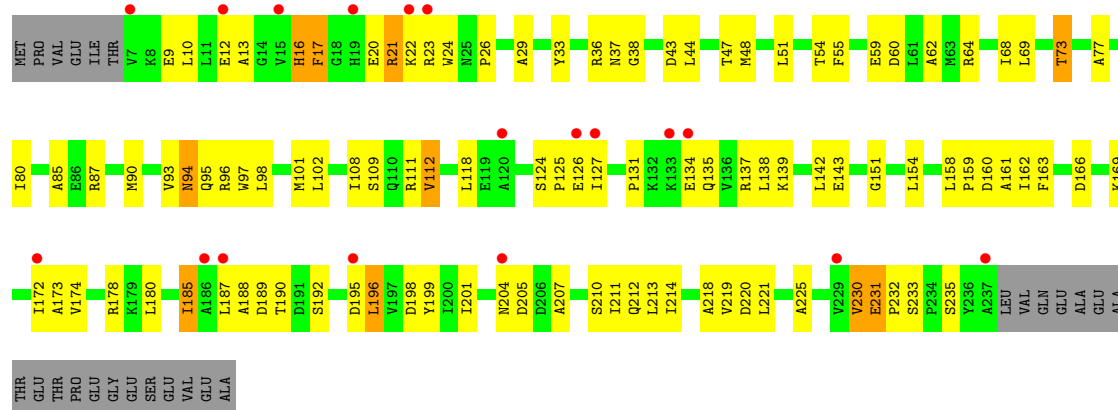




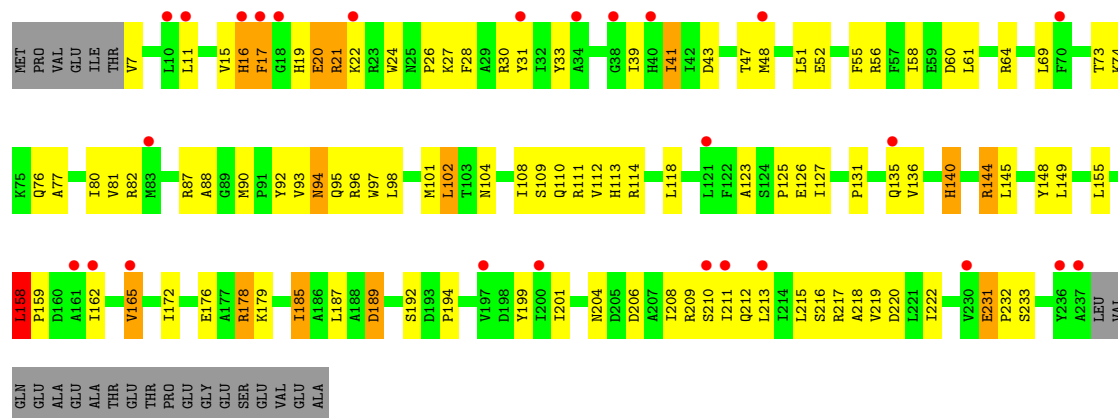
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G1373	C1296	A1227	C1030B	C970	C879	C773	A574	C490	C399	G302
A1374	C1297	C1228	G1030C	G971	C880	G777	G575	C401	C400	G316
A1299	C1162	G1163	A1030D	C972	C881	G778	G576	C402	C402	G316
G1300	C1163	G1166	G1031	C973	C882	G779	G577	C403	C403	A321
U1301	C1164	G1168	G1032	C974	C883	G780	G578	C404	C404	G324
A1377	G1169	A1168	G1033	C975	C886	G781	G579	C405	C405	G324
U1302	A1170	C1169	G1034	C976	C887	G782	G580	C406	C406	A325
G1303	A1171	G1170	G1035	C977	C888	G783	G581	C407	C407	G326
G1304	G1172	A1171	G1036	C978	C889	G784	G582	C408	C408	A327
G1305	C1173	G1173	G1037	C979	C890	G785	G583	C409	C409	C328
G1309	G1174	G1174	C1038	C980	C891	G786	G584	C410	C410	A329
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G1311	G1176	G1176	U1040	C982	C893	G788	G586	C412	C412	G331
G1312	G1177	G1177	U1041	C983	C894	G789	G587	C413	C413	G332
G1313	G1178	G1178	U1042	C984	C895	G790	G588	C414	C414	G335
U1314	G1179	A1179	C1043	C985	C896	G791	G589	C415	C415	G340
U1315	A1180	A1180	U1044	C986	C897	G792	G590	C416	C416	C341
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G1317	G1182	G1182	U1046	C988	C899	G794	G592	C418	C418	A344
A1318	G1183	G1183	G1047	C989	C900	G795	G593	C419	C419	C345
A1319	G1184	G1184	G1048	C990	C901	G796	G594	C420	C420	C346
C1320	G1185	G1185	G1049	C991	C902	G797	G595	C421	C421	C352
C1321	G1186	G1186	U1050	C992	C903	G798	G596	C422	C422	A353
G1322	G1187	G1187	U1051	C993	C904	G799	G597	C423	C423	G354
G1323	G1188	G1188	U1052	C994	C905	G800	G598	C424	C424	C355
C1324	G1189	G1189	U1053	C995	C906	G801	G599	C425	C425	C355
C1325	G1190	G1190	U1054	C996	C907	G802	G600	C426	C426	U359
C1326	G1191	G1191	U1055	C997	C908	G803	G601	C427	C427	A360
A1327	G1192	G1192	U1056	C998	C909	G804	G602	C428	C428	G361
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G1331	G1194	G1194	U1058	C1000	C911	G806	G604	C430	C430	A363
A1332	G1195	G1195	U1059	C1001	C912	G807	G605	C431	C431	A364
A1333	G1196	G1196	U1060	C1002	C913	G808	G606	C432	C432	U365
G1334	G1197	G1197	U1061	C1003	C914	G809	G607	C433	C433	C366
G1337	G1200	G1200	U1062	C1004	C915	G810	G608	C434	C434	U367
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G1342	G1202	G1202	U1064	C1006	C917	G812	G610	C436	C436	A368
G1343	G1203	G1203	U1065	C1007	C918	G813	G611	C437	C437	A373
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G1352	G1205	G1205	U1067	C1009	C920	G815	G613	C439	C439	U375
G1353	G1206	G1206	U1068	C1010	C921	G816	G614	C440	C440	G376
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A1428	U1212	U1212	U1070	C1012	C923	G818	G616	C442	C442	A378
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U1439	U1212	U1212	U1077	C1019	C930	G825	G623	C449	C449	C385
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G1440	G1216	G1216	U1079	U1020	C932	G827	G625	C451	C451	C390
G1441	G1217	G1217	U1080	U1021	C933	G828	G626	C452	C452	G391
G1442	G1218	G1218	U1081	U1022	C934	G829	G627	C453	C453	G392
G1443	G1219	G1219	U1082	U1023	C935	G830	G628	C454	C454	G455
G1444	G1220	G1220	U1083	U1024	C936	G831	G629	C455	C455	
G1445	G1221	G1221	U1084	U1025	C937	G832	G630	C456	C456	
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G1492	G1268	G1268	U1131	U1072	C984	G879	G677	C503	C503	
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G1498	G1274	G1274	U1137	U1078	C990	G885	G683	C509	C509	
G1499	G1275	G1275	U1138	U1079	C991	G886	G684	C510	C510	
G1500	G1276	G1276	U1139	U1080	C992	G887	G685	C511	C511	
G1501	G1277	G1277	U1140	U1081	C993	G888	G686	C512	C512	
G1502	G1278	G1278	U1141	U1082	C994	G889	G687	C513	C513	
G1503	G1279	G1279	U1142	U1083	C995	G890	G688	C514	C514	
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G1507	G1283	G1283	U1146	U1087	C999	G894	G692	C518	C518	
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G1512	G1288	G1288	U1151	U1092	C1004	G899	G697	C523	C523	
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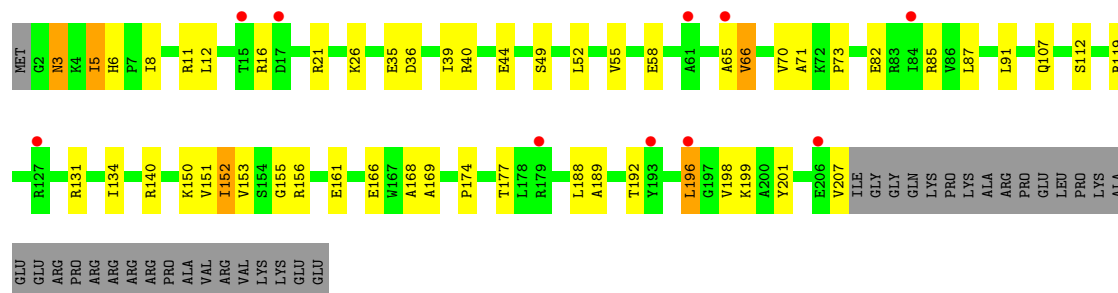
• Molecule 33: 30S ribosomal protein S2



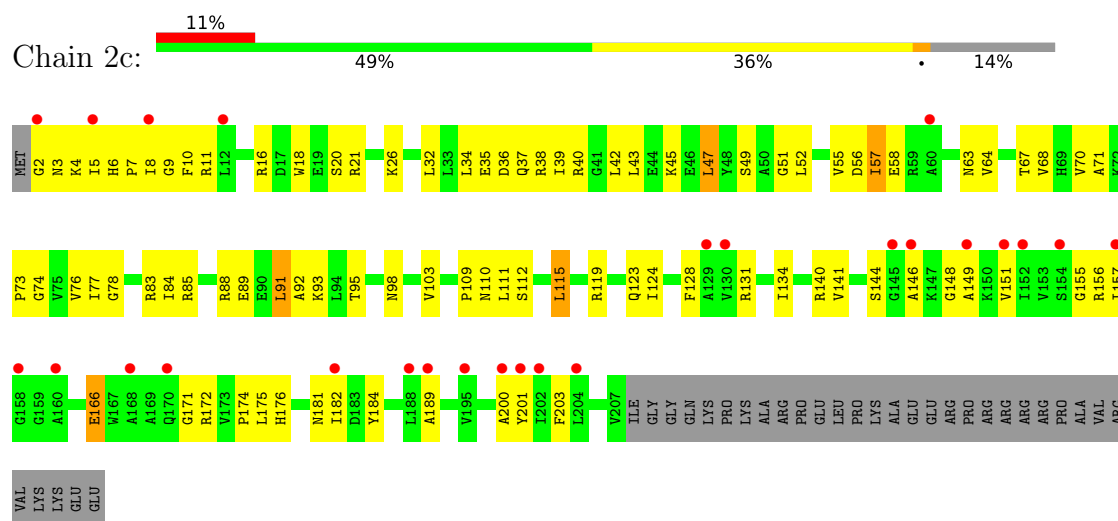
• Molecule 33: 30S ribosomal protein S2



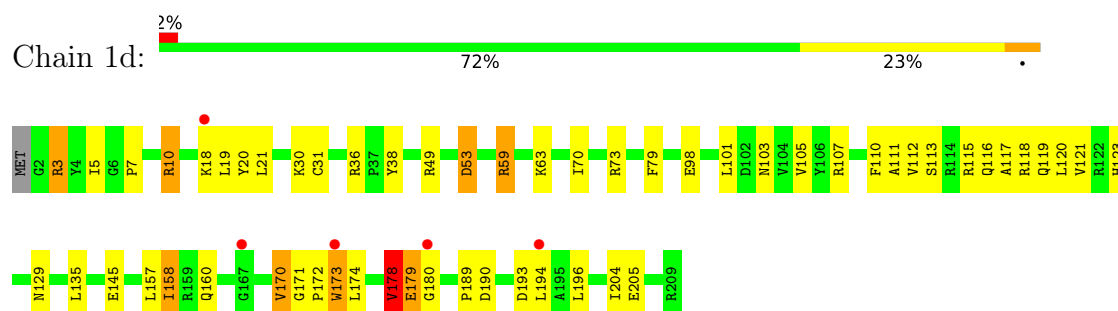
• Molecule 34: 30S ribosomal protein S3



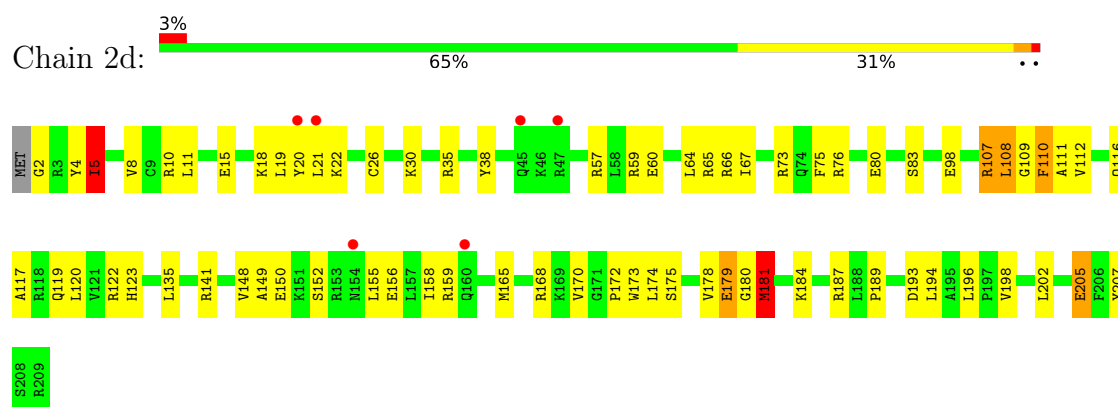
- Molecule 34: 30S ribosomal protein S3



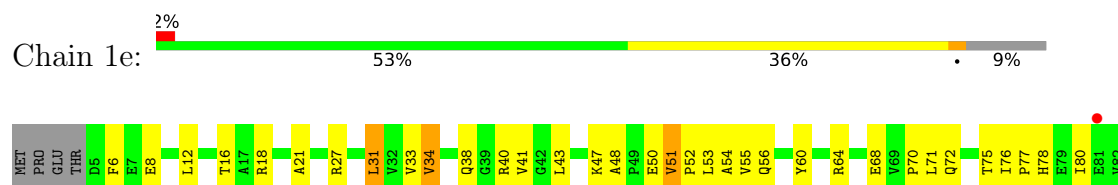
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

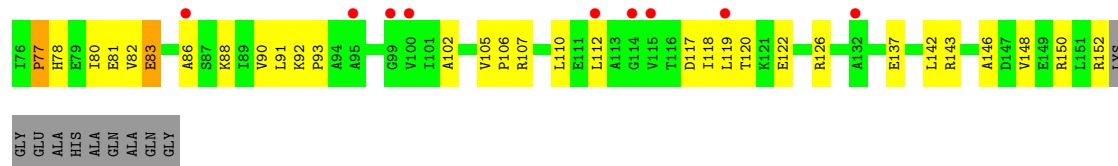
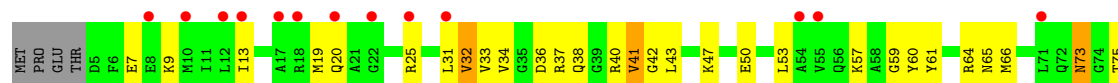


- Molecule 36: 30S ribosomal protein S5

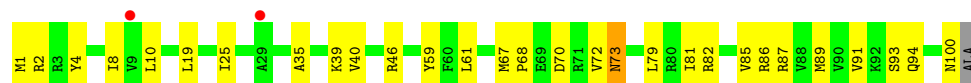




• Molecule 36: 30S ribosomal protein S5



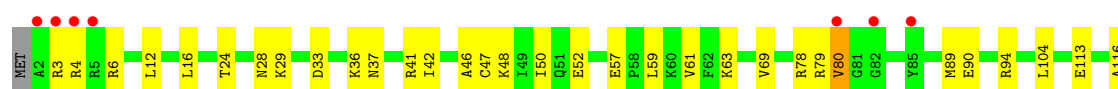
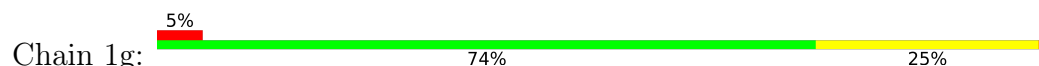
• Molecule 37: 30S ribosomal protein S6



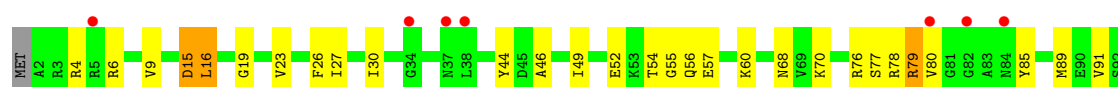
• Molecule 37: 30S ribosomal protein S6

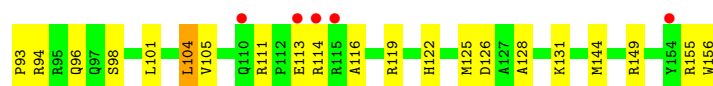


• Molecule 38: 30S ribosomal protein S7



• Molecule 38: 30S ribosomal protein S7





- Molecule 39: 30S ribosomal protein S8



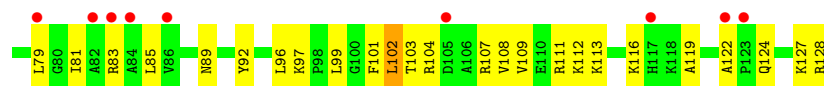
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

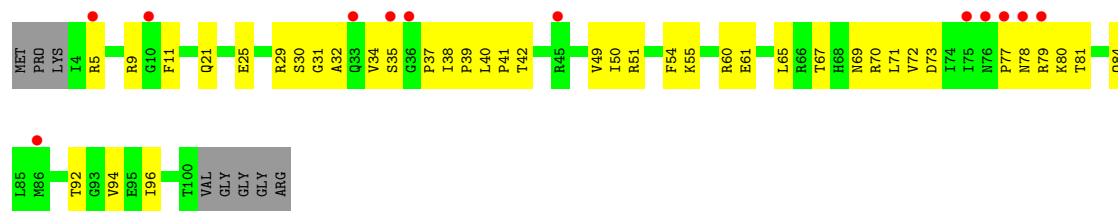


- Molecule 40: 30S ribosomal protein S9

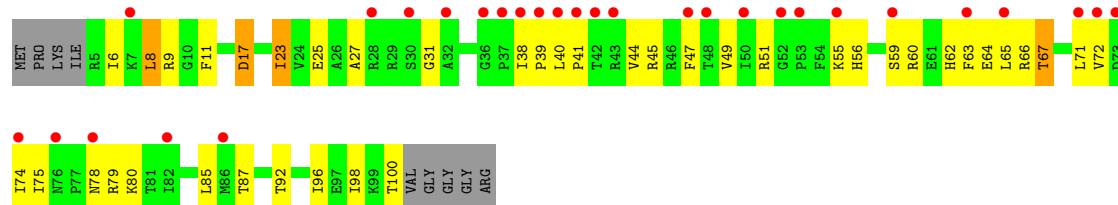


- Molecule 41: 30S ribosomal protein S10

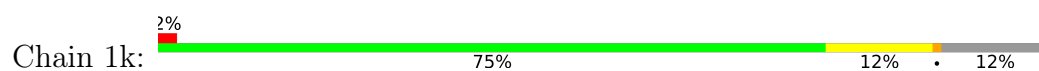




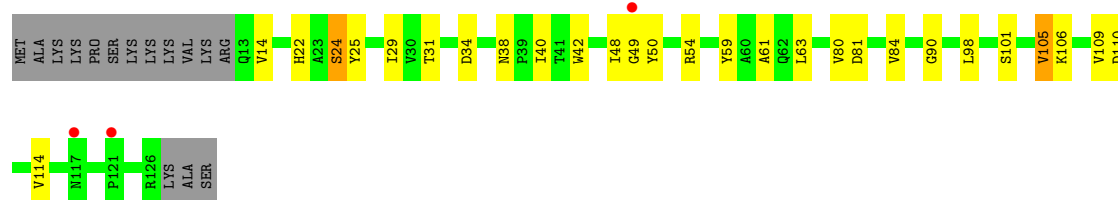
• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11

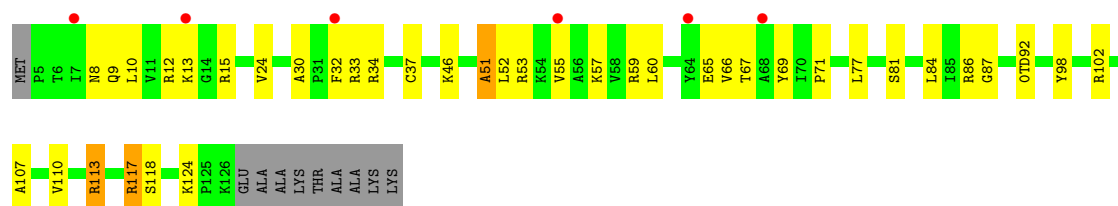


• Molecule 43: 30S ribosomal protein S12

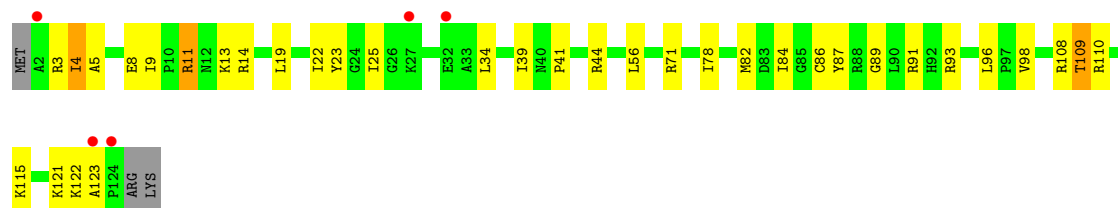
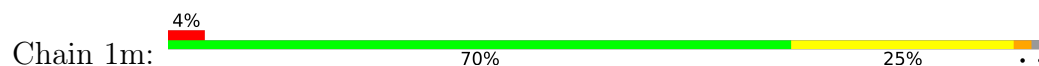


• Molecule 43: 30S ribosomal protein S12

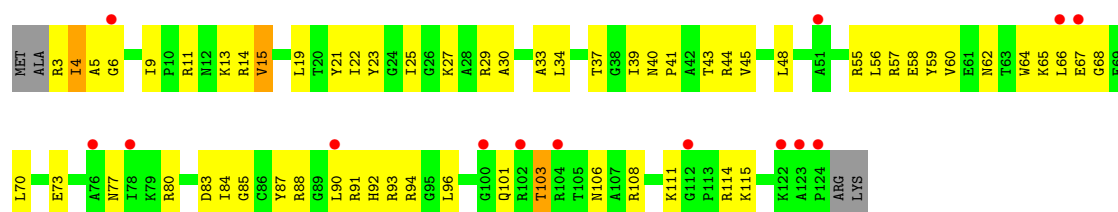




- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13



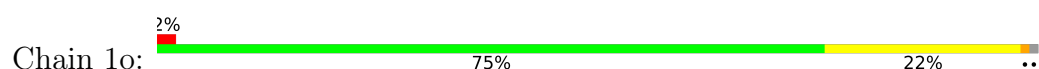
- Molecule 45: 30S ribosomal protein S14 type Z



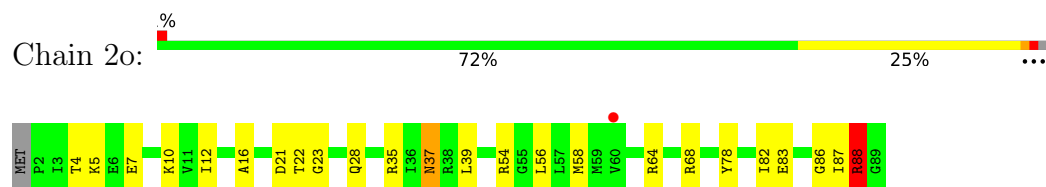
- Molecule 45: 30S ribosomal protein S14 type Z



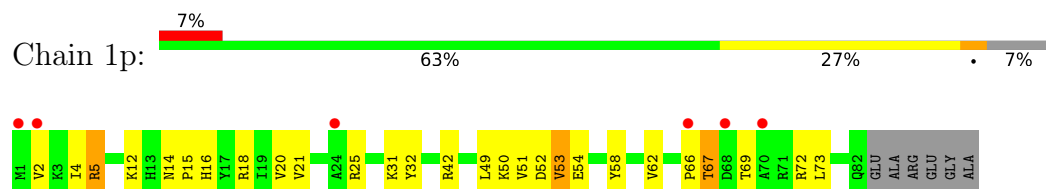
- Molecule 46: 30S ribosomal protein S15



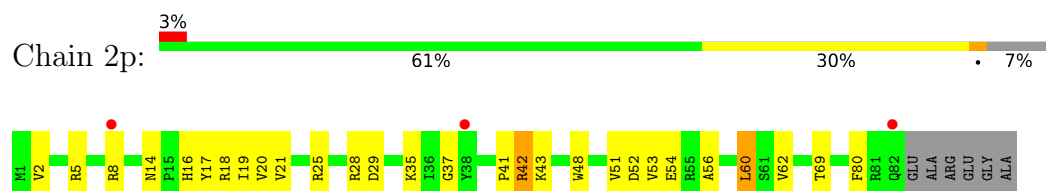
- Molecule 46: 30S ribosomal protein S15



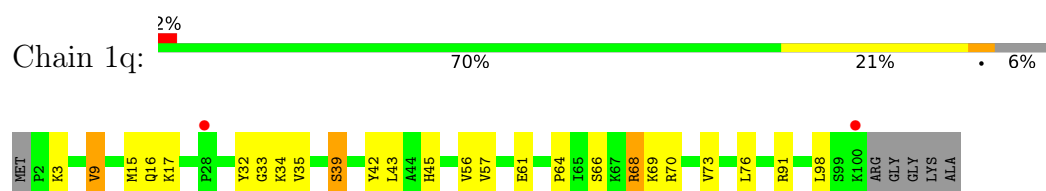
- Molecule 47: 30S ribosomal protein S16



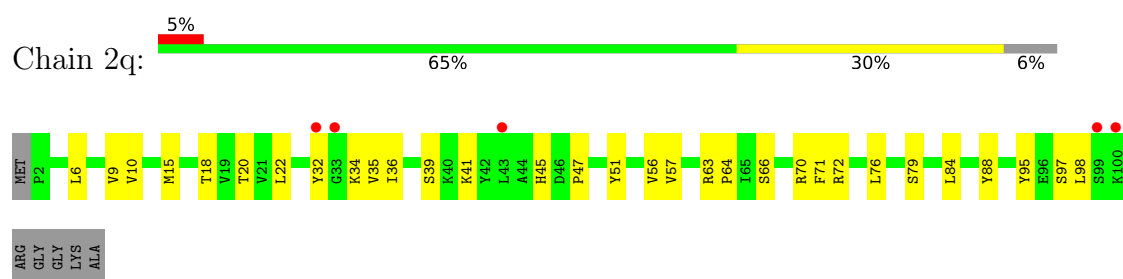
- Molecule 47: 30S ribosomal protein S16



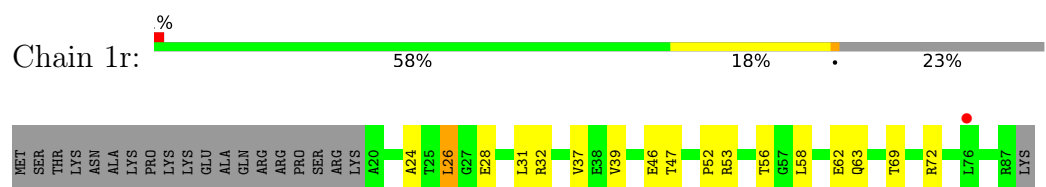
- Molecule 48: 30S ribosomal protein S17



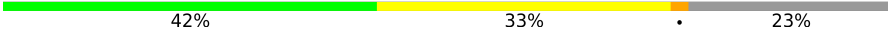
- Molecule 48: 30S ribosomal protein S17

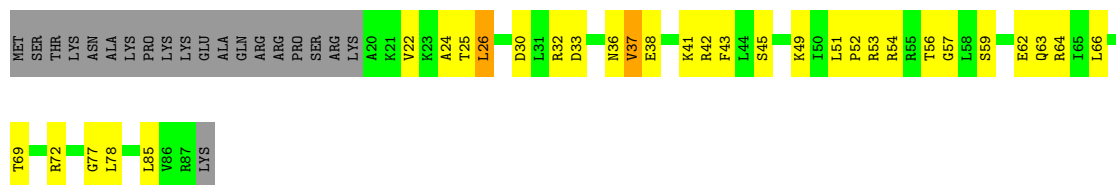


- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

Chain 2r: 



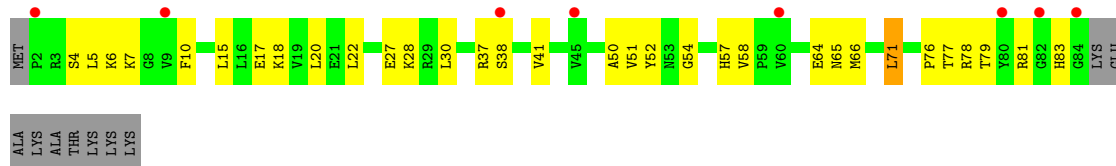
- Molecule 50: 30S ribosomal protein S19

Chain 1s: 



- Molecule 50: 30S ribosomal protein S19

Chain 2s: 



- Molecule 51: 30S ribosomal protein S20

Chain 1t: 



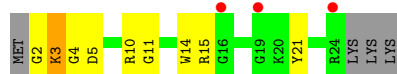
- Molecule 51: 30S ribosomal protein S20

Chain 2t: 

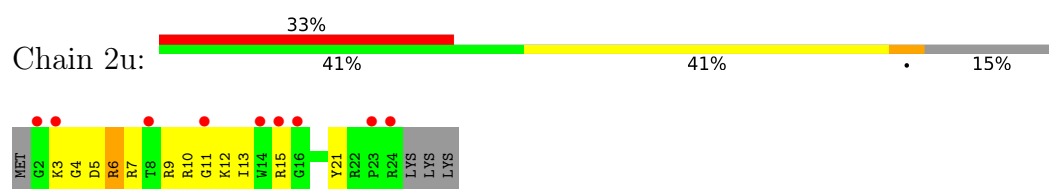


- Molecule 52: 30S ribosomal protein Thx

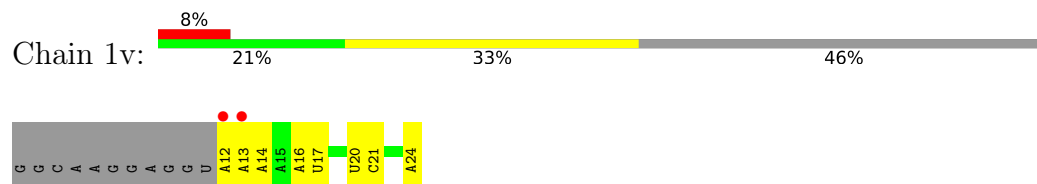
Chain 1u: 



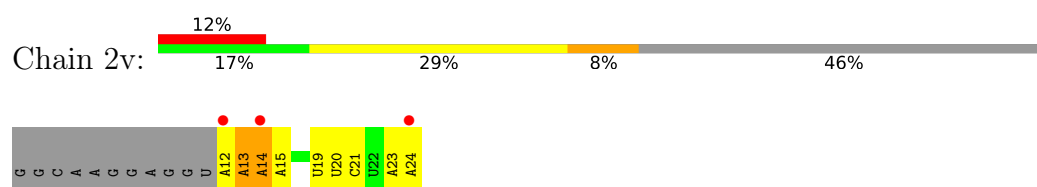
- Molecule 52: 30S ribosomal protein Thx



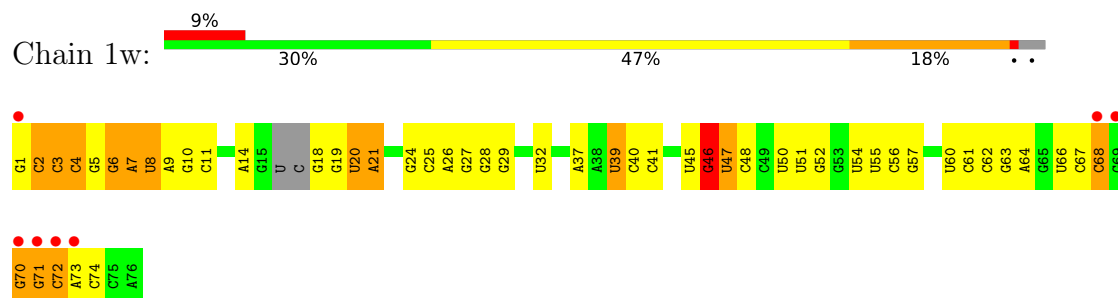
• Molecule 53: mRNA



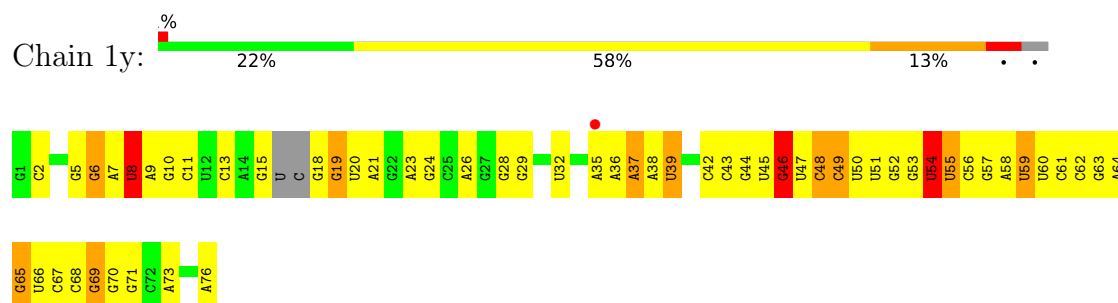
• Molecule 53: mRNA



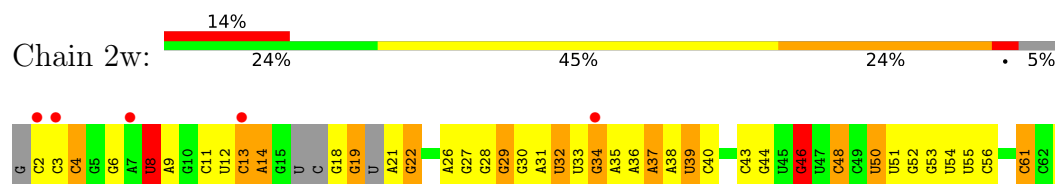
• Molecule 54: A-site and E-site tRNAs

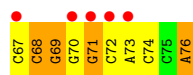


• Molecule 54: A-site and E-site tRNAs

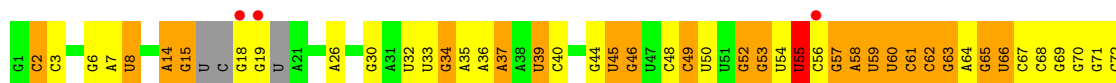


• Molecule 54: A-site and E-site tRNAs





• Molecule 54: A-site and E-site tRNAs



• Molecule 55: P-site tRNA



• Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.78Å 449.83Å 622.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.54 – 2.80 152.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (152.54-2.80) 94.0 (152.54-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.214 , 0.269 0.216 , 0.268	Depositor DCC
R_{free} test set	67418 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299109	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: MG, K, 4SU, 7MG, OMG, ZN, 4OC, MIA, PSU, 0TD, MA6, UR3, 5MC, 5MU, 2MU, M2G, SF4, 2MA, 2MG, EZG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	0/69009	0.46	1/107712 (0.0%)
1	2A	0.22	0/67293	0.41	1/105034 (0.0%)
2	1B	0.23	0/2882	0.43	0/4494
2	2B	0.20	0/2879	0.40	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.25	0/2186	0.52	1/2944 (0.0%)
4	1E	0.29	0/1592	0.54	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.26	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.48	2/2188 (0.1%)
6	1G	0.22	0/1448	0.45	0/1957
6	2G	0.19	0/1453	0.43	1/1963 (0.1%)
7	1H	0.24	0/1356	0.43	0/1834
7	2H	0.25	1/1356 (0.1%)	0.43	0/1834
8	1I	0.19	0/1112	0.41	0/1514
8	2I	0.18	0/1079	0.39	0/1475
9	1N	0.27	0/1144	0.48	0/1543
9	2N	0.20	0/1144	0.44	0/1543
10	1O	0.27	0/943	0.48	0/1269
10	2O	0.21	0/943	0.49	0/1269
11	1P	0.27	0/1152	0.49	0/1533
11	2P	0.23	0/1152	0.51	2/1533 (0.1%)
12	1Q	0.25	0/1143	0.45	0/1527
12	2Q	0.20	0/1143	0.46	0/1527
13	1R	0.26	0/982	0.50	0/1312
13	2R	0.21	0/982	0.45	0/1312
14	1S	0.22	0/883	0.49	0/1176
14	2S	0.20	0/880	0.46	0/1172
15	1T	0.24	0/1105	0.49	0/1477
15	2T	0.20	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.42	0/1301
17	1V	0.26	0/782	0.48	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.28	0/897	0.49	0/1205
18	2W	0.22	0/897	0.42	0/1205
19	1X	0.27	0/764	0.53	0/1025
19	2X	0.20	0/764	0.47	0/1025
20	1Y	0.25	0/819	0.50	0/1095
20	2Y	0.21	0/819	0.44	0/1095
21	1Z	0.25	0/1267	0.50	1/1717 (0.1%)
21	2Z	0.22	0/1299	0.46	0/1763
22	10	0.28	0/662	0.54	0/881
22	20	0.21	0/662	0.48	0/881
23	11	0.24	0/762	0.45	0/1014
23	21	0.23	0/762	0.47	0/1014
24	12	0.29	0/590	0.45	0/781
24	22	0.19	0/590	0.42	0/781
25	13	0.27	0/474	0.48	0/635
25	23	0.19	0/469	0.39	0/630
26	14	0.27	0/565	0.62	1/761 (0.1%)
26	24	0.25	0/545	0.52	0/737
27	15	0.29	0/469	0.49	0/635
27	25	0.23	0/469	0.41	0/635
28	16	0.27	0/460	0.54	0/613
28	26	0.22	0/456	0.46	0/608
29	17	0.30	0/426	0.55	0/561
29	27	0.28	0/426	0.56	0/561
30	18	0.29	0/525	0.50	0/691
30	28	0.22	0/525	0.43	0/691
31	19	0.26	0/310	0.49	0/407
31	29	0.21	0/310	0.44	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.38	1/56005 (0.0%)
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.22	0/1860	0.50	0/2518
34	1c	0.19	0/1572	0.40	0/2126
34	2c	0.21	0/1566	0.46	1/2119 (0.0%)
35	1d	0.19	0/1685	0.46	0/2262
35	2d	0.19	0/1704	0.46	0/2284
36	1e	0.20	0/1145	0.44	0/1543
36	2e	0.20	0/1149	0.48	0/1548
37	1f	0.19	0/823	0.41	0/1115
37	2f	0.19	0/829	0.37	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.22	0/1250	0.44	0/1679
38	2g	0.18	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.40	0/1494
39	2h	0.19	0/1108	0.40	0/1494
40	1i	0.20	0/1002	0.46	0/1346
40	2i	0.21	0/997	0.49	0/1343
41	1j	0.19	0/722	0.43	0/982
41	2j	0.24	0/727	0.52	0/988
42	1k	0.17	0/844	0.38	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.22	0/937	0.43	0/1260
43	2l	0.22	0/937	0.50	0/1260
44	1m	0.20	0/969	0.44	0/1302
44	2m	0.21	0/961	0.46	0/1291
45	1n	0.20	0/501	0.45	0/664
45	2n	0.26	0/501	0.53	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.19	0/739	0.43	0/985
47	1p	0.20	0/697	0.47	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.19	0/836	0.42	0/1117
48	2q	0.19	0/836	0.38	0/1117
49	1r	0.21	0/560	0.45	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.23	0/667	0.51	0/900
50	2s	0.26	0/661	0.61	0/893
51	1t	0.20	0/730	0.51	0/965
51	2t	0.21	0/729	0.46	0/965
52	1u	0.21	0/203	0.51	0/266
52	2u	0.23	0/203	0.48	0/266
53	1v	0.20	0/310	0.32	0/480
53	2v	0.23	0/310	0.36	0/480
54	1w	0.27	1/1606 (0.1%)	0.43	0/2497
54	1y	0.26	1/1606 (0.1%)	0.42	0/2497
54	2w	0.27	1/1556 (0.1%)	0.43	0/2418
54	2y	0.28	1/1583 (0.1%)	0.43	0/2459
55	1x	0.26	0/1725	0.41	0/2689
55	2x	0.25	1/1725 (0.1%)	0.39	0/2689
All	All	0.23	6/316686 (0.0%)	0.43	12/474113 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	O3'-P	5.30	1.61	1.56
7	2H	53	GLU	C-N	5.15	1.44	1.33
55	2x	8	4SU	O3'-P	5.15	1.61	1.56
54	1y	8	4SU	O3'-P	5.07	1.61	1.56
54	2y	8	4SU	O3'-P	5.06	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1Z	53	ILE	N-CA-C	-6.57	106.06	111.91
1	1A	2014	G	C2'-C3'-O3'	5.89	118.34	109.50
34	2c	84	ILE	N-CA-C	-5.64	105.59	112.76
26	14	54	GLY	N-CA-C	5.50	123.46	115.32
1	2A	1992	G	C2'-C3'-O3'	5.29	117.43	109.50

There are no chirality outliers.

There are no planarity outliers.

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	31192	685	0
1	2A	60322	0	30423	795	0
2	1B	2577	0	1305	25	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	52	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	40	0
5	1F	1584	0	1625	39	0
5	2F	1580	0	1619	48	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	48	0
7	1H	1330	0	1407	27	0
7	2H	1330	0	1407	45	0
8	1I	1097	0	1140	31	0
8	2I	1064	0	1082	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1N	1117	0	1184	16	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	23	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	28	0
12	2Q	1122	0	1179	35	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	23	0
14	1S	873	0	927	22	0
14	2S	870	0	923	37	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	33	0
16	1U	959	0	1019	19	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	7	0
17	2V	771	0	830	11	0
18	1W	886	0	940	16	0
18	2W	886	0	940	15	0
19	1X	750	0	814	15	0
19	2X	750	0	814	20	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	19	0
21	2Z	1271	0	1273	38	0
22	10	653	0	674	19	0
22	20	653	0	674	20	0
23	11	755	0	826	16	0
23	21	755	0	826	23	0
24	12	588	0	643	9	0
24	22	588	0	643	14	0
25	13	469	0	518	13	0
25	23	464	0	514	11	0
26	14	552	0	533	13	0
26	24	532	0	503	28	0
27	15	455	0	465	9	0
27	25	455	0	465	14	0
28	16	453	0	473	9	0
28	26	449	0	469	10	0
29	17	418	0	467	9	0
29	27	418	0	467	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	18	517	0	582	18	0
30	28	517	0	582	20	0
31	19	307	0	335	7	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	419	0
32	2a	32327	0	16339	579	0
33	1b	1846	0	1867	76	0
33	2b	1825	0	1828	80	0
34	1c	1548	0	1535	35	0
34	2c	1542	0	1517	66	0
35	1d	1655	0	1672	41	0
35	2d	1674	0	1714	53	0
36	1e	1129	0	1184	38	0
36	2e	1133	0	1191	42	0
37	1f	810	0	804	18	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	23	0
38	2g	1235	0	1249	31	0
39	1h	1088	0	1126	32	0
39	2h	1088	0	1126	35	0
40	1i	983	0	986	34	0
40	2i	978	0	966	40	0
41	1j	709	0	650	27	0
41	2j	714	0	672	31	0
42	1k	829	0	825	8	0
42	2k	833	0	836	14	0
43	1l	932	0	981	26	0
43	2l	932	0	981	30	0
44	1m	958	0	1002	23	0
44	2m	950	0	988	56	0
45	1n	492	0	529	19	0
45	2n	492	0	529	26	0
46	1o	728	0	760	13	0
46	2o	728	0	760	14	0
47	1p	681	0	697	21	0
47	2p	677	0	686	20	0
48	1q	823	0	891	18	0
48	2q	823	0	891	20	0
49	1r	555	0	618	11	0
49	2r	555	0	618	28	0
50	1s	652	0	662	19	0
50	2s	646	0	644	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1t	728	0	798	20	0
51	2t	727	0	796	13	0
52	1u	199	0	208	8	0
52	2u	199	0	208	12	0
53	1v	277	0	140	6	0
53	2v	277	0	140	8	0
54	1w	1592	0	819	42	0
54	1y	1585	0	804	51	0
54	2w	1544	0	788	46	0
54	2y	1565	0	795	45	0
55	1x	1625	0	827	11	0
55	2x	1625	0	828	23	0
56	10	5	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	2	0	0	0	0
56	15	6	0	0	0	0
56	16	3	0	0	0	0
56	17	5	0	0	0	0
56	18	3	0	0	0	0
56	19	1	0	0	0	0
56	1A	1063	0	0	0	0
56	1B	38	0	0	0	0
56	1D	14	0	0	0	0
56	1E	13	0	0	0	0
56	1F	9	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	7	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	3	0	0	0	0
56	1W	5	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	215	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1b	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1q	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	15	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	25	3	0	0	0	0
56	27	2	0	0	0	0
56	28	2	0	0	0	0
56	2A	754	0	0	0	0
56	2B	21	0	0	0	0
56	2D	7	0	0	0	0
56	2E	10	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	6	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	233	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2j	2	0	0	0	0
56	2l	4	0	0	0	0
56	2q	4	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	5	0	0	0	0
56	2w	9	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	2	0	0	0	0
57	2A	2	0	0	0	0
58	1A	25	0	0	2	0
58	2A	25	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	10	0	0	0	0
61	11	7	0	0	0	0
61	12	2	0	0	0	0
61	13	4	0	0	0	0
61	15	5	0	0	1	0
61	16	2	0	0	0	0
61	17	9	0	0	1	0
61	18	7	0	0	1	0
61	1A	1433	0	0	74	0
61	1B	65	0	0	2	0
61	1D	24	0	0	0	0
61	1E	30	0	0	4	0
61	1F	10	0	0	4	0
61	1G	8	0	0	2	0
61	1H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1I	2	0	0	0	0
61	1N	6	0	0	1	0
61	1O	8	0	0	0	0
61	1P	18	0	0	1	0
61	1Q	12	0	0	0	0
61	1R	12	0	0	0	0
61	1S	4	0	0	0	0
61	1T	7	0	0	0	0
61	1U	9	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	0	0
61	1X	8	0	0	1	0
61	1Y	2	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	315	0	0	20	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	6	0	0	0	0
61	1m	1	0	0	0	0
61	1n	1	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	1	0
61	1v	6	0	0	0	0
61	1w	20	0	0	1	0
61	1x	14	0	0	0	0
61	1y	2	0	0	0	0
61	20	4	0	0	0	0
61	21	8	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	4	0	0	0	0
61	26	1	0	0	0	0
61	27	4	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	885	0	0	53	0
61	2B	26	0	0	0	0
61	2D	18	0	0	4	0
61	2E	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2F	18	0	0	0	0
61	2I	4	0	0	0	0
61	2N	1	0	0	0	0
61	2P	12	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	6	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	1	0	0	0	0
61	2Y	1	0	0	1	0
61	2Z	2	0	0	0	0
61	2a	258	0	0	17	0
61	2c	1	0	0	0	0
61	2d	3	0	0	0	0
61	2e	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	1	0
61	2l	6	0	0	1	0
61	2o	1	0	0	0	0
61	2p	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	1	0
61	2t	5	0	0	0	0
61	2u	1	0	0	0	0
61	2v	2	0	0	1	0
61	2w	2	0	0	1	0
61	2x	6	0	0	0	0
61	2y	18	0	0	1	0
All	All	299109	0	196685	4585	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4585 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:2158:C:N4	1:1A:2177:G:H1	1.36	1.21
54:1w:6:G:H1	54:1w:67:C:N4	1.46	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2136:C:N4	1:2A:2155:G:H1	1.46	1.12
1:2A:2129:C:N4	1:2A:2159:G:H1	1.49	1.10
1:1A:1128:U:H3	1:1A:1132:A:N6	1.48	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	30	60
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	55
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	55
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	55
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	6	21
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	51
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	4	14
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	51
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	7	25
8	1I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	18	47
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18	47
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	5	19
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	7	25
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2P	147/150 (98%)	134 (91%)	11 (8%)	2 (1%)	9	30
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	47
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	47
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	25
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	41
14	2S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	6	22
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	44
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	44
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	12	38
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	38
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	12	38
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6	22
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	18	47
21	2Z	156/206 (76%)	132 (85%)	19 (12%)	5 (3%)	3	11
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	34
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	8	28
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	23
26	14	67/71 (94%)	55 (82%)	8 (12%)	4 (6%)	1	3
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5	19
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	27 (12%)	10 (4%)	2	7
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	2	8
34	1c	204/239 (85%)	190 (93%)	11 (5%)	3 (2%)	8	28
34	2c	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	3	13
35	1d	206/209 (99%)	190 (92%)	13 (6%)	3 (2%)	8	28
35	2d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	6	22
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	30
36	2e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	18	47
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	6	21
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	6	21
39	1h	135/138 (98%)	129 (96%)	4 (3%)	2 (2%)	8	28
39	2h	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	8	28
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2	7
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2	7
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	41
42	2k	112/129 (87%)	103 (92%)	6 (5%)	3 (3%)	4	15
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	16	44
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	102 (85%)	15 (12%)	3 (2%)	4	16
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	34
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	34
47	1p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	9	31
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	38
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10	34
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	4	16
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1	5
51	2t	94/106 (89%)	83 (88%)	5 (5%)	6 (6%)	1	3
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	6
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10425 (92%)	802 (7%)	143 (1%)	9	31

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
26	14	53	GLU
33	1b	22	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	196 (91%)	19 (9%)	9	29
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	54
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	35
4	2E	164/166 (99%)	149 (91%)	15 (9%)	9	28
5	1F	160/166 (96%)	140 (88%)	20 (12%)	4	15
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	27
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10	32
6	2G	143/156 (92%)	133 (93%)	10 (7%)	14	40
7	1H	144/148 (97%)	135 (94%)	9 (6%)	16	45
7	2H	144/148 (97%)	138 (96%)	6 (4%)	26	61
8	1I	113/124 (91%)	102 (90%)	11 (10%)	8	25
8	2I	105/124 (85%)	95 (90%)	10 (10%)	8	26
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	36
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	27
10	1O	100/100 (100%)	92 (92%)	8 (8%)	11	34
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	80
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17	46
11	2P	115/116 (99%)	109 (95%)	6 (5%)	21	53
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	39
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	28
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	24
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	14
14	1S	86/88 (98%)	78 (91%)	8 (9%)	8	27
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	33
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32	67
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	45
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	31
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	51
17	1V	80/82 (98%)	71 (89%)	9 (11%)	5	19
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	69
18	2W	90/92 (98%)	80 (89%)	10 (11%)	6	20
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	43
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	43
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10	33
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13	39
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6	20
21	2Z	137/179 (76%)	129 (94%)	8 (6%)	18	49
22	10	65/67 (97%)	62 (95%)	3 (5%)	24	58
22	20	65/67 (97%)	62 (95%)	3 (5%)	24	58
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	64
23	21	80/83 (96%)	79 (99%)	1 (1%)	61	86
24	12	65/67 (97%)	60 (92%)	5 (8%)	12	36
24	22	65/67 (97%)	64 (98%)	1 (2%)	57	84
25	13	51/52 (98%)	50 (98%)	1 (2%)	48	80
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	17
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	31
26	24	53/63 (84%)	49 (92%)	4 (8%)	12	37
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	24
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	47
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	64
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	34
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	38
29	27	41/42 (98%)	40 (98%)	1 (2%)	43	77
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	50
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	50
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	73
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	29
33	1b	192/220 (87%)	182 (95%)	10 (5%)	21	53
33	2b	187/220 (85%)	172 (92%)	15 (8%)	11	34
34	1c	142/188 (76%)	132 (93%)	10 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2c	140/188 (74%)	131 (94%)	9 (6%)	16	44
35	1d	169/181 (93%)	155 (92%)	14 (8%)	10	32
35	2d	173/181 (96%)	158 (91%)	15 (9%)	9	30
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	29
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14	40
37	1f	84/90 (93%)	80 (95%)	4 (5%)	23	56
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	57
38	1g	119/127 (94%)	113 (95%)	6 (5%)	22	54
38	2g	120/127 (94%)	112 (93%)	8 (7%)	15	42
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	29
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	35
40	1i	90/99 (91%)	85 (94%)	5 (6%)	19	50
40	2i	89/99 (90%)	84 (94%)	5 (6%)	19	50
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	36
41	2j	69/92 (75%)	62 (90%)	7 (10%)	7	23
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17	46
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	39
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	22
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	61
44	1m	93/101 (92%)	86 (92%)	7 (8%)	12	37
44	2m	92/101 (91%)	90 (98%)	2 (2%)	45	78
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	23
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	23
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	75
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	44
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	39
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	29
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	52
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	44
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	42
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	73
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17	47
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26	60
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	49
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50
All	All	9303/10064 (92%)	8644 (93%)	659 (7%)	13	39

5 of 659 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	2U	33	ARG
36	2e	25	ARG
18	2W	17	VAL
16	2U	17	ILE
27	25	16	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
44	1m	40	ASN
39	2h	82	HIS
7	2H	158	HIS
38	2g	68	ASN
47	2p	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	474 (16%)	28 (0%)
1	2A	2791/2915 (95%)	502 (17%)	22 (0%)
2	1B	120/121 (99%)	12 (10%)	2 (1%)
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1497/1521 (98%)	243 (16%)	0
32	2a	1501/1521 (98%)	271 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	72/76 (94%)	22 (30%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	1y	72/76 (94%)	21 (29%)	0
54	2w	69/76 (90%)	24 (34%)	0
54	2y	70/76 (92%)	27 (38%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9347/9620 (97%)	1654 (17%)	52 (0%)

5 of 1654 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	57	G

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1B	1	U
1	2A	271(M)	G
1	2A	1992	G
2	1B	65	C
1	2A	228	A

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

84 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
55	5MU	2x	54	55	19,22,23	1.33	5 (26%)	27,32,35	2.28	6 (22%)
54	5MU	1y	54	54	19,22,23	1.49	6 (31%)	27,32,35	2.02	5 (18%)
54	4SU	1y	8	54	18,21,22	1.74	4 (22%)	25,30,33	1.99	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	8,9,10	4.49	1 (12%)	6,11,13	2.53	3 (50%)
54	PSU	1w	39	54	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)
1	5MC	1A	1964	1	19,22,23	1.61	3 (15%)	26,32,35	1.26	3 (11%)
32	7MG	1a	527	32	23,26,27	1.44	5 (21%)	27,39,42	2.50	5 (18%)
1	5MU	1A	1937	1	19,22,23	1.43	5 (26%)	27,32,35	2.24	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.90	3 (14%)
54	4SU	2y	8	54	18,21,22	1.72	4 (22%)	25,30,33	2.42	6 (24%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.28	8 (24%)
54	5MU	1w	54	54	19,22,23	1.41	6 (31%)	27,32,35	2.15	7 (25%)
32	M2G	2a	966	32	24,27,28	1.27	4 (16%)	33,40,43	1.84	6 (18%)
1	2MU	2A	2552	1,56	19,22,24	1.27	2 (10%)	25,31,36	1.85	5 (20%)
1	4OC	2A	1920	1	19,22,24	0.76	0	25,31,35	0.83	0
1	OMG	2A	2251	1,56,55	23,26,27	1.21	2 (8%)	32,38,41	2.02	5 (15%)
1	PSU	1A	1939	1	18,21,22	1.37	2 (11%)	21,30,33	1.87	3 (14%)
1	5MU	1A	1961	1,56	19,22,23	1.31	4 (21%)	27,32,35	2.38	6 (22%)
54	7MG	2y	46	54	23,26,27	1.37	4 (17%)	27,39,42	2.62	6 (22%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
54	PSU	1w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
32	2MG	1a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.20	8 (24%)
54	MIA	2y	37	54	21,24,32	1.62	4 (19%)	30,35,47	2.03	8 (26%)
55	4SU	2x	8	56,55	18,21,22	2.07	6 (33%)	25,30,33	1.51	5 (20%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	1.96	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
54	7MG	2w	46	54	23,26,27	1.36	3 (13%)	27,39,42	2.53	7 (25%)
1	2MA	1A	2515	1,56	22,25,26	1.51	5 (22%)	32,37,40	2.18	7 (21%)
32	5MC	2a	1400	32	19,22,23	1.85	3 (15%)	26,32,35	1.20	3 (11%)
1	5MU	2A	1939	1,56	19,22,23	1.45	6 (31%)	27,32,35	2.25	6 (22%)
55	5MU	1x	54	56,55	19,22,23	1.41	5 (26%)	27,32,35	2.01	6 (22%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.86	3 (14%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.76	3 (11%)
1	OMG	1A	2263	1,56,55	23,26,27	1.23	3 (13%)	32,38,41	1.94	6 (18%)
54	4SU	2w	8	54	18,21,22	1.78	4 (22%)	25,30,33	2.39	5 (20%)
54	PSU	2y	32	54	18,21,22	1.32	2 (11%)	21,30,33	1.95	5 (23%)
43	0TD	1l	92	43	8,9,10	4.60	1 (12%)	6,11,13	3.35	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)
54	PSU	2w	32	54	18,21,22	1.35	3 (16%)	21,30,33	1.93	4 (19%)
1	5MU	2A	1915	1	19,22,23	1.43	4 (21%)	27,32,35	2.13	6 (22%)
55	5MC	1x	32	55	19,22,23	1.60	3 (15%)	26,32,35	1.22	3 (11%)
32	5MC	2a	1407	32	19,22,23	1.53	3 (15%)	26,32,35	1.22	3 (11%)
32	MA6	2a	1519	32	23,26,27	1.55	4 (17%)	33,38,41	2.40	13 (39%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.98	1 (4%)
32	PSU	1a	516	56,32	18,21,22	1.37	3 (16%)	21,30,33	1.93	5 (23%)
54	5MU	2y	54	54	19,22,23	1.48	5 (26%)	27,32,35	2.23	9 (33%)
1	2MU	1A	2564	1,56	19,22,24	1.35	3 (15%)	25,31,36	1.93	5 (20%)
1	PSU	1A	2617	1,56	18,21,22	1.35	3 (16%)	21,30,33	2.04	5 (23%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	21,30,33	2.17	4 (19%)
32	5MC	1a	967	32	19,22,23	1.52	3 (15%)	26,32,35	1.24	3 (11%)
54	MIA	1w	37	54	28,31,32	2.35	6 (21%)	38,44,47	2.62	12 (31%)
54	PSU	2y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.94	5 (23%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
54	PSU	2w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.80	4 (19%)
32	M2G	1a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.98	5 (15%)
1	4OC	1A	1942	1	19,22,24	0.79	0	25,31,35	0.87	0
1	5MC	2A	1942	1	19,22,23	1.66	3 (15%)	26,32,35	1.14	2 (7%)
54	PSU	2y	55	54	18,21,22	1.42	3 (16%)	21,30,33	1.93	4 (19%)
55	4SU	1x	8	55	18,21,22	2.21	4 (22%)	25,30,33	1.68	6 (24%)
32	5MC	1a	1400	32	19,22,23	1.57	3 (15%)	26,32,35	1.18	3 (11%)
1	PSU	1A	1933	1	18,21,22	1.44	2 (11%)	21,30,33	2.13	3 (14%)
1	5MC	2A	1962	1,56	19,22,23	1.52	3 (15%)	26,32,35	1.12	2 (7%)
1	2MA	2A	2503	1,56	22,25,26	1.48	5 (22%)	32,37,40	2.22	8 (25%)
32	UR3	1a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.71	2 (7%)
32	MA6	1a	1519	32	23,26,27	1.53	4 (17%)	33,38,41	2.24	13 (39%)
54	7MG	1y	46	54	23,26,27	1.34	2 (8%)	27,39,42	2.74	6 (22%)
54	7MG	1w	46	54	23,26,27	1.35	3 (13%)	27,39,42	2.66	7 (25%)
32	MA6	1a	1518	32	23,26,27	1.53	5 (21%)	33,38,41	2.28	13 (39%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.47	3 (15%)	26,32,35	1.11	2 (7%)
54	5MU	2w	54	54	19,22,23	1.30	4 (21%)	27,32,35	1.96	7 (25%)
54	4SU	1w	8	54	18,21,22	1.86	5 (27%)	25,30,33	2.17	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.06	2 (7%)
32	MA6	2a	1518	32	23,26,27	1.60	4 (17%)	33,38,41	2.26	12 (36%)
54	MIA	1y	37	54	21,24,32	1.63	4 (19%)	30,35,47	1.98	8 (26%)
54	MIA	2w	37	54	24,27,32	2.01	5 (20%)	32,39,47	2.44	9 (28%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.85	3 (14%)
32	7MG	2a	527	56,32	23,26,27	1.30	3 (13%)	27,39,42	2.68	7 (25%)
55	5MC	2x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.26	3 (11%)
32	4OC	2a	1402	56,32	20,23,24	0.74	0	25,32,35	1.02	1 (4%)
54	PSU	1y	55	54	18,21,22	1.34	2 (11%)	21,30,33	2.16	5 (23%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.18	2 (7%)
1	5MC	1A	1984	1,56	19,22,23	1.68	3 (15%)	26,32,35	1.25	4 (15%)

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
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	4/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	2MU	2A	2552	1,56	-	1/9/27/28	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
1	OMG	2A	2251	1,56,55	-	0/9/27/28	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	1/7/37/38	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	MIA	2y	37	54	-	3/7/25/34	0/3/3/3
55	4SU	2x	8	56,55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
1	2MA	1A	2515	1,56	-	1/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,56,55	-	0/9/27/28	0/3/3/3
54	4SU	2w	8	54	-	1/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	1/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	4OC	1A	1942	1	-	0/9/27/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	1/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/11/29/30	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
54	MIA	2w	37	54	-	4/11/29/34	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	56,32	-	3/7/37/38	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	56,32	-	2/9/29/30	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	0/7/25/26	0/2/2/2

The worst 5 of 260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.59	1.69	1.82
43	2l	92	0TD	CB-SB	-12.42	1.69	1.82
54	1w	37	MIA	C13-C14	7.07	1.53	1.32
32	2a	1400	5MC	C5-C4	6.99	1.49	1.44
54	1w	37	MIA	C2-S10	-6.65	1.70	1.75

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N9-C4-N3	9.84	139.87	125.46
54	1w	46	7MG	N9-C4-N3	9.32	139.12	125.46
54	2y	46	7MG	N9-C4-N3	9.20	138.95	125.46
32	2a	527	7MG	N9-C4-N3	9.04	138.71	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	N9-C4-N3	8.65	138.13	125.46

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C9
54	2w	32	PSU	C2'-C1'-C5-C4
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	C5-C6-N6-C12

There are no ring outliers.

42 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	54	5MU	2	0
54	1y	54	5MU	1	0
54	1y	8	4SU	3	0
54	1w	39	PSU	2	0
54	2y	8	4SU	3	0
32	2a	1207	2MG	2	0
32	2a	966	M2G	2	0
1	2A	1920	4OC	2	0
1	1A	1961	5MU	1	0
32	1a	1207	2MG	1	0
54	2w	46	7MG	1	0
32	2a	1400	5MC	1	0
1	2A	1939	5MU	1	0
54	2w	8	4SU	2	0
43	1l	92	0TD	3	0
1	2A	1915	5MU	1	0
32	2a	1519	MA6	3	0
32	1a	1402	4OC	1	0
1	1A	2564	2MU	2	0
32	1a	967	5MC	1	0
54	2y	39	PSU	1	0
54	2w	39	PSU	3	0
32	1a	966	M2G	1	0
1	1A	1942	4OC	1	0
1	2A	1942	5MC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	55	PSU	8	0
55	1x	8	4SU	2	0
1	2A	2503	2MA	1	0
32	1a	1498	UR3	1	0
32	1a	1519	MA6	2	0
54	1y	46	7MG	1	0
54	1w	46	7MG	2	0
32	1a	1518	MA6	3	0
32	1a	1404	5MC	2	0
32	2a	967	5MC	2	0
32	2a	1518	MA6	5	0
54	1y	37	MIA	2	0
54	2w	37	MIA	1	0
54	1y	39	PSU	1	0
32	2a	1402	4OC	2	0
54	1y	55	PSU	2	0
32	2a	1404	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2625 ligands modelled in this entry, 2621 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	EZG	2A	3746	-	26,26,26	3.33	4 (15%)	32,35,35	1.39	4 (12%)
60	SF4	1d	501	35	0,12,12	-	-	-		
60	SF4	2d	501	35	0,12,12	-	-	-		
58	EZG	1A	4030	-	26,26,26	2.59	4 (15%)	32,35,35	1.54	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EZG	2A	3746	-	-	8/24/26/26	0/2/2/2
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	501	35	-	-	0/6/5/5
58	EZG	1A	4030	-	-	5/24/26/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3746	EZG	OAC-NAY	13.76	1.46	1.22
58	1A	4030	EZG	CAT-CAW	-8.60	1.39	1.51
58	2A	3746	EZG	CAT-CAW	-7.86	1.40	1.51
58	1A	4030	EZG	OAC-NAY	7.61	1.35	1.22
58	1A	4030	EZG	CAU-NAY	-4.89	1.33	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4030	EZG	CAW-CAX-NAP	5.37	119.74	110.03
58	2A	3746	EZG	CA-CB-CG	-4.78	101.99	113.77
58	2A	3746	EZG	CAX-NAP-C	-3.12	117.83	123.25
58	1A	4030	EZG	CAT-CAW-CAX	2.89	116.89	111.72
58	1A	4030	EZG	CA-CB-CG	-2.73	107.03	113.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	2A	3746	EZG	O-C-CA-CB
58	2A	3746	EZG	NAP-C-CA-CB
58	2A	3746	EZG	NAP-C-CA-N
58	2A	3746	EZG	OAD-CAM-CAX-CAW
58	2A	3746	EZG	OAD-CAM-CAX-NAP

There are no ring outliers.

2 monomers are involved in 3 short contacts:

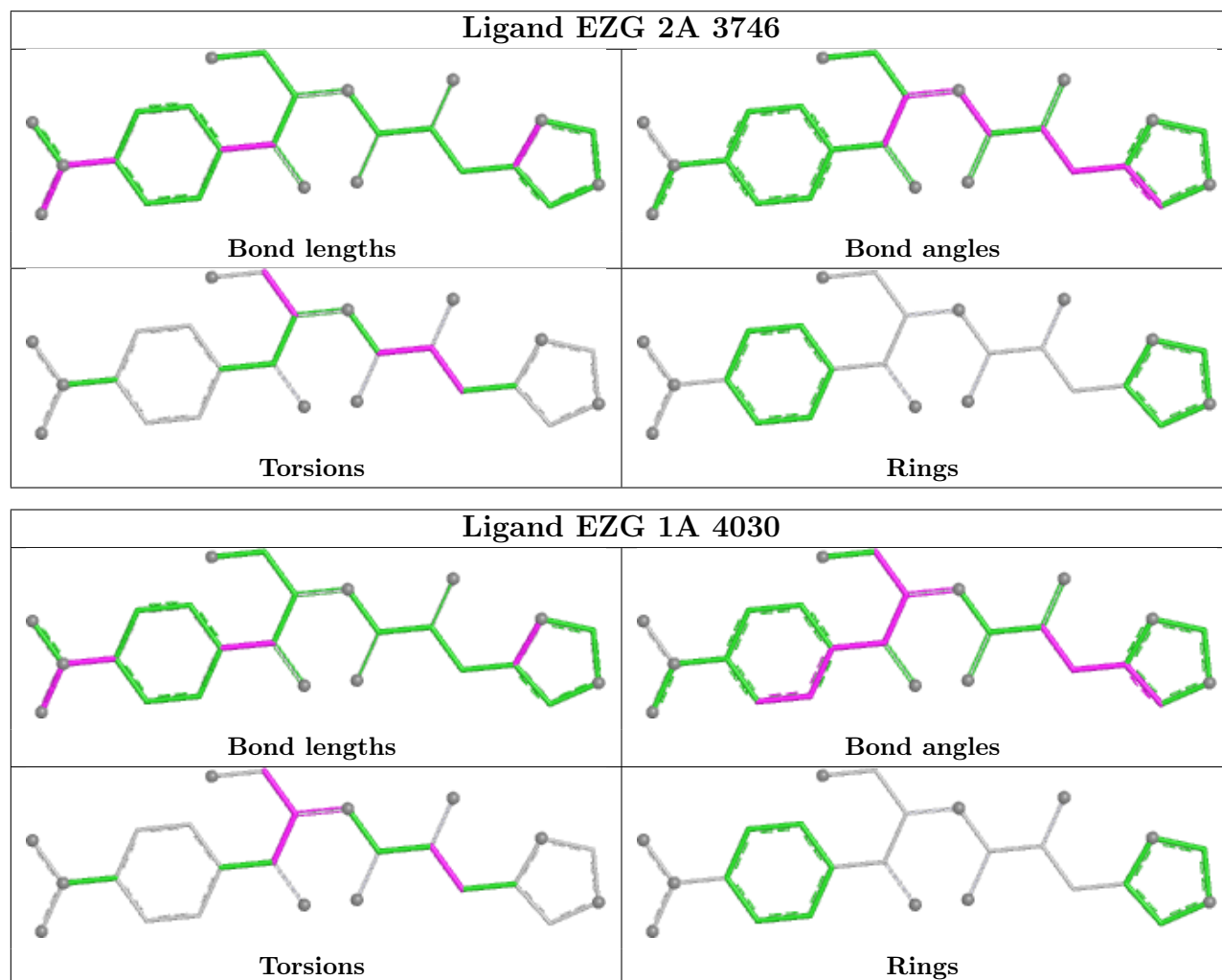
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3746	EZG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4030	EZG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	-0.52	46 (1%) 70 61	13, 30, 88, 101	0
1	2A	2789/2915 (95%)	-0.12	41 (1%) 72 63	25, 51, 87, 100	0
2	1B	120/121 (99%)	-0.46	0 100 100	23, 43, 57, 85	0
2	2B	120/121 (99%)	0.51	0 100 100	53, 71, 80, 89	0
3	1D	275/276 (99%)	-0.21	2 (0%) 84 77	16, 31, 46, 74	0
3	2D	275/276 (99%)	0.14	3 (1%) 78 70	23, 43, 56, 66	0
4	1E	204/206 (99%)	-0.22	0 100 100	13, 33, 54, 71	0
4	2E	204/206 (99%)	0.15	2 (0%) 79 72	28, 54, 67, 74	0
5	1F	203/210 (96%)	-0.17	0 100 100	15, 35, 62, 82	0
5	2F	203/210 (96%)	0.23	2 (0%) 79 72	30, 62, 74, 82	0
6	1G	181/182 (99%)	0.23	3 (1%) 69 60	35, 51, 69, 78	0
6	2G	181/182 (99%)	0.80	7 (3%) 43 34	56, 72, 78, 83	0
7	1H	174/180 (96%)	-0.03	2 (1%) 78 70	34, 46, 59, 66	0
7	2H	174/180 (96%)	0.76	7 (4%) 42 33	61, 75, 81, 86	0
8	1I	146/148 (98%)	0.44	2 (1%) 73 64	39, 67, 75, 81	0
8	2I	146/148 (98%)	0.48	2 (1%) 73 64	50, 66, 77, 81	0
9	1N	140/140 (100%)	-0.11	1 (0%) 84 77	21, 35, 55, 68	0
9	2N	140/140 (100%)	0.42	1 (0%) 84 77	43, 58, 72, 75	0
10	1O	122/122 (100%)	-0.26	0 100 100	22, 35, 50, 56	0
10	2O	122/122 (100%)	0.27	0 100 100	43, 54, 67, 70	0
11	1P	149/150 (99%)	-0.05	1 (0%) 84 77	14, 40, 62, 66	0
11	2P	149/150 (99%)	0.30	2 (1%) 75 66	30, 61, 75, 83	0
12	1Q	141/141 (100%)	-0.19	0 100 100	22, 36, 49, 72	0
12	2Q	141/141 (100%)	0.69	6 (4%) 40 31	41, 60, 70, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.17	0 100 100	18, 29, 44, 54	0
13	2R	118/118 (100%)	0.11	1 (0%) 82 75	33, 46, 55, 66	0
14	1S	110/112 (98%)	-0.05	0 100 100	32, 44, 55, 60	0
14	2S	110/112 (98%)	0.91	4 (3%) 46 37	58, 67, 76, 79	0
15	1T	131/146 (89%)	-0.12	2 (1%) 72 63	25, 39, 61, 71	0
15	2T	131/146 (89%)	0.31	0 100 100	46, 58, 69, 75	0
16	1U	116/118 (98%)	-0.41	0 100 100	14, 25, 42, 56	0
16	2U	116/118 (98%)	0.22	1 (0%) 81 74	35, 55, 67, 73	0
17	1V	101/101 (100%)	-0.30	0 100 100	19, 34, 53, 69	0
17	2V	101/101 (100%)	0.36	0 100 100	36, 63, 74, 78	0
18	1W	112/113 (99%)	-0.33	0 100 100	21, 26, 48, 71	0
18	2W	112/113 (99%)	0.22	0 100 100	33, 44, 59, 84	0
19	1X	95/96 (98%)	-0.13	1 (1%) 78 70	19, 31, 53, 75	0
19	2X	95/96 (98%)	0.34	0 100 100	40, 53, 64, 72	0
20	1Y	107/110 (97%)	0.01	1 (0%) 81 74	29, 43, 61, 72	0
20	2Y	107/110 (97%)	0.79	6 (5%) 30 23	54, 65, 74, 78	0
21	1Z	154/206 (74%)	0.46	6 (3%) 43 34	35, 57, 79, 85	0
21	2Z	160/206 (77%)	1.36	36 (22%) 2 1	61, 75, 84, 91	0
22	10	83/85 (97%)	-0.06	2 (2%) 59 49	18, 31, 51, 56	0
22	20	83/85 (97%)	0.71	4 (4%) 35 28	36, 58, 69, 74	0
23	11	97/98 (98%)	0.07	1 (1%) 79 72	20, 38, 62, 70	0
23	21	97/98 (98%)	0.37	4 (4%) 41 33	35, 50, 68, 73	0
24	12	70/72 (97%)	-0.06	1 (1%) 73 64	29, 41, 53, 64	0
24	22	70/72 (97%)	0.50	2 (2%) 53 43	47, 62, 70, 73	0
25	13	59/60 (98%)	-0.21	0 100 100	19, 31, 54, 72	0
25	23	59/60 (98%)	0.54	1 (1%) 69 60	48, 58, 70, 76	0
26	14	69/71 (97%)	0.55	3 (4%) 40 31	43, 65, 83, 84	0
26	24	69/71 (97%)	0.92	6 (8%) 16 11	67, 77, 86, 87	0
27	15	59/60 (98%)	-0.37	0 100 100	14, 28, 41, 50	0
27	25	59/60 (98%)	0.10	1 (1%) 69 60	32, 46, 56, 64	0
28	16	53/54 (98%)	-0.27	0 100 100	27, 36, 50, 54	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.55	1 (1%) 66 57	42, 54, 67, 68	0
29	17	48/49 (97%)	-0.24	0 100 100	16, 21, 50, 60	0
29	27	48/49 (97%)	-0.03	0 100 100	24, 35, 51, 60	0
30	18	64/65 (98%)	-0.18	1 (1%) 70 61	21, 27, 37, 55	0
30	28	64/65 (98%)	0.40	1 (1%) 70 61	40, 49, 58, 68	0
31	19	37/37 (100%)	-0.10	0 100 100	22, 33, 50, 55	0
31	29	37/37 (100%)	0.72	2 (5%) 31 24	53, 62, 71, 75	0
32	1a	1488/1521 (97%)	0.04	26 (1%) 69 60	32, 59, 86, 102	0
32	2a	1491/1521 (98%)	0.36	42 (2%) 55 45	43, 69, 89, 101	0
33	1b	231/256 (90%)	0.72	18 (7%) 19 14	59, 73, 82, 85	0
33	2b	231/256 (90%)	1.03	26 (11%) 10 7	64, 79, 85, 90	0
34	1c	206/239 (86%)	0.52	10 (4%) 35 27	51, 66, 74, 80	0
34	2c	206/239 (86%)	1.11	26 (12%) 8 6	66, 78, 82, 85	0
35	1d	208/209 (99%)	0.58	5 (2%) 59 49	50, 64, 76, 83	0
35	2d	208/209 (99%)	0.58	6 (2%) 53 43	53, 62, 72, 81	0
36	1e	148/162 (91%)	0.37	3 (2%) 65 56	48, 60, 70, 78	0
36	2e	148/162 (91%)	1.05	22 (14%) 5 4	58, 71, 79, 86	0
37	1f	100/101 (99%)	0.47	2 (2%) 65 56	48, 60, 69, 70	0
37	2f	100/101 (99%)	0.49	0 100 100	51, 63, 70, 76	0
38	1g	155/156 (99%)	0.52	8 (5%) 33 25	51, 62, 74, 88	0
38	2g	155/156 (99%)	0.69	12 (7%) 19 14	62, 71, 78, 84	0
39	1h	137/138 (99%)	0.54	2 (1%) 72 63	48, 61, 67, 72	0
39	2h	137/138 (99%)	0.77	6 (4%) 39 31	64, 71, 77, 85	0
40	1i	127/128 (99%)	0.93	10 (7%) 18 13	46, 69, 77, 83	0
40	2i	127/128 (99%)	1.43	30 (23%) 2 1	68, 77, 82, 88	0
41	1j	97/105 (92%)	1.05	12 (12%) 8 6	52, 71, 78, 83	0
41	2j	96/105 (91%)	1.52	29 (30%) 1 1	70, 78, 85, 87	0
42	1k	114/129 (88%)	0.34	2 (1%) 67 58	40, 58, 72, 79	0
42	2k	114/129 (88%)	0.48	3 (2%) 57 47	49, 66, 74, 78	0
43	1l	121/132 (91%)	0.06	2 (1%) 69 60	33, 47, 59, 66	0
43	2l	121/132 (91%)	0.62	6 (4%) 34 26	53, 61, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.43	5 (4%) 41 33	47, 59, 70, 74	0
44	2m	122/126 (96%)	1.01	14 (11%) 9 7	62, 75, 81, 85	0
45	1n	60/61 (98%)	0.50	1 (1%) 69 60	50, 59, 67, 71	0
45	2n	60/61 (98%)	1.70	20 (33%) 1 1	68, 77, 81, 87	0
46	1o	88/89 (98%)	0.25	2 (2%) 61 51	44, 59, 70, 75	0
46	2o	88/89 (98%)	0.36	1 (1%) 78 70	53, 65, 74, 75	0
47	1p	82/88 (93%)	0.99	6 (7%) 21 15	51, 61, 70, 75	0
47	2p	82/88 (93%)	0.79	3 (3%) 45 36	55, 62, 71, 75	0
48	1q	99/105 (94%)	0.56	2 (2%) 65 56	47, 59, 72, 75	0
48	2q	99/105 (94%)	0.65	5 (5%) 33 25	55, 65, 73, 75	0
49	1r	68/88 (77%)	0.23	1 (1%) 72 63	48, 61, 71, 73	0
49	2r	68/88 (77%)	0.36	0 100 100	57, 63, 73, 77	0
50	1s	83/93 (89%)	0.64	2 (2%) 59 49	49, 64, 73, 77	0
50	2s	83/93 (89%)	1.05	8 (9%) 13 10	71, 78, 84, 87	0
51	1t	96/106 (90%)	0.64	6 (6%) 26 19	50, 64, 73, 78	0
51	2t	96/106 (90%)	0.68	8 (8%) 17 12	52, 63, 76, 79	0
52	1u	23/27 (85%)	0.96	3 (13%) 7 6	52, 59, 63, 70	0
52	2u	23/27 (85%)	1.66	9 (39%) 1 0	67, 73, 80, 80	0
53	1v	13/24 (54%)	0.77	2 (15%) 5 4	42, 56, 81, 90	0
53	2v	13/24 (54%)	1.06	3 (23%) 2 1	59, 74, 91, 97	0
54	1w	67/76 (88%)	0.60	7 (10%) 11 8	32, 82, 93, 96	0
54	1y	67/76 (88%)	0.82	1 (1%) 72 63	28, 88, 96, 100	0
54	2w	65/76 (85%)	1.13	11 (16%) 4 3	54, 87, 95, 99	0
54	2y	66/76 (86%)	0.86	3 (4%) 38 30	49, 90, 94, 97	0
55	1x	72/77 (93%)	0.04	0 100 100	32, 58, 76, 85	0
55	2x	72/77 (93%)	0.49	1 (1%) 73 64	45, 71, 81, 83	0
All	All	20875/21748 (95%)	0.18	650 (3%) 51 41	13, 57, 83, 102	0

The worst 5 of 650 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	2c	168	ALA	5.9
21	2Z	172	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
44	2m	102	ARG	5.0
41	2j	65	LEU	4.8
32	2a	1033	G	4.8

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
54	PSU	1y	55	20/21	0.64	0.14	85,93,105,123	0
54	7MG	2y	46	24/25	0.66	0.13	83,92,97,112	0
54	7MG	2w	46	24/25	0.66	0.13	78,92,98,107	0
54	7MG	1w	46	24/25	0.68	0.13	76,87,106,118	0
54	5MU	1y	54	21/22	0.69	0.14	79,87,99,114	0
54	4SU	2y	8	20/21	0.69	0.14	83,95,104,112	0
54	5MU	2y	54	21/22	0.70	0.17	84,91,97,115	0
54	MIA	2y	37	22/30	0.71	0.11	69,81,100,111	0
54	4SU	1y	8	20/21	0.72	0.11	91,96,103,105	0
54	PSU	2y	55	20/21	0.72	0.15	85,92,104,109	0
54	7MG	1y	46	24/25	0.73	0.14	86,94,99,108	0
54	MIA	1y	37	22/30	0.74	0.15	70,78,88,93	0
54	4SU	2w	8	20/21	0.74	0.13	85,89,104,109	0
54	PSU	2y	32	20/21	0.76	0.13	69,84,92,94	0
54	PSU	2y	39	20/21	0.82	0.11	77,84,98,102	0
54	PSU	2w	55	20/21	0.83	0.09	75,81,89,94	0
54	PSU	1w	55	20/21	0.83	0.11	61,70,79,80	0
54	4SU	1w	8	20/21	0.84	0.11	74,81,92,95	0
32	2MG	2a	1207	24/25	0.85	0.11	74,77,86,91	0
55	PSU	2x	55	20/21	0.85	0.13	67,78,81,81	0
54	PSU	1y	32	20/21	0.86	0.11	71,81,88,90	0
43	0TD	2l	92	10/11	0.86	0.14	58,64,65,80	0
1	5MU	2A	1915	21/22	0.86	0.13	59,64,71,73	0
54	5MU	2w	54	21/22	0.87	0.10	68,75,81,83	0
55	5MU	2x	54	21/22	0.88	0.13	77,81,86,94	0
55	4SU	2x	8	20/21	0.88	0.13	69,73,78,81	0
54	PSU	2w	39	20/21	0.89	0.12	60,73,79,81	0
54	PSU	2w	32	20/21	0.89	0.13	67,78,88,89	0
32	PSU	2a	516	20/21	0.90	0.10	50,70,74,75	0
54	PSU	1y	39	20/21	0.90	0.09	70,77,87,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	2A	1917	20/21	0.91	0.10	55,60,65,69	0
55	PSU	1x	55	20/21	0.91	0.09	53,58,67,72	0
43	0TD	1l	92	10/11	0.91	0.12	43,48,51,69	0
55	5MU	1x	54	21/22	0.92	0.09	55,62,70,76	0
32	5MC	2a	1400	21/22	0.92	0.11	60,67,71,73	0
32	7MG	2a	527	24/25	0.92	0.10	46,56,67,71	0
55	5MC	2x	32	21/22	0.92	0.12	65,68,73,74	0
32	5MC	2a	967	21/22	0.92	0.11	62,67,71,73	0
1	4OC	2A	1920	21/23	0.93	0.10	53,58,64,66	0
1	5MC	2A	1942	21/22	0.93	0.12	49,56,62,66	0
32	4OC	2a	1402	22/23	0.93	0.11	52,58,64,67	0
32	5MC	2a	1404	21/22	0.93	0.11	47,51,56,61	0
1	PSU	2A	1911	20/21	0.93	0.09	50,60,65,67	0
1	PSU	1A	1939	20/21	0.93	0.09	38,46,53,54	0
32	M2G	2a	966	25/26	0.93	0.13	60,65,72,79	0
1	5MU	1A	1937	21/22	0.93	0.11	43,49,54,56	0
32	7MG	1a	527	24/25	0.94	0.10	34,42,51,55	0
32	2MG	1a	1207	24/25	0.94	0.09	57,62,67,68	0
54	PSU	1w	32	20/21	0.94	0.09	57,62,68,69	0
32	PSU	1a	516	20/21	0.94	0.09	32,49,53,54	0
32	5MC	2a	1407	21/22	0.94	0.09	44,48,55,60	0
32	MA6	2a	1518	24/25	0.94	0.10	47,59,63,66	0
32	MA6	2a	1519	24/25	0.94	0.11	47,56,64,66	0
55	4SU	1x	8	20/21	0.94	0.09	50,57,65,67	0
54	MIA	2w	37	25/30	0.94	0.13	60,68,74,78	0
55	5MC	1x	32	21/22	0.95	0.11	44,50,57,66	0
54	MIA	1w	37	29/30	0.95	0.12	41,51,60,64	0
32	M2G	1a	966	25/26	0.95	0.09	41,48,56,63	0
32	5MC	1a	1400	21/22	0.95	0.10	37,47,50,55	0
1	5MU	2A	1939	21/22	0.95	0.09	34,38,43,44	0
32	UR3	2a	1498	21/22	0.95	0.10	44,50,54,63	0
32	5MC	1a	967	21/22	0.95	0.09	45,50,58,64	0
54	PSU	1w	39	20/21	0.96	0.08	44,60,69,70	0
32	5MC	1a	1407	21/22	0.96	0.09	28,34,39,40	0
32	MA6	1a	1519	24/25	0.96	0.10	33,39,43,44	0
1	PSU	1A	1933	20/21	0.96	0.08	30,37,44,45	0
32	5MC	1a	1404	21/22	0.96	0.09	31,38,42,44	0
1	5MC	2A	1962	21/22	0.96	0.08	32,45,48,61	0
1	OMG	2A	2251	24/25	0.96	0.09	32,37,42,45	0
1	2MU	2A	2552	21/23	0.96	0.08	31,41,45,52	0
54	5MU	1w	54	21/22	0.96	0.07	44,60,67,72	0
1	5MC	1A	1984	21/22	0.97	0.07	24,31,36,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	2MA	2A	2503	23/24	0.97	0.08	24,33,37,46	0
1	2MU	1A	2564	21/23	0.97	0.07	18,23,28,31	0
1	4OC	1A	1942	21/23	0.97	0.08	32,39,45,47	0
32	4OC	1a	1402	22/23	0.97	0.09	38,42,47,53	0
1	5MU	1A	1961	21/22	0.97	0.06	19,23,26,32	0
1	5MC	1A	1964	21/22	0.97	0.08	30,39,46,50	0
32	MA6	1a	1518	24/25	0.98	0.07	31,38,40,40	0
1	PSU	2A	2605	20/21	0.98	0.06	27,31,37,38	0
1	2MA	1A	2515	23/24	0.98	0.06	11,16,19,22	0
1	OMG	1A	2263	24/25	0.98	0.07	14,18,24,25	0
1	PSU	1A	2617	20/21	0.98	0.06	16,20,25,28	0
32	UR3	1a	1498	21/22	0.98	0.07	27,39,42,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2y	3005	1/1	0.49	0.19	88,88,88,88	0
56	MG	2y	3006	1/1	0.50	0.15	88,88,88,88	0
56	MG	2A	3484	1/1	0.56	0.25	70,70,70,70	0
56	MG	2B	3013	1/1	0.61	0.16	74,74,74,74	0
56	MG	1B	236	1/1	0.61	0.14	65,65,65,65	0
56	MG	2A	3491	1/1	0.61	0.23	75,75,75,75	0
56	MG	1A	3801	1/1	0.62	0.16	71,71,71,71	0
56	MG	1a	3049	1/1	0.62	0.22	60,60,60,60	0
56	MG	2A	3560	1/1	0.62	0.15	50,50,50,50	0
56	MG	2A	3630	1/1	0.63	0.21	55,55,55,55	0
56	MG	1A	3986	1/1	0.63	0.15	67,67,67,67	0
56	MG	1y	103	1/1	0.64	0.34	82,82,82,82	0
56	MG	2a	1640	1/1	0.64	0.20	62,62,62,62	0
56	MG	2A	3550	1/1	0.65	0.13	58,58,58,58	0
56	MG	2A	3433	1/1	0.66	0.12	60,60,60,60	0
56	MG	1a	3026	1/1	0.67	0.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2v	3002	1/1	0.67	0.14	67,67,67,67	0
56	MG	2a	1810	1/1	0.68	0.15	81,81,81,81	0
56	MG	2A	3684	1/1	0.69	0.28	68,68,68,68	0
56	MG	1A	3458	1/1	0.70	0.31	68,68,68,68	0
56	MG	2a	1807	1/1	0.70	0.16	61,61,61,61	0
56	MG	1A	3653	1/1	0.70	0.20	20,20,20,20	0
56	MG	2j	8001	1/1	0.71	0.15	66,66,66,66	0
56	MG	2A	3420	1/1	0.71	0.20	67,67,67,67	0
56	MG	2A	3632	1/1	0.71	0.11	62,62,62,62	0
56	MG	28	102	1/1	0.71	0.34	64,64,64,64	0
56	MG	1A	3622	1/1	0.72	0.26	56,56,56,56	0
56	MG	2A	3570	1/1	0.72	0.33	56,56,56,56	0
56	MG	2a	1769	1/1	0.72	0.15	75,75,75,75	0
56	MG	2A	3618	1/1	0.73	0.11	71,71,71,71	0
56	MG	2a	1815	1/1	0.73	0.16	61,61,61,61	0
56	MG	1A	3863	1/1	0.73	0.19	56,56,56,56	0
56	MG	2A	3374	1/1	0.73	0.12	41,41,41,41	0
56	MG	1l	102	1/1	0.73	0.24	72,72,72,72	0
56	MG	2A	3695	1/1	0.73	0.16	58,58,58,58	0
56	MG	2B	3018	1/1	0.74	0.20	80,80,80,80	0
56	MG	2G	3001	1/1	0.74	0.12	60,60,60,60	0
56	MG	1e	201	1/1	0.74	0.09	59,59,59,59	0
56	MG	1A	3832	1/1	0.74	0.16	69,69,69,69	0
56	MG	2A	3648	1/1	0.75	0.12	46,46,46,46	0
56	MG	2a	1770	1/1	0.75	0.16	59,59,59,59	0
56	MG	1a	3149	1/1	0.75	0.31	76,76,76,76	0
56	MG	1D	304	1/1	0.75	0.59	43,43,43,43	0
56	MG	2A	3723	1/1	0.75	0.22	67,67,67,67	0
56	MG	2a	1617	1/1	0.75	0.22	73,73,73,73	0
56	MG	2B	3009	1/1	0.75	0.27	63,63,63,63	0
56	MG	2a	1661	1/1	0.75	0.20	63,63,63,63	0
56	MG	2a	1662	1/1	0.75	0.12	59,59,59,59	0
56	MG	1x	101	1/1	0.76	0.28	54,54,54,54	0
56	MG	1A	3527	1/1	0.76	0.17	66,66,66,66	0
56	MG	2A	3530	1/1	0.76	0.11	64,64,64,64	0
56	MG	1A	3898	1/1	0.76	0.18	71,71,71,71	0
56	MG	2a	1738	1/1	0.76	0.14	71,71,71,71	0
56	MG	1A	3931	1/1	0.76	0.13	47,47,47,47	0
56	MG	1A	3980	1/1	0.76	0.13	62,62,62,62	0
56	MG	1A	3960	1/1	0.77	0.17	51,51,51,51	0
56	MG	1a	3146	1/1	0.77	0.12	64,64,64,64	0
56	MG	1A	3802	1/1	0.77	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3720	1/1	0.77	0.08	97,97,97,97	0
56	MG	1a	3177	1/1	0.77	0.12	57,57,57,57	0
56	MG	2j	8002	1/1	0.77	0.14	62,62,62,62	0
56	MG	2A	3436	1/1	0.77	0.21	62,62,62,62	0
56	MG	1A	3951	1/1	0.77	0.14	62,62,62,62	0
56	MG	1B	232	1/1	0.77	0.13	66,66,66,66	0
56	MG	1A	3566	1/1	0.78	0.15	62,62,62,62	0
56	MG	2a	1674	1/1	0.78	0.20	55,55,55,55	0
56	MG	1A	3521	1/1	0.78	0.13	50,50,50,50	0
56	MG	2A	3457	1/1	0.78	0.17	58,58,58,58	0
56	MG	1A	3209	1/1	0.78	0.27	61,61,61,61	0
56	MG	2a	1788	1/1	0.78	0.08	55,55,55,55	0
56	MG	2a	1791	1/1	0.78	0.15	69,69,69,69	0
56	MG	1A	3859	1/1	0.78	0.16	61,61,61,61	0
56	MG	2A	3638	1/1	0.78	0.14	66,66,66,66	0
56	MG	2A	3400	1/1	0.78	0.20	72,72,72,72	0
56	MG	2a	1609	1/1	0.78	0.18	57,57,57,57	0
56	MG	2A	3650	1/1	0.78	0.16	52,52,52,52	0
56	MG	2a	1632	1/1	0.78	0.24	67,67,67,67	0
56	MG	2x	103	1/1	0.78	0.14	63,63,63,63	0
56	MG	2A	3532	1/1	0.78	0.16	62,62,62,62	0
56	MG	1A	3674	1/1	0.78	0.15	56,56,56,56	0
56	MG	2y	3007	1/1	0.78	0.24	81,81,81,81	0
56	MG	1A	3306	1/1	0.79	0.12	43,43,43,43	0
56	MG	2A	3285	1/1	0.79	0.16	58,58,58,58	0
56	MG	1A	3971	1/1	0.79	0.09	65,65,65,65	0
56	MG	2v	3003	1/1	0.79	0.16	66,66,66,66	0
56	MG	2w	106	1/1	0.79	0.23	59,59,59,59	0
56	MG	1A	3227	1/1	0.79	0.22	49,49,49,49	0
56	MG	1A	3679	1/1	0.79	0.15	14,14,14,14	0
56	MG	2A	3697	1/1	0.79	0.19	50,50,50,50	0
56	MG	1A	3760	1/1	0.79	0.13	44,44,44,44	0
56	MG	1A	3795	1/1	0.80	0.15	50,50,50,50	0
56	MG	2B	3012	1/1	0.80	0.12	75,75,75,75	0
56	MG	1A	3170	1/1	0.80	0.12	63,63,63,63	0
56	MG	1a	3037	1/1	0.80	0.30	61,61,61,61	0
56	MG	2A	3071	1/1	0.80	0.22	60,60,60,60	0
56	MG	2Z	8001	1/1	0.80	0.16	73,73,73,73	0
56	MG	2A	3208	1/1	0.80	0.11	49,49,49,49	0
56	MG	1A	3523	1/1	0.80	0.13	46,46,46,46	0
56	MG	2a	1821	1/1	0.80	0.18	66,66,66,66	0
56	MG	2a	1833	1/1	0.80	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3658	1/1	0.80	0.19	36,36,36,36	0
56	MG	1A	3465	1/1	0.80	0.38	55,55,55,55	0
56	MG	2A	3536	1/1	0.80	0.13	54,54,54,54	0
56	MG	1E	310	1/1	0.80	0.16	60,60,60,60	0
56	MG	2A	3408	1/1	0.80	0.12	53,53,53,53	0
56	MG	2a	1668	1/1	0.80	0.15	55,55,55,55	0
56	MG	1S	3003	1/1	0.80	0.15	61,61,61,61	0
56	MG	2a	1709	1/1	0.80	0.26	49,49,49,49	0
56	MG	2a	1724	1/1	0.80	0.20	73,73,73,73	0
56	MG	2a	1624	1/1	0.81	0.08	78,78,78,78	0
56	MG	1A	3942	1/1	0.81	0.12	47,47,47,47	0
56	MG	1A	3593	1/1	0.81	0.13	30,30,30,30	0
56	MG	1A	3691	1/1	0.81	0.17	55,55,55,55	0
56	MG	2A	3636	1/1	0.81	0.14	55,55,55,55	0
56	MG	2A	3533	1/1	0.81	0.16	52,52,52,52	0
56	MG	1a	3092	1/1	0.81	0.15	55,55,55,55	0
56	MG	2F	304	1/1	0.81	0.16	64,64,64,64	0
56	MG	2A	3539	1/1	0.81	0.26	59,59,59,59	0
56	MG	2U	202	1/1	0.81	0.27	55,55,55,55	0
56	MG	1A	3883	1/1	0.81	0.20	59,59,59,59	0
56	MG	1A	3730	1/1	0.81	0.18	42,42,42,42	0
56	MG	1A	3675	1/1	0.81	0.24	66,66,66,66	0
56	MG	2A	3604	1/1	0.81	0.20	58,58,58,58	0
56	MG	1A	3775	1/1	0.82	0.17	41,41,41,41	0
56	MG	2A	3366	1/1	0.82	0.22	67,67,67,67	0
56	MG	2a	1645	1/1	0.82	0.09	74,74,74,74	0
56	MG	16	103	1/1	0.82	0.11	56,56,56,56	0
56	MG	2A	3639	1/1	0.82	0.13	56,56,56,56	0
56	MG	2a	1663	1/1	0.82	0.18	48,48,48,48	0
56	MG	1A	3445	1/1	0.82	0.10	47,47,47,47	0
56	MG	1A	3568	1/1	0.82	0.08	30,30,30,30	0
56	MG	1A	3695	1/1	0.82	0.21	50,50,50,50	0
56	MG	2a	1719	1/1	0.82	0.18	55,55,55,55	0
56	MG	2A	3676	1/1	0.82	0.13	79,79,79,79	0
56	MG	2a	1730	1/1	0.82	0.14	65,65,65,65	0
56	MG	1a	3059	1/1	0.82	0.21	61,61,61,61	0
56	MG	2a	1740	1/1	0.82	0.13	60,60,60,60	0
56	MG	2a	1762	1/1	0.82	0.20	52,52,52,52	0
56	MG	2a	1765	1/1	0.82	0.28	64,64,64,64	0
56	MG	1A	3815	1/1	0.82	0.11	35,35,35,35	0
56	MG	1A	3828	1/1	0.82	0.17	62,62,62,62	0
56	MG	2a	1775	1/1	0.82	0.27	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1785	1/1	0.82	0.21	63,63,63,63	0
56	MG	1A	3706	1/1	0.82	0.12	27,27,27,27	0
56	MG	1a	3162	1/1	0.82	0.16	62,62,62,62	0
56	MG	2a	1802	1/1	0.82	0.26	69,69,69,69	0
56	MG	1B	221	1/1	0.82	0.09	36,36,36,36	0
56	MG	1a	3205	1/1	0.82	0.21	69,69,69,69	0
56	MG	1A	3242	1/1	0.82	0.16	59,59,59,59	0
56	MG	1r	3001	1/1	0.82	0.20	61,61,61,61	0
56	MG	2a	1824	1/1	0.82	0.23	63,63,63,63	0
56	MG	2a	1829	1/1	0.82	0.20	68,68,68,68	0
56	MG	1A	3735	1/1	0.82	0.14	22,22,22,22	0
56	MG	2A	3544	1/1	0.82	0.15	30,30,30,30	0
56	MG	1x	109	1/1	0.82	0.11	57,57,57,57	0
56	MG	1A	3741	1/1	0.82	0.18	40,40,40,40	0
56	MG	1A	3621	1/1	0.82	0.14	44,44,44,44	0
56	MG	2A	3098	1/1	0.82	0.18	68,68,68,68	0
56	MG	2a	1611	1/1	0.82	0.48	65,65,65,65	0
56	MG	2a	1616	1/1	0.82	0.65	67,67,67,67	0
56	MG	1A	3907	1/1	0.82	0.17	39,39,39,39	0
56	MG	2A	3246	1/1	0.82	0.16	48,48,48,48	0
56	MG	2A	3737	1/1	0.83	0.13	42,42,42,42	0
56	MG	2a	1727	1/1	0.83	0.21	87,87,87,87	0
56	MG	2A	3033	1/1	0.83	0.23	52,52,52,52	0
56	MG	1a	3050	1/1	0.83	0.16	50,50,50,50	0
56	MG	2A	3083	1/1	0.83	0.11	53,53,53,53	0
56	MG	1a	3052	1/1	0.83	0.26	58,58,58,58	0
56	MG	2B	3019	1/1	0.83	0.14	82,82,82,82	0
56	MG	2A	3140	1/1	0.83	0.19	60,60,60,60	0
56	MG	2A	3149	1/1	0.83	0.08	57,57,57,57	0
56	MG	2a	1772	1/1	0.83	0.12	54,54,54,54	0
56	MG	1A	3905	1/1	0.83	0.26	54,54,54,54	0
56	MG	1A	3831	1/1	0.83	0.26	68,68,68,68	0
56	MG	1a	3142	1/1	0.83	0.12	64,64,64,64	0
56	MG	1A	3916	1/1	0.83	0.10	54,54,54,54	0
56	MG	2a	1799	1/1	0.83	0.24	59,59,59,59	0
56	MG	1A	3606	1/1	0.83	0.14	61,61,61,61	0
56	MG	2a	1806	1/1	0.83	0.19	76,76,76,76	0
56	MG	1A	3833	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3752	1/1	0.83	0.30	36,36,36,36	0
56	MG	1a	3180	1/1	0.83	0.13	62,62,62,62	0
56	MG	2a	1630	1/1	0.83	0.34	57,57,57,57	0
56	MG	1A	3534	1/1	0.83	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3055	1/1	0.83	0.15	54,54,54,54	0
56	MG	2A	3656	1/1	0.83	0.17	68,68,68,68	0
56	MG	1A	3895	1/1	0.83	0.18	71,71,71,71	0
56	MG	1v	3001	1/1	0.83	0.33	72,72,72,72	0
56	MG	2A	3490	1/1	0.83	0.13	72,72,72,72	0
56	MG	1A	3790	1/1	0.83	0.20	27,27,27,27	0
56	MG	2w	105	1/1	0.83	0.12	72,72,72,72	0
56	MG	2A	3529	1/1	0.83	0.21	59,59,59,59	0
56	MG	2a	1681	1/1	0.83	0.14	69,69,69,69	0
56	MG	2a	1701	1/1	0.83	0.29	72,72,72,72	0
56	MG	1a	3038	1/1	0.83	0.26	55,55,55,55	0
56	MG	1B	213	1/1	0.83	0.12	55,55,55,55	0
56	MG	2A	3587	1/1	0.84	0.30	55,55,55,55	0
56	MG	1A	3761	1/1	0.84	0.16	48,48,48,48	0
56	MG	2A	3160	1/1	0.84	0.08	47,47,47,47	0
56	MG	2A	3619	1/1	0.84	0.11	60,60,60,60	0
56	MG	2A	3196	1/1	0.84	0.21	53,53,53,53	0
56	MG	2a	1692	1/1	0.84	0.33	60,60,60,60	0
56	MG	1A	3920	1/1	0.84	0.13	39,39,39,39	0
56	MG	2A	3215	1/1	0.84	0.12	58,58,58,58	0
56	MG	1a	3148	1/1	0.84	0.15	55,55,55,55	0
56	MG	2A	3257	1/1	0.84	0.20	57,57,57,57	0
56	MG	2A	3267	1/1	0.84	0.20	52,52,52,52	0
56	MG	1A	3698	1/1	0.84	0.08	41,41,41,41	0
56	MG	2A	3289	1/1	0.84	0.24	53,53,53,53	0
56	MG	2A	3334	1/1	0.84	0.18	58,58,58,58	0
56	MG	2A	3360	1/1	0.84	0.12	25,25,25,25	0
56	MG	1A	3858	1/1	0.84	0.20	54,54,54,54	0
56	MG	1a	3168	1/1	0.84	0.19	63,63,63,63	0
56	MG	1A	3700	1/1	0.84	0.10	27,27,27,27	0
56	MG	1A	3212	1/1	0.84	0.12	50,50,50,50	0
56	MG	1a	3186	1/1	0.84	0.18	48,48,48,48	0
56	MG	2a	1784	1/1	0.84	0.22	66,66,66,66	0
56	MG	1a	3194	1/1	0.84	0.10	59,59,59,59	0
56	MG	1a	3020	1/1	0.84	0.16	47,47,47,47	0
56	MG	1a	3207	1/1	0.84	0.15	41,41,41,41	0
56	MG	2A	3471	1/1	0.84	0.16	37,37,37,37	0
56	MG	2a	1801	1/1	0.84	0.33	63,63,63,63	0
56	MG	2B	3016	1/1	0.84	0.13	54,54,54,54	0
56	MG	1A	3882	1/1	0.84	0.12	62,62,62,62	0
56	MG	1A	3094	1/1	0.84	0.19	56,56,56,56	0
56	MG	1A	3321	1/1	0.84	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1812	1/1	0.84	0.26	64,64,64,64	0
56	MG	2A	3506	1/1	0.84	0.17	48,48,48,48	0
56	MG	2A	3508	1/1	0.84	0.20	57,57,57,57	0
56	MG	2A	3514	1/1	0.84	0.10	56,56,56,56	0
56	MG	2a	1828	1/1	0.84	0.26	64,64,64,64	0
56	MG	1A	4013	1/1	0.84	0.10	21,21,21,21	0
56	MG	1A	4037	1/1	0.84	0.25	28,28,28,28	0
56	MG	1A	3563	1/1	0.84	0.08	35,35,35,35	0
56	MG	2A	3002	1/1	0.84	0.43	61,61,61,61	0
56	MG	1a	3055	1/1	0.84	0.27	49,49,49,49	0
56	MG	1A	3356	1/1	0.84	0.13	48,48,48,48	0
56	MG	2w	104	1/1	0.84	0.12	83,83,83,83	0
56	MG	1a	3064	1/1	0.84	0.16	54,54,54,54	0
56	MG	1A	3631	1/1	0.84	0.12	32,32,32,32	0
56	MG	2A	3108	1/1	0.84	0.17	49,49,49,49	0
56	MG	2y	3003	1/1	0.84	0.13	59,59,59,59	0
56	MG	2a	1644	1/1	0.84	0.15	62,62,62,62	0
56	MG	2A	3565	1/1	0.84	0.09	45,45,45,45	0
56	MG	1a	3114	1/1	0.84	0.21	68,68,68,68	0
56	MG	2A	3486	1/1	0.85	0.15	53,53,53,53	0
56	MG	2a	1603	1/1	0.85	0.17	73,73,73,73	0
56	MG	1a	3072	1/1	0.85	0.57	54,54,54,54	0
56	MG	1A	3230	1/1	0.85	0.15	44,44,44,44	0
56	MG	2a	1783	1/1	0.85	0.20	62,62,62,62	0
56	MG	1a	3105	1/1	0.85	0.19	59,59,59,59	0
56	MG	1B	202	1/1	0.85	0.18	42,42,42,42	0
56	MG	1a	3141	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3516	1/1	0.85	0.21	62,62,62,62	0
56	MG	1A	3794	1/1	0.85	0.12	18,18,18,18	0
56	MG	1x	108	1/1	0.85	0.12	61,61,61,61	0
56	MG	1a	3036	1/1	0.85	0.26	49,49,49,49	0
56	MG	1A	3959	1/1	0.85	0.11	76,76,76,76	0
56	MG	2a	1648	1/1	0.85	0.11	63,63,63,63	0
56	MG	1A	3861	1/1	0.85	0.18	58,58,58,58	0
56	MG	1a	3155	1/1	0.85	0.14	53,53,53,53	0
56	MG	2A	3054	1/1	0.85	0.19	53,53,53,53	0
56	MG	1a	3161	1/1	0.85	0.11	53,53,53,53	0
56	MG	2a	1673	1/1	0.85	0.32	57,57,57,57	0
56	MG	2B	3011	1/1	0.85	0.23	69,69,69,69	0
56	MG	2a	1678	1/1	0.85	0.26	65,65,65,65	0
56	MG	2A	3075	1/1	0.85	0.14	51,51,51,51	0
56	MG	1A	3526	1/1	0.85	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
56	MG	1A	3881	1/1	0.85	0.11	44,44,44,44	0
56	MG	2q	204	1/1	0.85	0.19	65,65,65,65	0
56	MG	1A	3302	1/1	0.85	0.31	32,32,32,32	0
56	MG	2A	3443	1/1	0.85	0.11	34,34,34,34	0
56	MG	1A	3991	1/1	0.85	0.12	66,66,66,66	0
56	MG	1Z	3003	1/1	0.85	0.10	52,52,52,52	0
56	MG	2A	3477	1/1	0.85	0.12	64,64,64,64	0
56	MG	2a	1736	1/1	0.85	0.11	82,82,82,82	0
56	MG	2x	104	1/1	0.85	0.30	64,64,64,64	0
56	MG	2y	3001	1/1	0.85	0.14	64,64,64,64	0
56	MG	2U	203	1/1	0.85	0.11	55,55,55,55	0
56	MG	2W	201	1/1	0.85	0.10	50,50,50,50	0
56	MG	1A	3231	1/1	0.85	0.14	45,45,45,45	0
56	MG	25	504	1/1	0.85	0.36	67,67,67,67	0
56	MG	1A	3495	1/1	0.86	0.12	31,31,31,31	0
56	MG	1a	3073	1/1	0.86	0.28	59,59,59,59	0
56	MG	2A	3373	1/1	0.86	0.11	25,25,25,25	0
56	MG	2a	1680	1/1	0.86	0.24	45,45,45,45	0
56	MG	1x	103	1/1	0.86	0.14	54,54,54,54	0
56	MG	2A	3640	1/1	0.86	0.22	47,47,47,47	0
56	MG	2a	1698	1/1	0.86	0.22	60,60,60,60	0
56	MG	2A	3382	1/1	0.86	0.18	46,46,46,46	0
56	MG	1x	104	1/1	0.86	0.18	54,54,54,54	0
56	MG	2a	1712	1/1	0.86	0.24	63,63,63,63	0
56	MG	1A	3083	1/1	0.86	0.22	55,55,55,55	0
56	MG	1a	3097	1/1	0.86	0.17	62,62,62,62	0
56	MG	2A	3430	1/1	0.86	0.18	53,53,53,53	0
56	MG	2A	3677	1/1	0.86	0.12	48,48,48,48	0
56	MG	1Q	204	1/1	0.86	0.08	41,41,41,41	0
56	MG	1R	204	1/1	0.86	0.15	33,33,33,33	0
56	MG	2a	1739	1/1	0.86	0.09	57,57,57,57	0
56	MG	2A	3011	1/1	0.86	0.14	54,54,54,54	0
56	MG	2a	1748	1/1	0.86	0.16	60,60,60,60	0
56	MG	2A	3021	1/1	0.86	0.15	58,58,58,58	0
56	MG	2A	3469	1/1	0.86	0.12	39,39,39,39	0
56	MG	1A	3965	1/1	0.86	0.10	63,63,63,63	0
56	MG	2A	3753	1/1	0.86	0.10	52,52,52,52	0
56	MG	1A	3680	1/1	0.86	0.26	36,36,36,36	0
56	MG	2A	3480	1/1	0.86	0.13	47,47,47,47	0
56	MG	2A	3483	1/1	0.86	0.16	59,59,59,59	0
56	MG	10	105	1/1	0.86	0.14	50,50,50,50	0
56	MG	1A	3596	1/1	0.86	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2B	3017	1/1	0.86	0.12	61,61,61,61	0
56	MG	1A	3248	1/1	0.86	0.29	49,49,49,49	0
56	MG	1A	3844	1/1	0.86	0.10	23,23,23,23	0
56	MG	2D	304	1/1	0.86	0.12	53,53,53,53	0
56	MG	2A	3494	1/1	0.86	0.10	49,49,49,49	0
56	MG	1a	3160	1/1	0.86	0.13	52,52,52,52	0
56	MG	2R	3001	1/1	0.86	0.14	58,58,58,58	0
56	MG	2A	3117	1/1	0.86	0.18	61,61,61,61	0
56	MG	2A	3132	1/1	0.86	0.16	58,58,58,58	0
56	MG	1A	4009	1/1	0.86	0.16	41,41,41,41	0
56	MG	2A	3518	1/1	0.86	0.09	45,45,45,45	0
56	MG	2A	3521	1/1	0.86	0.17	63,63,63,63	0
56	MG	1A	3441	1/1	0.86	0.10	49,49,49,49	0
56	MG	2A	3154	1/1	0.86	0.23	51,51,51,51	0
56	MG	1A	3284	1/1	0.86	0.14	42,42,42,42	0
56	MG	1A	3061	1/1	0.86	0.11	39,39,39,39	0
56	MG	1A	3934	1/1	0.86	0.10	22,22,22,22	0
56	MG	2A	3538	1/1	0.86	0.22	49,49,49,49	0
56	MG	1B	220	1/1	0.86	0.13	57,57,57,57	0
56	MG	1A	3117	1/1	0.86	0.12	48,48,48,48	0
56	MG	2A	3253	1/1	0.86	0.34	68,68,68,68	0
56	MG	2a	1633	1/1	0.86	0.34	63,63,63,63	0
56	MG	1A	3493	1/1	0.86	0.21	23,23,23,23	0
56	MG	1B	235	1/1	0.86	0.15	55,55,55,55	0
56	MG	2A	3279	1/1	0.86	0.09	64,64,64,64	0
56	MG	1a	3063	1/1	0.86	0.26	53,53,53,53	0
56	MG	1A	3956	1/1	0.86	0.20	67,67,67,67	0
56	MG	2A	3296	1/1	0.86	0.27	54,54,54,54	0
56	MG	2A	3308	1/1	0.86	0.24	54,54,54,54	0
56	MG	1s	101	1/1	0.86	0.23	62,62,62,62	0
56	MG	2A	3621	1/1	0.87	0.07	49,49,49,49	0
56	MG	1a	3028	1/1	0.87	0.17	37,37,37,37	0
56	MG	2A	3376	1/1	0.87	0.12	45,45,45,45	0
56	MG	1A	3617	1/1	0.87	0.11	45,45,45,45	0
56	MG	2A	3390	1/1	0.87	0.11	58,58,58,58	0
56	MG	2A	3040	1/1	0.87	0.14	39,39,39,39	0
56	MG	2A	3046	1/1	0.87	0.14	58,58,58,58	0
56	MG	2A	3047	1/1	0.87	0.15	60,60,60,60	0
56	MG	1A	3823	1/1	0.87	0.23	50,50,50,50	0
56	MG	2a	1688	1/1	0.87	0.35	53,53,53,53	0
56	MG	1B	225	1/1	0.87	0.10	57,57,57,57	0
56	MG	1A	3620	1/1	0.87	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3672	1/1	0.87	0.24	46,46,46,46	0
56	MG	2a	1705	1/1	0.87	0.19	54,54,54,54	0
56	MG	2a	1706	1/1	0.87	0.24	54,54,54,54	0
56	MG	2A	3082	1/1	0.87	0.17	69,69,69,69	0
56	MG	1a	3163	1/1	0.87	0.18	47,47,47,47	0
56	MG	2a	1713	1/1	0.87	0.13	48,48,48,48	0
56	MG	2a	1714	1/1	0.87	0.33	68,68,68,68	0
56	MG	2A	3087	1/1	0.87	0.24	59,59,59,59	0
56	MG	2A	3093	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3472	1/1	0.87	0.12	42,42,42,42	0
56	MG	2A	3708	1/1	0.87	0.14	63,63,63,63	0
56	MG	1A	3592	1/1	0.87	0.11	30,30,30,30	0
56	MG	1A	3781	1/1	0.87	0.27	51,51,51,51	0
56	MG	1A	3783	1/1	0.87	0.17	31,31,31,31	0
56	MG	1A	3981	1/1	0.87	0.09	30,30,30,30	0
56	MG	2B	3002	1/1	0.87	0.11	62,62,62,62	0
56	MG	2a	1753	1/1	0.87	0.21	45,45,45,45	0
56	MG	2B	3006	1/1	0.87	0.14	65,65,65,65	0
56	MG	1a	3190	1/1	0.87	0.21	51,51,51,51	0
56	MG	2A	3141	1/1	0.87	0.18	40,40,40,40	0
56	MG	1N	201	1/1	0.87	0.26	45,45,45,45	0
56	MG	1a	3203	1/1	0.87	0.20	69,69,69,69	0
56	MG	2a	1773	1/1	0.87	0.09	70,70,70,70	0
56	MG	2B	3014	1/1	0.87	0.07	71,71,71,71	0
56	MG	2A	3501	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	3909	1/1	0.87	0.11	46,46,46,46	0
56	MG	2A	3191	1/1	0.87	0.23	56,56,56,56	0
56	MG	1A	3718	1/1	0.87	0.11	39,39,39,39	0
56	MG	1a	3209	1/1	0.87	0.36	60,60,60,60	0
56	MG	2E	307	1/1	0.87	0.12	60,60,60,60	0
56	MG	1A	3417	1/1	0.87	0.08	42,42,42,42	0
56	MG	1p	101	1/1	0.87	0.19	55,55,55,55	0
56	MG	2A	3522	1/1	0.87	0.16	49,49,49,49	0
56	MG	2T	3002	1/1	0.87	0.09	59,59,59,59	0
56	MG	1T	202	1/1	0.87	0.14	47,47,47,47	0
56	MG	1A	3169	1/1	0.87	0.10	53,53,53,53	0
56	MG	2V	3002	1/1	0.87	0.09	56,56,56,56	0
56	MG	1A	4027	1/1	0.87	0.13	61,61,61,61	0
56	MG	2A	3277	1/1	0.87	0.12	54,54,54,54	0
56	MG	1a	3110	1/1	0.87	0.14	50,50,50,50	0
56	MG	27	101	1/1	0.87	0.07	44,44,44,44	0
56	MG	2A	3281	1/1	0.87	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3134	1/1	0.87	0.23	30,30,30,30	0
56	MG	2a	1604	1/1	0.87	0.18	48,48,48,48	0
56	MG	1a	3121	1/1	0.87	0.13	54,54,54,54	0
56	MG	2r	3002	1/1	0.87	0.12	64,64,64,64	0
56	MG	2A	3291	1/1	0.87	0.14	55,55,55,55	0
56	MG	2a	1615	1/1	0.87	0.09	54,54,54,54	0
56	MG	16	101	1/1	0.87	0.11	35,35,35,35	0
56	MG	1A	3697	1/1	0.87	0.16	27,27,27,27	0
56	MG	2A	3567	1/1	0.87	0.12	44,44,44,44	0
56	MG	2A	3310	1/1	0.87	0.20	58,58,58,58	0
56	MG	1y	102	1/1	0.87	0.20	83,83,83,83	0
56	MG	2A	3592	1/1	0.87	0.13	43,43,43,43	0
56	MG	2A	3601	1/1	0.87	0.20	53,53,53,53	0
56	MG	1a	3144	1/1	0.87	0.20	66,66,66,66	0
56	MG	1B	203	1/1	0.87	0.12	39,39,39,39	0
56	MG	1A	3806	1/1	0.87	0.10	45,45,45,45	0
56	MG	1a	3045	1/1	0.88	0.20	52,52,52,52	0
56	MG	2a	1637	1/1	0.88	0.13	52,52,52,52	0
56	MG	2A	3273	1/1	0.88	0.35	57,57,57,57	0
56	MG	2a	1642	1/1	0.88	0.17	55,55,55,55	0
56	MG	2A	3586	1/1	0.88	0.08	44,44,44,44	0
56	MG	1A	3443	1/1	0.88	0.09	32,32,32,32	0
56	MG	1A	3779	1/1	0.88	0.09	50,50,50,50	0
56	MG	2a	1659	1/1	0.88	0.16	47,47,47,47	0
56	MG	1A	3545	1/1	0.88	0.11	25,25,25,25	0
56	MG	1A	3082	1/1	0.88	0.11	40,40,40,40	0
56	MG	1w	101	1/1	0.88	0.15	74,74,74,74	0
56	MG	2a	1667	1/1	0.88	0.12	61,61,61,61	0
56	MG	1w	102	1/1	0.88	0.10	76,76,76,76	0
56	MG	1w	106	1/1	0.88	0.09	70,70,70,70	0
56	MG	2A	3623	1/1	0.88	0.23	46,46,46,46	0
56	MG	1w	110	1/1	0.88	0.14	75,75,75,75	0
56	MG	1A	3904	1/1	0.88	0.14	71,71,71,71	0
56	MG	2A	3316	1/1	0.88	0.09	53,53,53,53	0
56	MG	1a	3061	1/1	0.88	0.13	56,56,56,56	0
56	MG	2A	3337	1/1	0.88	0.18	27,27,27,27	0
56	MG	2a	1693	1/1	0.88	0.06	75,75,75,75	0
56	MG	1A	3307	1/1	0.88	0.12	49,49,49,49	0
56	MG	1A	3906	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3308	1/1	0.88	0.10	49,49,49,49	0
56	MG	1A	3570	1/1	0.88	0.13	57,57,57,57	0
56	MG	1a	3075	1/1	0.88	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1710	1/1	0.88	0.12	64,64,64,64	0
56	MG	1a	3077	1/1	0.88	0.18	42,42,42,42	0
56	MG	1B	231	1/1	0.88	0.13	59,59,59,59	0
56	MG	2A	3018	1/1	0.88	0.14	51,51,51,51	0
56	MG	1A	3586	1/1	0.88	0.16	17,17,17,17	0
56	MG	1A	3241	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3036	1/1	0.88	0.13	48,48,48,48	0
56	MG	2A	3705	1/1	0.88	0.11	64,64,64,64	0
56	MG	1A	3922	1/1	0.88	0.10	49,49,49,49	0
56	MG	2A	3710	1/1	0.88	0.09	76,76,76,76	0
56	MG	2A	3719	1/1	0.88	0.10	70,70,70,70	0
56	MG	1A	3924	1/1	0.88	0.12	34,34,34,34	0
56	MG	2A	3442	1/1	0.88	0.09	23,23,23,23	0
56	MG	2a	1752	1/1	0.88	0.11	62,62,62,62	0
56	MG	1a	3118	1/1	0.88	0.18	65,65,65,65	0
56	MG	2A	3738	1/1	0.88	0.17	63,63,63,63	0
56	MG	2a	1763	1/1	0.88	0.16	72,72,72,72	0
56	MG	2A	3049	1/1	0.88	0.21	53,53,53,53	0
56	MG	1D	313	1/1	0.88	0.16	52,52,52,52	0
56	MG	1E	308	1/1	0.88	0.10	28,28,28,28	0
56	MG	1A	3333	1/1	0.88	0.16	43,43,43,43	0
56	MG	1a	3143	1/1	0.88	0.13	74,74,74,74	0
56	MG	1G	3003	1/1	0.88	0.08	51,51,51,51	0
56	MG	2a	1777	1/1	0.88	0.20	55,55,55,55	0
56	MG	1A	3506	1/1	0.88	0.08	24,24,24,24	0
56	MG	1A	3510	1/1	0.88	0.15	50,50,50,50	0
56	MG	2B	3015	1/1	0.88	0.18	51,51,51,51	0
56	MG	1A	3713	1/1	0.88	0.12	48,48,48,48	0
56	MG	1A	3616	1/1	0.88	0.09	58,58,58,58	0
56	MG	1A	3513	1/1	0.88	0.15	29,29,29,29	0
56	MG	2A	3131	1/1	0.88	0.11	40,40,40,40	0
56	MG	1A	3288	1/1	0.88	0.10	47,47,47,47	0
56	MG	2a	1804	1/1	0.88	0.23	48,48,48,48	0
56	MG	10	104	1/1	0.88	0.16	49,49,49,49	0
56	MG	1A	3964	1/1	0.88	0.12	45,45,45,45	0
56	MG	2a	1808	1/1	0.88	0.14	58,58,58,58	0
56	MG	1A	3737	1/1	0.88	0.09	29,29,29,29	0
56	MG	1A	3849	1/1	0.88	0.10	35,35,35,35	0
56	MG	1A	3289	1/1	0.88	0.16	41,41,41,41	0
56	MG	2a	1820	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3163	1/1	0.88	0.08	44,44,44,44	0
56	MG	2A	3168	1/1	0.88	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
56	MG	1a	3018	1/1	0.88	0.09	55,55,55,55	0
56	MG	1A	3425	1/1	0.88	0.10	34,34,34,34	0
56	MG	2a	1831	1/1	0.88	0.06	53,53,53,53	0
56	MG	2A	3201	1/1	0.88	0.07	55,55,55,55	0
56	MG	2g	8001	1/1	0.88	0.08	59,59,59,59	0
56	MG	20	3001	1/1	0.88	0.20	52,52,52,52	0
56	MG	2A	3202	1/1	0.88	0.12	56,56,56,56	0
56	MG	2l	202	1/1	0.88	0.16	66,66,66,66	0
56	MG	2q	202	1/1	0.88	0.20	59,59,59,59	0
56	MG	2q	203	1/1	0.88	0.11	75,75,75,75	0
56	MG	1A	3226	1/1	0.88	0.30	49,49,49,49	0
56	MG	2A	3213	1/1	0.88	0.15	50,50,50,50	0
56	MG	1A	3638	1/1	0.88	0.10	56,56,56,56	0
56	MG	1A	3997	1/1	0.88	0.09	45,45,45,45	0
56	MG	2v	3004	1/1	0.88	0.15	73,73,73,73	0
56	MG	2A	3545	1/1	0.88	0.13	45,45,45,45	0
56	MG	2A	3547	1/1	0.88	0.21	47,47,47,47	0
56	MG	1A	3774	1/1	0.88	0.15	56,56,56,56	0
56	MG	2A	3551	1/1	0.88	0.24	48,48,48,48	0
56	MG	2A	3552	1/1	0.88	0.13	35,35,35,35	0
56	MG	2a	1623	1/1	0.88	0.17	46,46,46,46	0
56	MG	1A	4012	1/1	0.88	0.14	47,47,47,47	0
56	MG	2a	1625	1/1	0.88	0.28	67,67,67,67	0
56	MG	2A	3562	1/1	0.88	0.10	40,40,40,40	0
56	MG	2A	3260	1/1	0.88	0.07	48,48,48,48	0
56	MG	2A	3097	1/1	0.89	0.09	42,42,42,42	0
56	MG	2A	3503	1/1	0.89	0.12	54,54,54,54	0
56	MG	1A	3952	1/1	0.89	0.20	50,50,50,50	0
56	MG	2A	3102	1/1	0.89	0.11	44,44,44,44	0
56	MG	1A	3463	1/1	0.89	0.12	38,38,38,38	0
56	MG	1A	3152	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3119	1/1	0.89	0.16	41,41,41,41	0
56	MG	1A	3257	1/1	0.89	0.10	34,34,34,34	0
56	MG	1Z	3004	1/1	0.89	0.14	41,41,41,41	0
56	MG	2A	3528	1/1	0.89	0.13	58,58,58,58	0
56	MG	10	103	1/1	0.89	0.20	54,54,54,54	0
56	MG	1A	3320	1/1	0.89	0.28	48,48,48,48	0
56	MG	1a	3176	1/1	0.89	0.14	59,59,59,59	0
56	MG	1A	3707	1/1	0.89	0.10	45,45,45,45	0
56	MG	2A	3158	1/1	0.89	0.28	49,49,49,49	0
56	MG	1A	3261	1/1	0.89	0.11	35,35,35,35	0
56	MG	1A	3977	1/1	0.89	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3263	1/1	0.89	0.15	48,48,48,48	0
56	MG	2A	3170	1/1	0.89	0.17	44,44,44,44	0
56	MG	2a	1643	1/1	0.89	0.12	61,61,61,61	0
56	MG	2A	3185	1/1	0.89	0.22	46,46,46,46	0
56	MG	1a	3017	1/1	0.89	0.26	57,57,57,57	0
56	MG	1A	3721	1/1	0.89	0.29	53,53,53,53	0
56	MG	2a	1655	1/1	0.89	0.09	67,67,67,67	0
56	MG	2a	1656	1/1	0.89	0.29	68,68,68,68	0
56	MG	1A	3618	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3553	1/1	0.89	0.18	57,57,57,57	0
56	MG	1a	3021	1/1	0.89	0.17	40,40,40,40	0
56	MG	2A	3561	1/1	0.89	0.10	56,56,56,56	0
56	MG	2a	1666	1/1	0.89	0.29	51,51,51,51	0
56	MG	1A	3282	1/1	0.89	0.08	56,56,56,56	0
56	MG	2A	3212	1/1	0.89	0.13	59,59,59,59	0
56	MG	1a	3212	1/1	0.89	0.21	41,41,41,41	0
56	MG	1A	3996	1/1	0.89	0.09	49,49,49,49	0
56	MG	2A	3571	1/1	0.89	0.13	57,57,57,57	0
56	MG	2A	3583	1/1	0.89	0.25	40,40,40,40	0
56	MG	2A	3217	1/1	0.89	0.10	51,51,51,51	0
56	MG	2a	1684	1/1	0.89	0.22	49,49,49,49	0
56	MG	2A	3228	1/1	0.89	0.30	38,38,38,38	0
56	MG	2a	1691	1/1	0.89	0.11	56,56,56,56	0
56	MG	2A	3233	1/1	0.89	0.10	42,42,42,42	0
56	MG	2A	3593	1/1	0.89	0.15	47,47,47,47	0
56	MG	2A	3241	1/1	0.89	0.10	55,55,55,55	0
56	MG	2a	1700	1/1	0.89	0.12	62,62,62,62	0
56	MG	1l	203	1/1	0.89	0.11	50,50,50,50	0
56	MG	2A	3605	1/1	0.89	0.11	42,42,42,42	0
56	MG	2A	3613	1/1	0.89	0.08	61,61,61,61	0
56	MG	2a	1707	1/1	0.89	0.10	68,68,68,68	0
56	MG	2a	1708	1/1	0.89	0.17	61,61,61,61	0
56	MG	1m	201	1/1	0.89	0.21	57,57,57,57	0
56	MG	1A	3383	1/1	0.89	0.06	42,42,42,42	0
56	MG	2A	3259	1/1	0.89	0.15	53,53,53,53	0
56	MG	1A	4004	1/1	0.89	0.25	55,55,55,55	0
56	MG	1A	3869	1/1	0.89	0.14	19,19,19,19	0
56	MG	2a	1717	1/1	0.89	0.09	66,66,66,66	0
56	MG	1A	3870	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3397	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3624	1/1	0.89	0.22	26,26,26,26	0
56	MG	1A	3759	1/1	0.89	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1w	107	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3642	1/1	0.89	0.15	43,43,43,43	0
56	MG	1A	4042	1/1	0.89	0.08	40,40,40,40	0
56	MG	1A	4060	1/1	0.89	0.33	19,19,19,19	0
56	MG	2A	3653	1/1	0.89	0.11	37,37,37,37	0
56	MG	2A	3654	1/1	0.89	0.16	33,33,33,33	0
56	MG	1A	3398	1/1	0.89	0.08	37,37,37,37	0
56	MG	2a	1757	1/1	0.89	0.14	48,48,48,48	0
56	MG	1A	3414	1/1	0.89	0.09	55,55,55,55	0
56	MG	2A	3663	1/1	0.89	0.17	47,47,47,47	0
56	MG	2A	3664	1/1	0.89	0.23	41,41,41,41	0
56	MG	2A	3671	1/1	0.89	0.16	29,29,29,29	0
56	MG	1A	3644	1/1	0.89	0.13	12,12,12,12	0
56	MG	1a	3069	1/1	0.89	0.39	59,59,59,59	0
56	MG	1x	114	1/1	0.89	0.13	67,67,67,67	0
56	MG	2A	3678	1/1	0.89	0.17	71,71,71,71	0
56	MG	2A	3682	1/1	0.89	0.15	61,61,61,61	0
56	MG	2a	1780	1/1	0.89	0.10	57,57,57,57	0
56	MG	1A	3019	1/1	0.89	0.10	32,32,32,32	0
56	MG	2A	3690	1/1	0.89	0.10	58,58,58,58	0
56	MG	2A	3692	1/1	0.89	0.21	52,52,52,52	0
56	MG	2A	3348	1/1	0.89	0.17	47,47,47,47	0
56	MG	2a	1789	1/1	0.89	0.18	54,54,54,54	0
56	MG	2A	3354	1/1	0.89	0.13	53,53,53,53	0
56	MG	2a	1798	1/1	0.89	0.10	60,60,60,60	0
56	MG	2A	3701	1/1	0.89	0.11	50,50,50,50	0
56	MG	1A	3666	1/1	0.89	0.09	50,50,50,50	0
56	MG	1y	104	1/1	0.89	0.08	44,44,44,44	0
56	MG	1A	3672	1/1	0.89	0.23	68,68,68,68	0
56	MG	2A	3714	1/1	0.89	0.15	50,50,50,50	0
56	MG	2A	3003	1/1	0.89	0.12	49,49,49,49	0
56	MG	1A	3285	1/1	0.89	0.10	34,34,34,34	0
56	MG	2A	3017	1/1	0.89	0.23	59,59,59,59	0
56	MG	1A	3103	1/1	0.89	0.11	33,33,33,33	0
56	MG	2a	1813	1/1	0.89	0.17	54,54,54,54	0
56	MG	1A	3201	1/1	0.89	0.16	42,42,42,42	0
56	MG	2A	3402	1/1	0.89	0.20	49,49,49,49	0
56	MG	1a	3100	1/1	0.89	0.17	61,61,61,61	0
56	MG	2a	1822	1/1	0.89	0.19	52,52,52,52	0
56	MG	2B	3003	1/1	0.89	0.20	60,60,60,60	0
56	MG	2A	3409	1/1	0.89	0.15	54,54,54,54	0
56	MG	2A	3414	1/1	0.89	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
56	MG	1A	3065	1/1	0.89	0.22	62,62,62,62	0
56	MG	2A	3429	1/1	0.89	0.12	59,59,59,59	0
56	MG	1D	301	1/1	0.89	0.16	44,44,44,44	0
56	MG	2A	3041	1/1	0.89	0.10	46,46,46,46	0
56	MG	2A	3044	1/1	0.89	0.16	61,61,61,61	0
56	MG	1A	3923	1/1	0.89	0.17	39,39,39,39	0
56	MG	1A	3682	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3445	1/1	0.89	0.13	47,47,47,47	0
56	MG	2A	3446	1/1	0.89	0.12	32,32,32,32	0
56	MG	1E	307	1/1	0.89	0.10	50,50,50,50	0
56	MG	2D	307	1/1	0.89	0.15	35,35,35,35	0
56	MG	1a	3138	1/1	0.89	0.18	66,66,66,66	0
56	MG	2A	3065	1/1	0.89	0.20	52,52,52,52	0
56	MG	1A	3690	1/1	0.89	0.16	42,42,42,42	0
56	MG	1A	3447	1/1	0.89	0.17	47,47,47,47	0
56	MG	2A	3079	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3081	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3808	1/1	0.89	0.09	34,34,34,34	0
56	MG	2V	3001	1/1	0.89	0.10	46,46,46,46	0
56	MG	1A	3947	1/1	0.89	0.10	49,49,49,49	0
56	MG	1O	205	1/1	0.89	0.13	57,57,57,57	0
56	MG	2A	3088	1/1	0.89	0.08	40,40,40,40	0
56	MG	1A	3087	1/1	0.89	0.12	47,47,47,47	0
56	MG	2I	3001	1/1	0.90	0.13	36,36,36,36	0
56	MG	1A	3121	1/1	0.90	0.14	33,33,33,33	0
56	MG	1A	3496	1/1	0.90	0.09	35,35,35,35	0
56	MG	1A	3958	1/1	0.90	0.08	32,32,32,32	0
56	MG	2A	3517	1/1	0.90	0.11	51,51,51,51	0
56	MG	1A	3598	1/1	0.90	0.17	48,48,48,48	0
56	MG	2a	1607	1/1	0.90	0.36	73,73,73,73	0
56	MG	2A	3520	1/1	0.90	0.11	52,52,52,52	0
56	MG	1a	3195	1/1	0.90	0.15	45,45,45,45	0
56	MG	1A	3200	1/1	0.90	0.07	44,44,44,44	0
56	MG	1A	3961	1/1	0.90	0.08	36,36,36,36	0
56	MG	2A	3186	1/1	0.90	0.25	51,51,51,51	0
56	MG	2a	1620	1/1	0.90	0.32	64,64,64,64	0
56	MG	1A	3822	1/1	0.90	0.08	45,45,45,45	0
56	MG	2A	3531	1/1	0.90	0.07	60,60,60,60	0
56	MG	2A	3193	1/1	0.90	0.31	51,51,51,51	0
56	MG	1A	3610	1/1	0.90	0.21	45,45,45,45	0
56	MG	2a	1631	1/1	0.90	0.13	66,66,66,66	0
56	MG	2A	3199	1/1	0.90	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3001	1/1	0.90	0.19	52,52,52,52	0
56	MG	1a	3004	1/1	0.90	0.12	50,50,50,50	0
56	MG	1A	3968	1/1	0.90	0.07	55,55,55,55	0
56	MG	2A	3210	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3211	1/1	0.90	0.13	68,68,68,68	0
56	MG	1A	3825	1/1	0.90	0.24	43,43,43,43	0
56	MG	1A	3826	1/1	0.90	0.13	27,27,27,27	0
56	MG	1A	3508	1/1	0.90	0.12	26,26,26,26	0
56	MG	1A	3703	1/1	0.90	0.10	24,24,24,24	0
56	MG	2A	3558	1/1	0.90	0.19	50,50,50,50	0
56	MG	2A	3220	1/1	0.90	0.08	49,49,49,49	0
56	MG	2A	3223	1/1	0.90	0.12	45,45,45,45	0
56	MG	1A	3705	1/1	0.90	0.14	39,39,39,39	0
56	MG	1a	3031	1/1	0.90	0.22	54,54,54,54	0
56	MG	2A	3238	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3568	1/1	0.90	0.22	47,47,47,47	0
56	MG	2A	3569	1/1	0.90	0.11	63,63,63,63	0
56	MG	2a	1671	1/1	0.90	0.11	58,58,58,58	0
56	MG	2A	3240	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3234	1/1	0.90	0.19	43,43,43,43	0
56	MG	2a	1676	1/1	0.90	0.17	48,48,48,48	0
56	MG	2A	3582	1/1	0.90	0.13	44,44,44,44	0
56	MG	1w	104	1/1	0.90	0.09	36,36,36,36	0
56	MG	2A	3248	1/1	0.90	0.06	44,44,44,44	0
56	MG	2a	1682	1/1	0.90	0.12	48,48,48,48	0
56	MG	1A	3839	1/1	0.90	0.10	34,34,34,34	0
56	MG	2A	3256	1/1	0.90	0.06	46,46,46,46	0
56	MG	1A	3843	1/1	0.90	0.11	66,66,66,66	0
56	MG	2A	3599	1/1	0.90	0.12	61,61,61,61	0
56	MG	1a	3043	1/1	0.90	0.26	50,50,50,50	0
56	MG	1A	3433	1/1	0.90	0.12	50,50,50,50	0
56	MG	2A	3261	1/1	0.90	0.20	50,50,50,50	0
56	MG	2A	3263	1/1	0.90	0.11	54,54,54,54	0
56	MG	1a	3046	1/1	0.90	0.20	54,54,54,54	0
56	MG	1a	3048	1/1	0.90	0.11	43,43,43,43	0
56	MG	1A	3436	1/1	0.90	0.17	62,62,62,62	0
56	MG	1A	3852	1/1	0.90	0.12	55,55,55,55	0
56	MG	2A	3624	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3625	1/1	0.90	0.15	52,52,52,52	0
56	MG	2a	1711	1/1	0.90	0.30	67,67,67,67	0
56	MG	1A	3016	1/1	0.90	0.11	40,40,40,40	0
56	MG	1A	4016	1/1	0.90	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4021	1/1	0.90	0.08	47,47,47,47	0
56	MG	1a	3060	1/1	0.90	0.11	50,50,50,50	0
56	MG	2A	3293	1/1	0.90	0.28	46,46,46,46	0
56	MG	1A	3135	1/1	0.90	0.19	23,23,23,23	0
56	MG	1A	3860	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3727	1/1	0.90	0.11	42,42,42,42	0
56	MG	1A	4053	1/1	0.90	0.12	42,42,42,42	0
56	MG	1A	3056	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3336	1/1	0.90	0.17	58,58,58,58	0
56	MG	1A	3733	1/1	0.90	0.17	55,55,55,55	0
56	MG	2a	1745	1/1	0.90	0.20	64,64,64,64	0
56	MG	2A	3022	1/1	0.90	0.09	38,38,38,38	0
56	MG	2a	1750	1/1	0.90	0.09	60,60,60,60	0
56	MG	2a	1751	1/1	0.90	0.13	87,87,87,87	0
56	MG	2A	3662	1/1	0.90	0.18	28,28,28,28	0
56	MG	2A	3350	1/1	0.90	0.09	50,50,50,50	0
56	MG	2A	3024	1/1	0.90	0.10	50,50,50,50	0
56	MG	2A	3358	1/1	0.90	0.13	47,47,47,47	0
56	MG	2A	3031	1/1	0.90	0.19	57,57,57,57	0
56	MG	2A	3362	1/1	0.90	0.20	58,58,58,58	0
56	MG	1A	3626	1/1	0.90	0.11	23,23,23,23	0
56	MG	1A	3628	1/1	0.90	0.09	16,16,16,16	0
56	MG	2a	1771	1/1	0.90	0.25	62,62,62,62	0
56	MG	2A	3680	1/1	0.90	0.09	62,62,62,62	0
56	MG	1a	3081	1/1	0.90	0.11	67,67,67,67	0
56	MG	1A	3630	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3744	1/1	0.90	0.13	41,41,41,41	0
56	MG	2a	1778	1/1	0.90	0.21	68,68,68,68	0
56	MG	2A	3383	1/1	0.90	0.12	56,56,56,56	0
56	MG	2A	3694	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3387	1/1	0.90	0.13	50,50,50,50	0
56	MG	1a	3099	1/1	0.90	0.09	72,72,72,72	0
56	MG	1A	3382	1/1	0.90	0.09	41,41,41,41	0
56	MG	1B	226	1/1	0.90	0.10	67,67,67,67	0
56	MG	2A	3707	1/1	0.90	0.10	47,47,47,47	0
56	MG	2a	1793	1/1	0.90	0.18	53,53,53,53	0
56	MG	2a	1797	1/1	0.90	0.23	70,70,70,70	0
56	MG	1A	3542	1/1	0.90	0.15	44,44,44,44	0
56	MG	1A	3456	1/1	0.90	0.14	33,33,33,33	0
56	MG	2A	3410	1/1	0.90	0.19	61,61,61,61	0
56	MG	2A	3413	1/1	0.90	0.15	55,55,55,55	0
56	MG	1A	3650	1/1	0.90	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3722	1/1	0.90	0.18	47,47,47,47	0
56	MG	1A	3292	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3422	1/1	0.90	0.14	49,49,49,49	0
56	MG	2A	3428	1/1	0.90	0.07	43,43,43,43	0
56	MG	2A	3742	1/1	0.90	0.08	52,52,52,52	0
56	MG	1a	3123	1/1	0.90	0.08	60,60,60,60	0
56	MG	1A	3459	1/1	0.90	0.19	53,53,53,53	0
56	MG	1A	3461	1/1	0.90	0.18	55,55,55,55	0
56	MG	2B	3004	1/1	0.90	0.12	60,60,60,60	0
56	MG	1A	3386	1/1	0.90	0.06	33,33,33,33	0
56	MG	2B	3008	1/1	0.90	0.19	59,59,59,59	0
56	MG	2A	3086	1/1	0.90	0.15	62,62,62,62	0
56	MG	1A	3580	1/1	0.90	0.09	18,18,18,18	0
56	MG	1A	3789	1/1	0.90	0.14	44,44,44,44	0
56	MG	1A	3584	1/1	0.90	0.10	44,44,44,44	0
56	MG	2A	3449	1/1	0.90	0.21	63,63,63,63	0
56	MG	2A	3094	1/1	0.90	0.10	47,47,47,47	0
56	MG	2A	3095	1/1	0.90	0.08	52,52,52,52	0
56	MG	1E	312	1/1	0.90	0.14	44,44,44,44	0
56	MG	1A	3166	1/1	0.90	0.16	31,31,31,31	0
56	MG	1a	3154	1/1	0.90	0.13	59,59,59,59	0
56	MG	2D	301	1/1	0.90	0.19	54,54,54,54	0
56	MG	1A	3681	1/1	0.90	0.06	23,23,23,23	0
56	MG	2t	3001	1/1	0.90	0.20	53,53,53,53	0
56	MG	2A	3481	1/1	0.90	0.24	58,58,58,58	0
56	MG	1A	3796	1/1	0.90	0.09	33,33,33,33	0
56	MG	1O	207	1/1	0.90	0.11	54,54,54,54	0
56	MG	2w	102	1/1	0.90	0.18	78,78,78,78	0
56	MG	2A	3127	1/1	0.90	0.18	56,56,56,56	0
56	MG	2A	3489	1/1	0.90	0.20	48,48,48,48	0
56	MG	1A	3935	1/1	0.90	0.15	43,43,43,43	0
56	MG	2w	109	1/1	0.90	0.15	63,63,63,63	0
56	MG	2x	102	1/1	0.90	0.20	57,57,57,57	0
56	MG	1A	3798	1/1	0.90	0.28	45,45,45,45	0
56	MG	2A	3493	1/1	0.90	0.07	28,28,28,28	0
56	MG	2A	3139	1/1	0.90	0.14	41,41,41,41	0
56	MG	2A	3498	1/1	0.90	0.07	46,46,46,46	0
56	MG	1A	3799	1/1	0.90	0.31	29,29,29,29	0
56	MG	1A	3078	1/1	0.90	0.23	26,26,26,26	0
56	MG	1V	202	1/1	0.90	0.13	44,44,44,44	0
58	EZG	2A	3746	25/25	0.90	0.15	35,43,49,51	0
56	MG	2a	1628	1/1	0.91	0.28	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3309	1/1	0.91	0.20	52,52,52,52	0
56	MG	2A	3580	1/1	0.91	0.09	39,39,39,39	0
56	MG	2A	3078	1/1	0.91	0.18	54,54,54,54	0
56	MG	1A	3518	1/1	0.91	0.18	41,41,41,41	0
56	MG	2a	1634	1/1	0.91	0.22	59,59,59,59	0
56	MG	2A	3584	1/1	0.91	0.06	50,50,50,50	0
56	MG	2A	3319	1/1	0.91	0.25	62,62,62,62	0
56	MG	2A	3329	1/1	0.91	0.13	46,46,46,46	0
56	MG	2A	3589	1/1	0.91	0.20	45,45,45,45	0
56	MG	2A	3590	1/1	0.91	0.08	50,50,50,50	0
56	MG	1a	3156	1/1	0.91	0.09	50,50,50,50	0
56	MG	1a	3159	1/1	0.91	0.12	41,41,41,41	0
56	MG	2a	1651	1/1	0.91	0.07	60,60,60,60	0
56	MG	2a	1653	1/1	0.91	0.16	67,67,67,67	0
56	MG	1a	3002	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3339	1/1	0.91	0.18	58,58,58,58	0
56	MG	1A	4041	1/1	0.91	0.31	35,35,35,35	0
56	MG	1A	3919	1/1	0.91	0.15	42,42,42,42	0
56	MG	2A	3353	1/1	0.91	0.13	35,35,35,35	0
56	MG	1A	3609	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3750	1/1	0.91	0.09	31,31,31,31	0
56	MG	1A	3171	1/1	0.91	0.07	29,29,29,29	0
56	MG	1A	3522	1/1	0.91	0.15	30,30,30,30	0
56	MG	2A	3364	1/1	0.91	0.10	45,45,45,45	0
56	MG	2a	1672	1/1	0.91	0.18	50,50,50,50	0
56	MG	1a	3027	1/1	0.91	0.22	58,58,58,58	0
56	MG	1A	3126	1/1	0.91	0.33	21,21,21,21	0
56	MG	1A	3143	1/1	0.91	0.18	37,37,37,37	0
56	MG	2A	3103	1/1	0.91	0.09	46,46,46,46	0
56	MG	2A	3104	1/1	0.91	0.10	51,51,51,51	0
56	MG	1a	3032	1/1	0.91	0.14	54,54,54,54	0
56	MG	2A	3111	1/1	0.91	0.14	36,36,36,36	0
56	MG	1A	3619	1/1	0.91	0.12	36,36,36,36	0
56	MG	1B	222	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3126	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3406	1/1	0.91	0.17	40,40,40,40	0
56	MG	1A	3692	1/1	0.91	0.09	29,29,29,29	0
56	MG	2a	1697	1/1	0.91	0.15	64,64,64,64	0
56	MG	2A	3655	1/1	0.91	0.13	53,53,53,53	0
56	MG	1a	3042	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3943	1/1	0.91	0.10	38,38,38,38	0
56	MG	2a	1702	1/1	0.91	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3044	1/1	0.91	0.19	46,46,46,46	0
56	MG	1a	3214	1/1	0.91	0.20	58,58,58,58	0
56	MG	1b	3002	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3669	1/1	0.91	0.11	27,27,27,27	0
56	MG	1A	3392	1/1	0.91	0.07	38,38,38,38	0
56	MG	1A	3314	1/1	0.91	0.08	42,42,42,42	0
56	MG	2A	3156	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3853	1/1	0.91	0.12	38,38,38,38	0
56	MG	2A	3432	1/1	0.91	0.19	56,56,56,56	0
56	MG	1A	3855	1/1	0.91	0.12	49,49,49,49	0
56	MG	2A	3435	1/1	0.91	0.12	47,47,47,47	0
56	MG	1B	237	1/1	0.91	0.12	46,46,46,46	0
56	MG	2a	1720	1/1	0.91	0.11	66,66,66,66	0
56	MG	2A	3689	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3439	1/1	0.91	0.08	49,49,49,49	0
56	MG	2a	1729	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3204	1/1	0.91	0.08	39,39,39,39	0
56	MG	2A	3693	1/1	0.91	0.12	68,68,68,68	0
56	MG	1a	3053	1/1	0.91	0.21	56,56,56,56	0
56	MG	2A	3172	1/1	0.91	0.09	48,48,48,48	0
56	MG	1A	3399	1/1	0.91	0.05	42,42,42,42	0
56	MG	2a	1744	1/1	0.91	0.09	67,67,67,67	0
56	MG	2A	3698	1/1	0.91	0.15	58,58,58,58	0
56	MG	1a	3058	1/1	0.91	0.22	58,58,58,58	0
56	MG	2A	3187	1/1	0.91	0.14	54,54,54,54	0
56	MG	1D	309	1/1	0.91	0.10	28,28,28,28	0
56	MG	1A	3205	1/1	0.91	0.31	28,28,28,28	0
56	MG	2A	3195	1/1	0.91	0.08	50,50,50,50	0
56	MG	1A	3262	1/1	0.91	0.14	33,33,33,33	0
56	MG	2A	3716	1/1	0.91	0.08	44,44,44,44	0
56	MG	2A	3198	1/1	0.91	0.08	43,43,43,43	0
56	MG	1A	3423	1/1	0.91	0.09	38,38,38,38	0
56	MG	1A	3346	1/1	0.91	0.09	43,43,43,43	0
56	MG	1a	3067	1/1	0.91	0.20	46,46,46,46	0
56	MG	2A	3735	1/1	0.91	0.07	45,45,45,45	0
56	MG	1A	3429	1/1	0.91	0.15	29,29,29,29	0
56	MG	2A	3488	1/1	0.91	0.09	53,53,53,53	0
56	MG	2a	1774	1/1	0.91	0.26	44,44,44,44	0
56	MG	1F	309	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3750	1/1	0.91	0.18	40,40,40,40	0
56	MG	1A	3877	1/1	0.91	0.14	28,28,28,28	0
56	MG	2A	3757	1/1	0.91	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	111	1/1	0.91	0.17	64,64,64,64	0
56	MG	1A	3504	1/1	0.91	0.10	48,48,48,48	0
56	MG	1a	3076	1/1	0.91	0.18	48,48,48,48	0
56	MG	2A	3495	1/1	0.91	0.17	60,60,60,60	0
56	MG	2B	3007	1/1	0.91	0.12	56,56,56,56	0
56	MG	1O	201	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	3347	1/1	0.91	0.17	42,42,42,42	0
56	MG	2a	1794	1/1	0.91	0.29	58,58,58,58	0
56	MG	2A	3221	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3086	1/1	0.91	0.18	55,55,55,55	0
56	MG	2A	3224	1/1	0.91	0.17	54,54,54,54	0
56	MG	2a	1800	1/1	0.91	0.15	61,61,61,61	0
56	MG	2A	3510	1/1	0.91	0.08	50,50,50,50	0
56	MG	1a	3094	1/1	0.91	0.15	40,40,40,40	0
56	MG	1A	3887	1/1	0.91	0.11	16,16,16,16	0
56	MG	2A	3012	1/1	0.91	0.08	44,44,44,44	0
56	MG	1A	3990	1/1	0.91	0.08	38,38,38,38	0
56	MG	1A	3889	1/1	0.91	0.16	39,39,39,39	0
56	MG	1A	3805	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3247	1/1	0.91	0.18	63,63,63,63	0
56	MG	2A	3523	1/1	0.91	0.09	37,37,37,37	0
56	MG	2a	1814	1/1	0.91	0.26	63,63,63,63	0
56	MG	2E	305	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3525	1/1	0.91	0.19	52,52,52,52	0
56	MG	2A	3526	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3897	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3251	1/1	0.91	0.17	49,49,49,49	0
56	MG	2T	3001	1/1	0.91	0.11	52,52,52,52	0
56	MG	1X	105	1/1	0.91	0.07	44,44,44,44	0
56	MG	2U	201	1/1	0.91	0.11	49,49,49,49	0
56	MG	2A	3255	1/1	0.91	0.09	54,54,54,54	0
56	MG	2d	503	1/1	0.91	0.23	56,56,56,56	0
56	MG	1Y	502	1/1	0.91	0.08	67,67,67,67	0
56	MG	1Z	3002	1/1	0.91	0.24	46,46,46,46	0
56	MG	2A	3258	1/1	0.91	0.20	58,58,58,58	0
56	MG	1A	3437	1/1	0.91	0.12	52,52,52,52	0
56	MG	2W	202	1/1	0.91	0.14	46,46,46,46	0
56	MG	1a	3129	1/1	0.91	0.20	65,65,65,65	0
56	MG	1A	3511	1/1	0.91	0.12	20,20,20,20	0
56	MG	2A	3042	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3812	1/1	0.91	0.11	43,43,43,43	0
56	MG	2A	3549	1/1	0.91	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3268	1/1	0.91	0.14	47,47,47,47	0
56	MG	1A	3673	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	4014	1/1	0.91	0.20	33,33,33,33	0
56	MG	1A	3365	1/1	0.91	0.11	39,39,39,39	0
56	MG	2A	3052	1/1	0.91	0.08	36,36,36,36	0
56	MG	13	101	1/1	0.91	0.12	39,39,39,39	0
56	MG	2a	1614	1/1	0.91	0.18	52,52,52,52	0
56	MG	2A	3058	1/1	0.91	0.13	65,65,65,65	0
56	MG	1A	3740	1/1	0.91	0.11	46,46,46,46	0
56	MG	1A	3910	1/1	0.91	0.09	32,32,32,32	0
56	MG	2a	1618	1/1	0.91	0.09	51,51,51,51	0
56	MG	2A	3073	1/1	0.91	0.08	38,38,38,38	0
56	MG	2A	3303	1/1	0.91	0.16	35,35,35,35	0
56	MG	2A	3306	1/1	0.91	0.21	47,47,47,47	0
56	MG	16	104	1/1	0.91	0.22	38,38,38,38	0
56	MG	2a	1626	1/1	0.91	0.25	50,50,50,50	0
56	MG	1A	3969	1/1	0.92	0.08	41,41,41,41	0
56	MG	2A	3556	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3722	1/1	0.92	0.09	29,29,29,29	0
56	MG	2a	1619	1/1	0.92	0.16	53,53,53,53	0
56	MG	2A	3559	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3290	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3066	1/1	0.92	0.17	40,40,40,40	0
56	MG	1A	3074	1/1	0.92	0.12	24,24,24,24	0
56	MG	2A	3563	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3979	1/1	0.92	0.09	56,56,56,56	0
56	MG	2a	1629	1/1	0.92	0.15	73,73,73,73	0
56	MG	1A	3179	1/1	0.92	0.27	23,23,23,23	0
56	MG	1A	3407	1/1	0.92	0.14	45,45,45,45	0
56	MG	1a	3151	1/1	0.92	0.22	62,62,62,62	0
56	MG	1A	3413	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3092	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3572	1/1	0.92	0.09	66,66,66,66	0
56	MG	2a	1638	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3578	1/1	0.92	0.15	27,27,27,27	0
56	MG	2A	3311	1/1	0.92	0.15	50,50,50,50	0
56	MG	2A	3312	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3314	1/1	0.92	0.21	40,40,40,40	0
56	MG	1A	3023	1/1	0.92	0.15	43,43,43,43	0
56	MG	2A	3085	1/1	0.92	0.11	48,48,48,48	0
56	MG	1a	3158	1/1	0.92	0.10	47,47,47,47	0
56	MG	11	104	1/1	0.92	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3420	1/1	0.92	0.07	49,49,49,49	0
56	MG	2A	3089	1/1	0.92	0.10	40,40,40,40	0
56	MG	2A	3338	1/1	0.92	0.16	42,42,42,42	0
56	MG	15	107	1/1	0.92	0.12	45,45,45,45	0
56	MG	2A	3346	1/1	0.92	0.17	48,48,48,48	0
56	MG	2A	3347	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3342	1/1	0.92	0.16	21,21,21,21	0
56	MG	2A	3606	1/1	0.92	0.13	49,49,49,49	0
56	MG	1A	3025	1/1	0.92	0.28	42,42,42,42	0
56	MG	2A	3617	1/1	0.92	0.09	43,43,43,43	0
56	MG	2A	3352	1/1	0.92	0.14	50,50,50,50	0
56	MG	1a	3164	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3426	1/1	0.92	0.09	44,44,44,44	0
56	MG	2a	1675	1/1	0.92	0.10	53,53,53,53	0
56	MG	1a	3170	1/1	0.92	0.14	66,66,66,66	0
56	MG	1A	3871	1/1	0.92	0.10	59,59,59,59	0
56	MG	1A	3758	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3626	1/1	0.92	0.20	46,46,46,46	0
56	MG	2A	3627	1/1	0.92	0.22	50,50,50,50	0
56	MG	2A	3629	1/1	0.92	0.11	62,62,62,62	0
56	MG	1a	3178	1/1	0.92	0.09	54,54,54,54	0
56	MG	2A	3631	1/1	0.92	0.09	53,53,53,53	0
56	MG	1A	3106	1/1	0.92	0.24	24,24,24,24	0
56	MG	1a	3183	1/1	0.92	0.10	51,51,51,51	0
56	MG	1a	3006	1/1	0.92	0.23	59,59,59,59	0
56	MG	2A	3375	1/1	0.92	0.12	36,36,36,36	0
56	MG	1a	3015	1/1	0.92	0.08	48,48,48,48	0
56	MG	1a	3193	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3431	1/1	0.92	0.18	34,34,34,34	0
56	MG	2a	1704	1/1	0.92	0.07	52,52,52,52	0
56	MG	1A	3432	1/1	0.92	0.05	31,31,31,31	0
56	MG	1a	3196	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3394	1/1	0.92	0.11	29,29,29,29	0
56	MG	1a	3200	1/1	0.92	0.13	41,41,41,41	0
56	MG	1A	4022	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3147	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3524	1/1	0.92	0.16	20,20,20,20	0
56	MG	1A	3648	1/1	0.92	0.09	20,20,20,20	0
56	MG	1A	3525	1/1	0.92	0.08	9,9,9,9	0
56	MG	2A	3412	1/1	0.92	0.08	47,47,47,47	0
56	MG	2a	1716	1/1	0.92	0.08	43,43,43,43	0
56	MG	1a	3210	1/1	0.92	0.22	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3351	1/1	0.92	0.06	34,34,34,34	0
56	MG	2A	3675	1/1	0.92	0.29	62,62,62,62	0
56	MG	2a	1722	1/1	0.92	0.10	79,79,79,79	0
56	MG	1A	4045	1/1	0.92	0.30	39,39,39,39	0
56	MG	2A	3164	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3166	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	4047	1/1	0.92	0.18	29,29,29,29	0
56	MG	1A	3659	1/1	0.92	0.17	40,40,40,40	0
56	MG	2A	3431	1/1	0.92	0.07	24,24,24,24	0
56	MG	2A	3687	1/1	0.92	0.17	65,65,65,65	0
56	MG	1A	4058	1/1	0.92	0.18	69,69,69,69	0
56	MG	2a	1743	1/1	0.92	0.09	70,70,70,70	0
56	MG	2A	3177	1/1	0.92	0.11	36,36,36,36	0
56	MG	2A	3434	1/1	0.92	0.18	46,46,46,46	0
56	MG	2A	3180	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	4059	1/1	0.92	0.07	22,22,22,22	0
56	MG	1A	3355	1/1	0.92	0.20	30,30,30,30	0
56	MG	2A	3441	1/1	0.92	0.14	62,62,62,62	0
56	MG	1A	3670	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3188	1/1	0.92	0.14	57,57,57,57	0
56	MG	2a	1759	1/1	0.92	0.13	50,50,50,50	0
56	MG	1A	3291	1/1	0.92	0.11	38,38,38,38	0
56	MG	1t	3001	1/1	0.92	0.21	57,57,57,57	0
56	MG	2A	3448	1/1	0.92	0.08	33,33,33,33	0
56	MG	2a	1767	1/1	0.92	0.08	39,39,39,39	0
56	MG	2A	3194	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3243	1/1	0.92	0.12	25,25,25,25	0
56	MG	2A	3460	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3464	1/1	0.92	0.11	29,29,29,29	0
56	MG	2A	3465	1/1	0.92	0.20	42,42,42,42	0
56	MG	2A	3466	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	3376	1/1	0.92	0.08	31,31,31,31	0
56	MG	2A	3725	1/1	0.92	0.12	47,47,47,47	0
56	MG	2A	3470	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3548	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3913	1/1	0.92	0.15	39,39,39,39	0
56	MG	2A	3474	1/1	0.92	0.11	35,35,35,35	0
56	MG	2A	3200	1/1	0.92	0.12	50,50,50,50	0
56	MG	2a	1786	1/1	0.92	0.19	66,66,66,66	0
56	MG	2A	3478	1/1	0.92	0.26	38,38,38,38	0
56	MG	1A	3556	1/1	0.92	0.15	20,20,20,20	0
56	MG	1A	3379	1/1	0.92	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1792	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3203	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3565	1/1	0.92	0.11	26,26,26,26	0
56	MG	1w	111	1/1	0.92	0.09	69,69,69,69	0
56	MG	1A	3297	1/1	0.92	0.09	35,35,35,35	0
56	MG	1B	233	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3683	1/1	0.92	0.28	41,41,41,41	0
56	MG	1x	107	1/1	0.92	0.17	46,46,46,46	0
56	MG	2A	3492	1/1	0.92	0.12	49,49,49,49	0
56	MG	1A	3450	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	3930	1/1	0.92	0.10	33,33,33,33	0
56	MG	1A	3811	1/1	0.92	0.09	32,32,32,32	0
56	MG	1D	303	1/1	0.92	0.14	26,26,26,26	0
56	MG	1A	3933	1/1	0.92	0.18	54,54,54,54	0
56	MG	1A	3109	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	3457	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3237	1/1	0.92	0.07	43,43,43,43	0
56	MG	2A	3509	1/1	0.92	0.08	52,52,52,52	0
56	MG	2a	1816	1/1	0.92	0.09	48,48,48,48	0
56	MG	1E	305	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3513	1/1	0.92	0.12	52,52,52,52	0
56	MG	1a	3074	1/1	0.92	0.17	49,49,49,49	0
56	MG	2F	301	1/1	0.92	0.10	35,35,35,35	0
56	MG	2F	302	1/1	0.92	0.09	50,50,50,50	0
56	MG	1A	3939	1/1	0.92	0.08	44,44,44,44	0
56	MG	2A	3242	1/1	0.92	0.10	47,47,47,47	0
56	MG	2Q	3003	1/1	0.92	0.16	52,52,52,52	0
56	MG	2A	3244	1/1	0.92	0.11	47,47,47,47	0
56	MG	2R	3004	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	3581	1/1	0.92	0.10	19,19,19,19	0
56	MG	1A	3040	1/1	0.92	0.06	30,30,30,30	0
56	MG	1A	3387	1/1	0.92	0.11	37,37,37,37	0
56	MG	2l	204	1/1	0.92	0.08	43,43,43,43	0
56	MG	1F	302	1/1	0.92	0.08	30,30,30,30	0
56	MG	1A	3949	1/1	0.92	0.07	18,18,18,18	0
56	MG	1A	3391	1/1	0.92	0.06	46,46,46,46	0
56	MG	1I	3001	1/1	0.92	0.08	64,64,64,64	0
56	MG	1A	3225	1/1	0.92	0.13	40,40,40,40	0
56	MG	1A	3044	1/1	0.92	0.12	37,37,37,37	0
56	MG	1a	3106	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3597	1/1	0.92	0.07	50,50,50,50	0
56	MG	2w	101	1/1	0.92	0.34	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	20	3003	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3466	1/1	0.92	0.12	39,39,39,39	0
56	MG	25	503	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	3834	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3480	1/1	0.92	0.21	35,35,35,35	0
56	MG	1A	3841	1/1	0.92	0.11	33,33,33,33	0
56	MG	2A	3048	1/1	0.92	0.22	57,57,57,57	0
56	MG	1A	3482	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3278	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3489	1/1	0.92	0.16	30,30,30,30	0
56	MG	2A	3280	1/1	0.92	0.10	50,50,50,50	0
56	MG	2a	1612	1/1	0.92	0.33	58,58,58,58	0
56	MG	1V	203	1/1	0.92	0.10	63,63,63,63	0
58	EZG	1A	4030	25/25	0.92	0.12	19,29,40,41	0
56	MG	2A	3283	1/1	0.92	0.08	42,42,42,42	0
56	MG	2A	3497	1/1	0.93	0.23	63,63,63,63	0
56	MG	1a	3007	1/1	0.93	0.08	50,50,50,50	0
56	MG	1a	3008	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3168	1/1	0.93	0.09	43,43,43,43	0
56	MG	1q	201	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3460	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3590	1/1	0.93	0.26	36,36,36,36	0
56	MG	1a	3019	1/1	0.93	0.10	54,54,54,54	0
56	MG	23	101	1/1	0.93	0.13	54,54,54,54	0
56	MG	25	502	1/1	0.93	0.20	47,47,47,47	0
56	MG	2A	3512	1/1	0.93	0.17	55,55,55,55	0
56	MG	1A	3301	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3226	1/1	0.93	0.21	42,42,42,42	0
56	MG	1A	3251	1/1	0.93	0.30	25,25,25,25	0
56	MG	2a	1601	1/1	0.93	0.11	46,46,46,46	0
56	MG	2a	1602	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3231	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3232	1/1	0.93	0.18	54,54,54,54	0
56	MG	1a	3023	1/1	0.93	0.17	44,44,44,44	0
56	MG	2A	3234	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3235	1/1	0.93	0.06	40,40,40,40	0
56	MG	1a	3024	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3524	1/1	0.93	0.07	61,61,61,61	0
56	MG	1A	3714	1/1	0.93	0.07	26,26,26,26	0
56	MG	1A	3716	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3305	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3719	1/1	0.93	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3039	1/1	0.93	0.08	26,26,26,26	0
56	MG	1a	3033	1/1	0.93	0.11	57,57,57,57	0
56	MG	2a	1621	1/1	0.93	0.12	65,65,65,65	0
56	MG	2a	1622	1/1	0.93	0.10	39,39,39,39	0
56	MG	1A	3469	1/1	0.93	0.21	43,43,43,43	0
56	MG	1x	105	1/1	0.93	0.24	59,59,59,59	0
56	MG	2A	3249	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3250	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3868	1/1	0.93	0.09	24,24,24,24	0
56	MG	2A	3542	1/1	0.93	0.09	36,36,36,36	0
56	MG	1A	4029	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3477	1/1	0.93	0.07	32,32,32,32	0
56	MG	2A	3546	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3608	1/1	0.93	0.27	54,54,54,54	0
56	MG	1A	3388	1/1	0.93	0.10	30,30,30,30	0
56	MG	1A	3873	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3875	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	4048	1/1	0.93	0.26	31,31,31,31	0
56	MG	2a	1641	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3001	1/1	0.93	0.25	44,44,44,44	0
56	MG	2A	3262	1/1	0.93	0.05	44,44,44,44	0
56	MG	1A	4052	1/1	0.93	0.13	31,31,31,31	0
56	MG	2A	3266	1/1	0.93	0.19	54,54,54,54	0
56	MG	1A	3027	1/1	0.93	0.34	27,27,27,27	0
56	MG	2A	3007	1/1	0.93	0.08	32,32,32,32	0
56	MG	2A	3008	1/1	0.93	0.08	34,34,34,34	0
56	MG	1A	3036	1/1	0.93	0.14	26,26,26,26	0
56	MG	1A	3739	1/1	0.93	0.17	29,29,29,29	0
56	MG	1A	3396	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	4065	1/1	0.93	0.13	36,36,36,36	0
56	MG	1B	201	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3313	1/1	0.93	0.11	35,35,35,35	0
56	MG	2A	3284	1/1	0.93	0.06	37,37,37,37	0
56	MG	1A	3048	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3576	1/1	0.93	0.15	52,52,52,52	0
56	MG	2a	1670	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3286	1/1	0.93	0.06	46,46,46,46	0
56	MG	2A	3287	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3581	1/1	0.93	0.07	28,28,28,28	0
56	MG	1B	208	1/1	0.93	0.18	59,59,59,59	0
56	MG	1B	211	1/1	0.93	0.33	45,45,45,45	0
56	MG	1a	3066	1/1	0.93	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3892	1/1	0.93	0.17	33,33,33,33	0
56	MG	1B	218	1/1	0.93	0.11	40,40,40,40	0
56	MG	2A	3298	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3299	1/1	0.93	0.18	43,43,43,43	0
56	MG	2A	3300	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3747	1/1	0.93	0.07	31,31,31,31	0
56	MG	2a	1689	1/1	0.93	0.21	57,57,57,57	0
56	MG	2a	1690	1/1	0.93	0.16	57,57,57,57	0
56	MG	2A	3304	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3600	1/1	0.93	0.11	56,56,56,56	0
56	MG	1A	3896	1/1	0.93	0.14	42,42,42,42	0
56	MG	2a	1695	1/1	0.93	0.15	56,56,56,56	0
56	MG	2A	3602	1/1	0.93	0.24	62,62,62,62	0
56	MG	1A	3317	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3505	1/1	0.93	0.11	31,31,31,31	0
56	MG	1A	3900	1/1	0.93	0.09	44,44,44,44	0
56	MG	1B	229	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3615	1/1	0.93	0.09	66,66,66,66	0
56	MG	2A	3616	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3050	1/1	0.93	0.07	38,38,38,38	0
56	MG	1a	3080	1/1	0.93	0.17	46,46,46,46	0
56	MG	1B	230	1/1	0.93	0.13	42,42,42,42	0
56	MG	2A	3318	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3055	1/1	0.93	0.16	44,44,44,44	0
56	MG	2A	3322	1/1	0.93	0.07	55,55,55,55	0
56	MG	1a	3089	1/1	0.93	0.09	40,40,40,40	0
56	MG	1a	3091	1/1	0.93	0.23	46,46,46,46	0
56	MG	1A	3264	1/1	0.93	0.10	39,39,39,39	0
56	MG	2A	3069	1/1	0.93	0.05	39,39,39,39	0
56	MG	1A	3409	1/1	0.93	0.19	54,54,54,54	0
56	MG	2a	1718	1/1	0.93	0.09	55,55,55,55	0
56	MG	1a	3096	1/1	0.93	0.16	47,47,47,47	0
56	MG	2A	3343	1/1	0.93	0.15	36,36,36,36	0
56	MG	1A	3281	1/1	0.93	0.21	29,29,29,29	0
56	MG	1A	3329	1/1	0.93	0.05	41,41,41,41	0
56	MG	2a	1726	1/1	0.93	0.11	64,64,64,64	0
56	MG	1A	3766	1/1	0.93	0.11	36,36,36,36	0
56	MG	1a	3102	1/1	0.93	0.13	39,39,39,39	0
56	MG	2A	3351	1/1	0.93	0.07	43,43,43,43	0
56	MG	2a	1731	1/1	0.93	0.11	56,56,56,56	0
56	MG	1a	3104	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3769	1/1	0.93	0.14	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3332	1/1	0.93	0.07	34,34,34,34	0
56	MG	1a	3109	1/1	0.93	0.15	30,30,30,30	0
56	MG	1A	3914	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3188	1/1	0.93	0.05	12,12,12,12	0
56	MG	1A	3334	1/1	0.93	0.14	22,22,22,22	0
56	MG	2A	3659	1/1	0.93	0.14	41,41,41,41	0
56	MG	1A	3640	1/1	0.93	0.10	36,36,36,36	0
56	MG	2A	3369	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3370	1/1	0.93	0.22	44,44,44,44	0
56	MG	1A	3336	1/1	0.93	0.08	35,35,35,35	0
56	MG	1a	3124	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3784	1/1	0.93	0.12	57,57,57,57	0
56	MG	1a	3134	1/1	0.93	0.24	47,47,47,47	0
56	MG	2A	3099	1/1	0.93	0.08	38,38,38,38	0
56	MG	1A	3340	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3386	1/1	0.93	0.18	43,43,43,43	0
56	MG	1A	3926	1/1	0.93	0.10	18,18,18,18	0
56	MG	1A	3341	1/1	0.93	0.15	38,38,38,38	0
56	MG	2A	3683	1/1	0.93	0.14	42,42,42,42	0
56	MG	1A	3196	1/1	0.93	0.07	34,34,34,34	0
56	MG	2A	3685	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3396	1/1	0.93	0.10	29,29,29,29	0
56	MG	1F	303	1/1	0.93	0.08	35,35,35,35	0
56	MG	2A	3401	1/1	0.93	0.13	32,32,32,32	0
56	MG	2A	3113	1/1	0.93	0.23	48,48,48,48	0
56	MG	2a	1779	1/1	0.93	0.09	60,60,60,60	0
56	MG	2A	3115	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3116	1/1	0.93	0.16	55,55,55,55	0
56	MG	1a	3145	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3118	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3107	1/1	0.93	0.14	24,24,24,24	0
56	MG	1A	3237	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3668	1/1	0.93	0.07	22,22,22,22	0
56	MG	2A	3706	1/1	0.93	0.06	42,42,42,42	0
56	MG	2A	3417	1/1	0.93	0.15	35,35,35,35	0
56	MG	2A	3419	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3130	1/1	0.93	0.24	51,51,51,51	0
56	MG	2A	3421	1/1	0.93	0.10	39,39,39,39	0
56	MG	1A	3938	1/1	0.93	0.17	40,40,40,40	0
56	MG	1N	204	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3133	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	3528	1/1	0.93	0.13	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3349	1/1	0.93	0.08	39,39,39,39	0
56	MG	1O	206	1/1	0.93	0.08	60,60,60,60	0
56	MG	2a	1805	1/1	0.93	0.09	53,53,53,53	0
56	MG	2A	3726	1/1	0.93	0.11	43,43,43,43	0
56	MG	2A	3728	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3146	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3538	1/1	0.93	0.06	45,45,45,45	0
56	MG	2a	1811	1/1	0.93	0.10	71,71,71,71	0
56	MG	1P	203	1/1	0.93	0.28	33,33,33,33	0
56	MG	1A	3945	1/1	0.93	0.10	30,30,30,30	0
56	MG	1A	3803	1/1	0.93	0.12	41,41,41,41	0
56	MG	2A	3440	1/1	0.93	0.11	51,51,51,51	0
56	MG	2A	3755	1/1	0.93	0.39	48,48,48,48	0
56	MG	1S	3002	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3350	1/1	0.93	0.12	44,44,44,44	0
56	MG	2A	3161	1/1	0.93	0.13	46,46,46,46	0
56	MG	2a	1823	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3439	1/1	0.93	0.11	37,37,37,37	0
56	MG	2a	1827	1/1	0.93	0.16	58,58,58,58	0
56	MG	1A	3678	1/1	0.93	0.16	22,22,22,22	0
56	MG	1A	3071	1/1	0.93	0.09	31,31,31,31	0
56	MG	2a	1830	1/1	0.93	0.14	71,71,71,71	0
56	MG	1A	3158	1/1	0.93	0.07	31,31,31,31	0
56	MG	1A	3559	1/1	0.93	0.15	15,15,15,15	0
56	MG	2B	3010	1/1	0.93	0.08	64,64,64,64	0
56	MG	2A	3458	1/1	0.93	0.14	40,40,40,40	0
56	MG	1A	3562	1/1	0.93	0.07	18,18,18,18	0
56	MG	2A	3173	1/1	0.93	0.08	45,45,45,45	0
56	MG	1A	3444	1/1	0.93	0.07	18,18,18,18	0
56	MG	2l	203	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3073	1/1	0.93	0.29	42,42,42,42	0
56	MG	2q	201	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3468	1/1	0.93	0.09	40,40,40,40	0
56	MG	1a	3189	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3361	1/1	0.93	0.33	57,57,57,57	0
56	MG	1A	3967	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3293	1/1	0.93	0.29	51,51,51,51	0
56	MG	2A	3190	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	3829	1/1	0.93	0.12	43,43,43,43	0
56	MG	1l	103	1/1	0.93	0.10	31,31,31,31	0
56	MG	2E	306	1/1	0.93	0.18	43,43,43,43	0
56	MG	1a	3199	1/1	0.93	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2w	103	1/1	0.93	0.09	44,44,44,44	0
56	MG	2E	310	1/1	0.93	0.07	50,50,50,50	0
56	MG	1A	3970	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3693	1/1	0.93	0.12	40,40,40,40	0
56	MG	2F	303	1/1	0.93	0.29	55,55,55,55	0
56	MG	1A	3975	1/1	0.93	0.13	51,51,51,51	0
56	MG	1A	3366	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3574	1/1	0.93	0.10	16,16,16,16	0
56	MG	1A	3373	1/1	0.93	0.10	41,41,41,41	0
56	MG	2y	3002	1/1	0.93	0.19	51,51,51,51	0
56	MG	1A	3836	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3295	1/1	0.93	0.07	38,38,38,38	0
56	MG	2A	3206	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3989	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3702	1/1	0.93	0.05	23,23,23,23	0
56	MG	1l	202	1/1	0.93	0.08	85,85,85,85	0
59	ZN	24	501	1/1	0.93	0.08	103,103,103,103	0
56	MG	2E	301	1/1	0.94	0.08	33,33,33,33	0
56	MG	2E	302	1/1	0.94	0.12	44,44,44,44	0
56	MG	2E	303	1/1	0.94	0.05	50,50,50,50	0
56	MG	1A	3901	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3732	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3454	1/1	0.94	0.13	52,52,52,52	0
56	MG	2A	3150	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3357	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3057	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3060	1/1	0.94	0.09	26,26,26,26	0
56	MG	2A	3159	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3228	1/1	0.94	0.12	40,40,40,40	0
56	MG	2Q	3001	1/1	0.94	0.17	54,54,54,54	0
56	MG	1A	3294	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3374	1/1	0.94	0.10	40,40,40,40	0
56	MG	1E	311	1/1	0.94	0.27	36,36,36,36	0
56	MG	1a	3153	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3603	1/1	0.94	0.12	43,43,43,43	0
56	MG	1E	313	1/1	0.94	0.07	25,25,25,25	0
56	MG	2A	3171	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3745	1/1	0.94	0.09	33,33,33,33	0
56	MG	2U	205	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3746	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3175	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3482	1/1	0.94	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3112	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3378	1/1	0.94	0.14	27,27,27,27	0
56	MG	2A	3181	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3182	1/1	0.94	0.26	43,43,43,43	0
56	MG	2A	3184	1/1	0.94	0.08	52,52,52,52	0
56	MG	1G	3004	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	3467	1/1	0.94	0.22	49,49,49,49	0
56	MG	1A	3018	1/1	0.94	0.14	43,43,43,43	0
56	MG	1N	202	1/1	0.94	0.06	36,36,36,36	0
56	MG	1a	3165	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3611	1/1	0.94	0.10	45,45,45,45	0
56	MG	1N	205	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3927	1/1	0.94	0.19	37,37,37,37	0
56	MG	2A	3499	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3928	1/1	0.94	0.09	37,37,37,37	0
56	MG	2a	1605	1/1	0.94	0.18	61,61,61,61	0
56	MG	2A	3502	1/1	0.94	0.07	42,42,42,42	0
56	MG	2a	1608	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3471	1/1	0.94	0.28	45,45,45,45	0
56	MG	2a	1610	1/1	0.94	0.07	63,63,63,63	0
56	MG	1A	3474	1/1	0.94	0.18	38,38,38,38	0
56	MG	2A	3507	1/1	0.94	0.12	67,67,67,67	0
56	MG	1a	3181	1/1	0.94	0.10	41,41,41,41	0
56	MG	1a	3182	1/1	0.94	0.15	45,45,45,45	0
56	MG	1P	201	1/1	0.94	0.23	16,16,16,16	0
56	MG	1A	3381	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3767	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3204	1/1	0.94	0.05	43,43,43,43	0
56	MG	2A	3515	1/1	0.94	0.11	44,44,44,44	0
56	MG	1A	3479	1/1	0.94	0.06	30,30,30,30	0
56	MG	1R	205	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3936	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3298	1/1	0.94	0.06	40,40,40,40	0
56	MG	1A	3046	1/1	0.94	0.11	50,50,50,50	0
56	MG	1a	3197	1/1	0.94	0.06	39,39,39,39	0
56	MG	2a	1627	1/1	0.94	0.30	53,53,53,53	0
56	MG	2A	3214	1/1	0.94	0.23	49,49,49,49	0
56	MG	1A	3941	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3172	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3219	1/1	0.94	0.21	54,54,54,54	0
56	MG	1W	3003	1/1	0.94	0.11	33,33,33,33	0
56	MG	1a	3204	1/1	0.94	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3623	1/1	0.94	0.15	41,41,41,41	0
56	MG	2a	1636	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3944	1/1	0.94	0.06	39,39,39,39	0
56	MG	1A	3492	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3227	1/1	0.94	0.05	40,40,40,40	0
56	MG	2A	3535	1/1	0.94	0.12	27,27,27,27	0
56	MG	1A	3625	1/1	0.94	0.16	10,10,10,10	0
56	MG	2A	3537	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3229	1/1	0.94	0.10	34,34,34,34	0
56	MG	2A	3230	1/1	0.94	0.06	41,41,41,41	0
56	MG	2a	1646	1/1	0.94	0.22	71,71,71,71	0
56	MG	2a	1647	1/1	0.94	0.15	80,80,80,80	0
56	MG	1A	3304	1/1	0.94	0.17	41,41,41,41	0
56	MG	2a	1650	1/1	0.94	0.28	68,68,68,68	0
56	MG	1A	3494	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3791	1/1	0.94	0.13	23,23,23,23	0
56	MG	1A	3793	1/1	0.94	0.17	26,26,26,26	0
56	MG	1A	3629	1/1	0.94	0.11	60,60,60,60	0
56	MG	2a	1658	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3548	1/1	0.94	0.16	51,51,51,51	0
56	MG	2a	1660	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3238	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3239	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3239	1/1	0.94	0.22	64,64,64,64	0
56	MG	1n	502	1/1	0.94	0.30	51,51,51,51	0
56	MG	1A	3636	1/1	0.94	0.16	21,21,21,21	0
56	MG	13	102	1/1	0.94	0.18	46,46,46,46	0
56	MG	15	101	1/1	0.94	0.15	27,27,27,27	0
56	MG	2A	3245	1/1	0.94	0.10	59,59,59,59	0
56	MG	15	105	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3174	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3068	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3182	1/1	0.94	0.06	33,33,33,33	0
56	MG	2A	3564	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3646	1/1	0.94	0.14	19,19,19,19	0
56	MG	2a	1679	1/1	0.94	0.13	44,44,44,44	0
56	MG	2A	3566	1/1	0.94	0.18	56,56,56,56	0
56	MG	1w	103	1/1	0.94	0.20	68,68,68,68	0
56	MG	1A	3029	1/1	0.94	0.13	17,17,17,17	0
56	MG	1A	3192	1/1	0.94	0.13	54,54,54,54	0
56	MG	1a	3003	1/1	0.94	0.15	56,56,56,56	0
56	MG	1w	108	1/1	0.94	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3318	1/1	0.94	0.08	46,46,46,46	0
56	MG	1A	3654	1/1	0.94	0.14	37,37,37,37	0
56	MG	2A	3577	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3408	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3515	1/1	0.94	0.12	11,11,11,11	0
56	MG	1a	3009	1/1	0.94	0.14	32,32,32,32	0
56	MG	1a	3011	1/1	0.94	0.08	41,41,41,41	0
56	MG	2a	1699	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3265	1/1	0.94	0.10	46,46,46,46	0
56	MG	1x	106	1/1	0.94	0.17	66,66,66,66	0
56	MG	1a	3013	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3816	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3252	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	3984	1/1	0.94	0.10	52,52,52,52	0
56	MG	2A	3591	1/1	0.94	0.11	34,34,34,34	0
56	MG	1x	112	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3410	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3595	1/1	0.94	0.13	59,59,59,59	0
56	MG	1x	115	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3988	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3824	1/1	0.94	0.10	33,33,33,33	0
56	MG	1a	3022	1/1	0.94	0.11	48,48,48,48	0
56	MG	2a	1715	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3030	1/1	0.94	0.33	20,20,20,20	0
56	MG	1A	3322	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3993	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3609	1/1	0.94	0.26	36,36,36,36	0
56	MG	1A	3138	1/1	0.94	0.26	30,30,30,30	0
56	MG	2A	3614	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1723	1/1	0.94	0.21	57,57,57,57	0
56	MG	1A	3419	1/1	0.94	0.12	42,42,42,42	0
56	MG	2a	1725	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3009	1/1	0.94	0.12	29,29,29,29	0
56	MG	1a	3029	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	4001	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3014	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3330	1/1	0.94	0.08	28,28,28,28	0
56	MG	2A	3622	1/1	0.94	0.09	55,55,55,55	0
56	MG	2a	1737	1/1	0.94	0.07	57,57,57,57	0
56	MG	1A	4006	1/1	0.94	0.18	41,41,41,41	0
56	MG	1a	3034	1/1	0.94	0.15	44,44,44,44	0
56	MG	1A	4007	1/1	0.94	0.16	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1741	1/1	0.94	0.18	57,57,57,57	0
56	MG	1A	3331	1/1	0.94	0.07	39,39,39,39	0
56	MG	2A	3025	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3027	1/1	0.94	0.13	32,32,32,32	0
56	MG	2A	3028	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3030	1/1	0.94	0.10	25,25,25,25	0
56	MG	1A	3140	1/1	0.94	0.30	23,23,23,23	0
56	MG	2A	3633	1/1	0.94	0.12	66,66,66,66	0
56	MG	2A	3032	1/1	0.94	0.11	41,41,41,41	0
56	MG	2A	3637	1/1	0.94	0.09	53,53,53,53	0
56	MG	2a	1758	1/1	0.94	0.11	52,52,52,52	0
56	MG	1a	3041	1/1	0.94	0.15	51,51,51,51	0
56	MG	1A	3043	1/1	0.94	0.10	19,19,19,19	0
56	MG	1A	3427	1/1	0.94	0.33	29,29,29,29	0
56	MG	2A	3321	1/1	0.94	0.13	44,44,44,44	0
56	MG	2A	3643	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3644	1/1	0.94	0.23	57,57,57,57	0
56	MG	2A	3647	1/1	0.94	0.19	51,51,51,51	0
56	MG	1A	3540	1/1	0.94	0.11	46,46,46,46	0
56	MG	2A	3324	1/1	0.94	0.05	40,40,40,40	0
56	MG	2A	3328	1/1	0.94	0.23	45,45,45,45	0
56	MG	1A	3687	1/1	0.94	0.11	33,33,33,33	0
56	MG	1A	3147	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3335	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3045	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3335	1/1	0.94	0.15	33,33,33,33	0
56	MG	1A	3547	1/1	0.94	0.07	22,22,22,22	0
56	MG	1A	4035	1/1	0.94	0.05	38,38,38,38	0
56	MG	1A	4036	1/1	0.94	0.19	29,29,29,29	0
56	MG	2A	3667	1/1	0.94	0.08	63,63,63,63	0
56	MG	2A	3668	1/1	0.94	0.17	41,41,41,41	0
56	MG	2A	3345	1/1	0.94	0.13	63,63,63,63	0
56	MG	1A	3269	1/1	0.94	0.20	35,35,35,35	0
56	MG	1A	3694	1/1	0.94	0.24	51,51,51,51	0
56	MG	2A	3673	1/1	0.94	0.17	47,47,47,47	0
56	MG	2A	3053	1/1	0.94	0.07	30,30,30,30	0
56	MG	1A	3854	1/1	0.94	0.12	46,46,46,46	0
56	MG	2a	1795	1/1	0.94	0.09	64,64,64,64	0
56	MG	1A	3549	1/1	0.94	0.09	30,30,30,30	0
56	MG	1A	4046	1/1	0.94	0.22	20,20,20,20	0
56	MG	2A	3063	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3857	1/1	0.94	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3551	1/1	0.94	0.13	17,17,17,17	0
56	MG	2A	3359	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3339	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3070	1/1	0.94	0.10	33,33,33,33	0
56	MG	1A	3699	1/1	0.94	0.05	25,25,25,25	0
56	MG	1A	4055	1/1	0.94	0.25	31,31,31,31	0
56	MG	1a	3068	1/1	0.94	0.22	62,62,62,62	0
56	MG	2A	3076	1/1	0.94	0.16	45,45,45,45	0
56	MG	2A	3372	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	4056	1/1	0.94	0.15	33,33,33,33	0
56	MG	1A	3558	1/1	0.94	0.09	16,16,16,16	0
56	MG	1A	3862	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3273	1/1	0.94	0.05	38,38,38,38	0
56	MG	2A	3377	1/1	0.94	0.17	37,37,37,37	0
56	MG	1A	3276	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	4066	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3704	1/1	0.94	0.14	28,28,28,28	0
56	MG	1A	3277	1/1	0.94	0.08	37,37,37,37	0
56	MG	2A	3389	1/1	0.94	0.07	35,35,35,35	0
56	MG	2a	1825	1/1	0.94	0.18	56,56,56,56	0
56	MG	1A	3280	1/1	0.94	0.17	26,26,26,26	0
56	MG	1B	205	1/1	0.94	0.21	45,45,45,45	0
56	MG	1a	3090	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3397	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3207	1/1	0.94	0.23	52,52,52,52	0
56	MG	1B	210	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3096	1/1	0.94	0.06	42,42,42,42	0
56	MG	2e	3001	1/1	0.94	0.10	60,60,60,60	0
56	MG	1a	3093	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3708	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3876	1/1	0.94	0.07	34,34,34,34	0
56	MG	2A	3100	1/1	0.94	0.12	59,59,59,59	0
56	MG	1B	217	1/1	0.94	0.10	44,44,44,44	0
56	MG	2A	3748	1/1	0.94	0.06	27,27,27,27	0
56	MG	2A	3749	1/1	0.94	0.17	34,34,34,34	0
56	MG	1A	3105	1/1	0.94	0.10	30,30,30,30	0
56	MG	1A	3878	1/1	0.94	0.09	16,16,16,16	0
56	MG	2A	3105	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	3879	1/1	0.94	0.11	18,18,18,18	0
56	MG	2B	3001	1/1	0.94	0.12	75,75,75,75	0
56	MG	2A	3109	1/1	0.94	0.20	39,39,39,39	0
56	MG	1a	3103	1/1	0.94	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3157	1/1	0.94	0.13	50,50,50,50	0
56	MG	1B	223	1/1	0.94	0.06	51,51,51,51	0
56	MG	1A	3715	1/1	0.94	0.06	23,23,23,23	0
56	MG	1A	3222	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3717	1/1	0.94	0.10	45,45,45,45	0
56	MG	1a	3112	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3124	1/1	0.94	0.10	48,48,48,48	0
56	MG	2w	108	1/1	0.94	0.06	68,68,68,68	0
56	MG	1A	3448	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3223	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3893	1/1	0.94	0.17	27,27,27,27	0
56	MG	2A	3437	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3583	1/1	0.94	0.15	22,22,22,22	0
56	MG	1A	3455	1/1	0.94	0.27	28,28,28,28	0
56	MG	1A	3725	1/1	0.94	0.12	30,30,30,30	0
56	MG	1a	3130	1/1	0.94	0.16	46,46,46,46	0
56	MG	2B	3021	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3075	1/1	0.94	0.12	34,34,34,34	0
56	MG	1a	3135	1/1	0.94	0.08	52,52,52,52	0
56	MG	2D	305	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	3588	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	3600	1/1	0.95	0.14	50,50,50,50	0
56	MG	2W	203	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3013	1/1	0.95	0.04	27,27,27,27	0
56	MG	1A	3602	1/1	0.95	0.15	48,48,48,48	0
56	MG	1B	209	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3246	1/1	0.95	0.15	37,37,37,37	0
56	MG	1a	3062	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3472	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3385	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3476	1/1	0.95	0.13	27,27,27,27	0
56	MG	1A	3247	1/1	0.95	0.10	27,27,27,27	0
56	MG	28	101	1/1	0.95	0.17	49,49,49,49	0
56	MG	1A	3190	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3902	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3903	1/1	0.95	0.05	23,23,23,23	0
56	MG	1A	3613	1/1	0.95	0.07	30,30,30,30	0
56	MG	1B	224	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3137	1/1	0.95	0.12	40,40,40,40	0
56	MG	2a	1606	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3390	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3269	1/1	0.95	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3543	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3270	1/1	0.95	0.15	34,34,34,34	0
56	MG	2A	3271	1/1	0.95	0.09	45,45,45,45	0
56	MG	1B	228	1/1	0.95	0.04	24,24,24,24	0
56	MG	2A	3275	1/1	0.95	0.05	37,37,37,37	0
56	MG	2A	3276	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	3748	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3749	1/1	0.95	0.18	31,31,31,31	0
56	MG	1a	3084	1/1	0.95	0.11	54,54,54,54	0
56	MG	1a	3086	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3485	1/1	0.95	0.08	21,21,21,21	0
56	MG	1A	3911	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3487	1/1	0.95	0.10	34,34,34,34	0
56	MG	1A	3756	1/1	0.95	0.15	27,27,27,27	0
56	MG	2A	3051	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3052	1/1	0.95	0.05	31,31,31,31	0
56	MG	1A	3491	1/1	0.95	0.14	17,17,17,17	0
56	MG	1a	3095	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3315	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3292	1/1	0.95	0.12	31,31,31,31	0
56	MG	1A	3921	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3294	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3062	1/1	0.95	0.26	47,47,47,47	0
56	MG	2A	3297	1/1	0.95	0.22	51,51,51,51	0
56	MG	1A	3198	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3064	1/1	0.95	0.12	44,44,44,44	0
56	MG	1D	307	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3573	1/1	0.95	0.08	37,37,37,37	0
56	MG	2a	1639	1/1	0.95	0.06	60,60,60,60	0
56	MG	1A	3762	1/1	0.95	0.06	12,12,12,12	0
56	MG	1A	3765	1/1	0.95	0.11	19,19,19,19	0
56	MG	1E	301	1/1	0.95	0.18	26,26,26,26	0
56	MG	2A	3307	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3925	1/1	0.95	0.08	12,12,12,12	0
56	MG	1A	3104	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3074	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3319	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3141	1/1	0.95	0.11	38,38,38,38	0
56	MG	2a	1649	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3773	1/1	0.95	0.07	15,15,15,15	0
56	MG	2A	3588	1/1	0.95	0.10	52,52,52,52	0
56	MG	2a	1652	1/1	0.95	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
56	MG	2A	3315	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3503	1/1	0.95	0.12	22,22,22,22	0
56	MG	1A	3053	1/1	0.95	0.11	43,43,43,43	0
56	MG	1a	3120	1/1	0.95	0.12	43,43,43,43	0
56	MG	1F	301	1/1	0.95	0.26	23,23,23,23	0
56	MG	2A	3594	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3144	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3597	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3598	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3326	1/1	0.95	0.12	25,25,25,25	0
56	MG	2A	3325	1/1	0.95	0.11	63,63,63,63	0
56	MG	1a	3125	1/1	0.95	0.20	42,42,42,42	0
56	MG	1a	3126	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3332	1/1	0.95	0.21	56,56,56,56	0
56	MG	2A	3333	1/1	0.95	0.10	25,25,25,25	0
56	MG	1a	3127	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3607	1/1	0.95	0.07	48,48,48,48	0
56	MG	2A	3608	1/1	0.95	0.13	48,48,48,48	0
56	MG	1F	305	1/1	0.95	0.18	28,28,28,28	0
56	MG	2a	1677	1/1	0.95	0.15	55,55,55,55	0
56	MG	1F	306	1/1	0.95	0.07	36,36,36,36	0
56	MG	1F	307	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3507	1/1	0.95	0.13	24,24,24,24	0
56	MG	1A	3637	1/1	0.95	0.07	20,20,20,20	0
56	MG	1a	3139	1/1	0.95	0.18	56,56,56,56	0
56	MG	1A	3785	1/1	0.95	0.10	35,35,35,35	0
56	MG	2a	1687	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3940	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3265	1/1	0.95	0.07	26,26,26,26	0
56	MG	1A	3509	1/1	0.95	0.12	31,31,31,31	0
56	MG	2A	3349	1/1	0.95	0.10	30,30,30,30	0
56	MG	1A	3412	1/1	0.95	0.18	37,37,37,37	0
56	MG	1A	3062	1/1	0.95	0.08	12,12,12,12	0
56	MG	2a	1694	1/1	0.95	0.09	66,66,66,66	0
56	MG	2A	3106	1/1	0.95	0.15	50,50,50,50	0
56	MG	2a	1696	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3006	1/1	0.95	0.08	33,33,33,33	0
56	MG	2A	3628	1/1	0.95	0.10	40,40,40,40	0
56	MG	1O	202	1/1	0.95	0.06	56,56,56,56	0
56	MG	1a	3150	1/1	0.95	0.16	65,65,65,65	0
56	MG	2A	3112	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3649	1/1	0.95	0.09	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3274	1/1	0.95	0.16	40,40,40,40	0
56	MG	2A	3635	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3950	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3418	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3047	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3955	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3656	1/1	0.95	0.15	25,25,25,25	0
56	MG	2A	3641	1/1	0.95	0.16	50,50,50,50	0
56	MG	2A	3125	1/1	0.95	0.24	32,32,32,32	0
56	MG	1A	3221	1/1	0.95	0.10	21,21,21,21	0
56	MG	1S	3001	1/1	0.95	0.08	47,47,47,47	0
56	MG	2A	3128	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3662	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3804	1/1	0.95	0.12	45,45,45,45	0
56	MG	2A	3652	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3279	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3384	1/1	0.95	0.10	27,27,27,27	0
56	MG	1U	203	1/1	0.95	0.12	23,23,23,23	0
56	MG	2A	3136	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3657	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3963	1/1	0.95	0.05	33,33,33,33	0
56	MG	1A	3424	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3069	1/1	0.95	0.09	27,27,27,27	0
56	MG	2A	3145	1/1	0.95	0.14	48,48,48,48	0
56	MG	1X	102	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	3966	1/1	0.95	0.09	41,41,41,41	0
56	MG	2a	1733	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3810	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3671	1/1	0.95	0.06	14,14,14,14	0
56	MG	2A	3403	1/1	0.95	0.12	29,29,29,29	0
56	MG	2A	3405	1/1	0.95	0.11	35,35,35,35	0
56	MG	1A	3337	1/1	0.95	0.31	27,27,27,27	0
56	MG	1A	3162	1/1	0.95	0.07	24,24,24,24	0
56	MG	1A	3113	1/1	0.95	0.22	27,27,27,27	0
56	MG	1A	3972	1/1	0.95	0.06	49,49,49,49	0
56	MG	2A	3411	1/1	0.95	0.12	27,27,27,27	0
56	MG	2a	1747	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3819	1/1	0.95	0.11	29,29,29,29	0
56	MG	1a	3191	1/1	0.95	0.08	53,53,53,53	0
56	MG	1a	3192	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3415	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3283	1/1	0.95	0.20	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3418	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3677	1/1	0.95	0.10	18,18,18,18	0
56	MG	1A	3537	1/1	0.95	0.08	30,30,30,30	0
56	MG	2a	1760	1/1	0.95	0.28	60,60,60,60	0
56	MG	1A	3070	1/1	0.95	0.15	23,23,23,23	0
56	MG	1A	3026	1/1	0.95	0.11	30,30,30,30	0
56	MG	2a	1764	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3426	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3427	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3985	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3434	1/1	0.95	0.20	47,47,47,47	0
56	MG	2A	3700	1/1	0.95	0.10	61,61,61,61	0
56	MG	1a	3202	1/1	0.95	0.12	45,45,45,45	0
56	MG	2A	3702	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3703	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3286	1/1	0.95	0.15	34,34,34,34	0
56	MG	2A	3178	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3058	1/1	0.95	0.11	33,33,33,33	0
56	MG	1A	3229	1/1	0.95	0.10	28,28,28,28	0
56	MG	1A	3440	1/1	0.95	0.10	28,28,28,28	0
56	MG	2A	3713	1/1	0.95	0.14	26,26,26,26	0
56	MG	18	101	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3715	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3550	1/1	0.95	0.15	26,26,26,26	0
56	MG	2A	3438	1/1	0.95	0.09	36,36,36,36	0
56	MG	1a	3211	1/1	0.95	0.13	35,35,35,35	0
56	MG	2a	1790	1/1	0.95	0.23	50,50,50,50	0
56	MG	2A	3721	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3128	1/1	0.95	0.15	27,27,27,27	0
56	MG	1A	3837	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3998	1/1	0.95	0.08	55,55,55,55	0
56	MG	1a	3005	1/1	0.95	0.08	41,41,41,41	0
56	MG	2a	1796	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3444	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3731	1/1	0.95	0.06	37,37,37,37	0
56	MG	2A	3733	1/1	0.95	0.24	30,30,30,30	0
56	MG	1l	201	1/1	0.95	0.17	31,31,31,31	0
56	MG	1A	3352	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3354	1/1	0.95	0.08	39,39,39,39	0
56	MG	2a	1803	1/1	0.95	0.35	51,51,51,51	0
56	MG	1A	3129	1/1	0.95	0.13	27,27,27,27	0
56	MG	2A	3744	1/1	0.95	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3451	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3560	1/1	0.95	0.14	26,26,26,26	0
56	MG	1A	3845	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3752	1/1	0.95	0.10	61,61,61,61	0
56	MG	1a	3012	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3130	1/1	0.95	0.15	10,10,10,10	0
56	MG	1a	3014	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3850	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3236	1/1	0.95	0.16	35,35,35,35	0
56	MG	2A	3205	1/1	0.95	0.16	55,55,55,55	0
56	MG	2a	1818	1/1	0.95	0.06	48,48,48,48	0
56	MG	2a	1819	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3449	1/1	0.95	0.07	52,52,52,52	0
56	MG	2A	3207	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3097	1/1	0.95	0.04	24,24,24,24	0
56	MG	1A	3451	1/1	0.95	0.11	24,24,24,24	0
56	MG	1A	3454	1/1	0.95	0.14	30,30,30,30	0
56	MG	2A	3475	1/1	0.95	0.12	37,37,37,37	0
56	MG	2a	1826	1/1	0.95	0.08	55,55,55,55	0
56	MG	2A	3476	1/1	0.95	0.19	44,44,44,44	0
56	MG	1w	105	1/1	0.95	0.10	64,64,64,64	0
56	MG	1A	3362	1/1	0.95	0.12	33,33,33,33	0
56	MG	1A	4033	1/1	0.95	0.28	25,25,25,25	0
56	MG	1A	3575	1/1	0.95	0.08	11,11,11,11	0
56	MG	2a	1832	1/1	0.95	0.10	37,37,37,37	0
56	MG	2A	3216	1/1	0.95	0.18	51,51,51,51	0
56	MG	1A	3180	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3218	1/1	0.95	0.06	39,39,39,39	0
56	MG	1A	3101	1/1	0.95	0.16	28,28,28,28	0
56	MG	2A	3487	1/1	0.95	0.11	62,62,62,62	0
56	MG	1A	4039	1/1	0.95	0.14	33,33,33,33	0
56	MG	2l	201	1/1	0.95	0.05	51,51,51,51	0
56	MG	2D	302	1/1	0.95	0.08	39,39,39,39	0
56	MG	2D	303	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3710	1/1	0.95	0.10	28,28,28,28	0
56	MG	1A	3711	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3867	1/1	0.95	0.09	19,19,19,19	0
56	MG	2A	3225	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3712	1/1	0.95	0.11	34,34,34,34	0
56	MG	2r	3001	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3367	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3369	1/1	0.95	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
56	MG	2v	3001	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	3299	1/1	0.95	0.18	28,28,28,28	0
56	MG	1x	110	1/1	0.95	0.20	59,59,59,59	0
56	MG	1A	3300	1/1	0.95	0.16	29,29,29,29	0
56	MG	2A	3500	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3183	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3464	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3186	1/1	0.95	0.08	27,27,27,27	0
56	MG	1y	101	1/1	0.95	0.05	35,35,35,35	0
56	MG	2O	8001	1/1	0.95	0.13	56,56,56,56	0
56	MG	2w	107	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3236	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3720	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3595	1/1	0.95	0.17	40,40,40,40	0
56	MG	2R	3002	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	4061	1/1	0.95	0.14	38,38,38,38	0
56	MG	2A	3511	1/1	0.95	0.09	39,39,39,39	0
56	MG	1a	3047	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4063	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3303	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3006	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3136	1/1	0.95	0.05	21,21,21,21	0
57	K	1A	4028	1/1	0.95	0.05	40,40,40,40	0
56	MG	1A	3244	1/1	0.95	0.06	34,34,34,34	0
56	MG	1A	3728	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3599	1/1	0.95	0.05	15,15,15,15	0
56	MG	1A	3546	1/1	0.96	0.06	14,14,14,14	0
56	MG	1A	4017	1/1	0.96	0.13	37,37,37,37	0
56	MG	2X	3001	1/1	0.96	0.05	46,46,46,46	0
56	MG	2X	3002	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3435	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3846	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	4025	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	4026	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3847	1/1	0.96	0.11	18,18,18,18	0
56	MG	1x	113	1/1	0.96	0.13	58,58,58,58	0
56	MG	1A	3054	1/1	0.96	0.06	26,26,26,26	0
56	MG	1A	4032	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3072	1/1	0.96	0.12	27,27,27,27	0
56	MG	27	102	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	4034	1/1	0.96	0.31	28,28,28,28	0
56	MG	1A	3145	1/1	0.96	0.32	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3035	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3252	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3216	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3696	1/1	0.96	0.17	46,46,46,46	0
56	MG	1A	3555	1/1	0.96	0.12	29,29,29,29	0
56	MG	2A	3004	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3217	1/1	0.96	0.15	19,19,19,19	0
56	MG	1A	3004	1/1	0.96	0.16	21,21,21,21	0
56	MG	1A	3151	1/1	0.96	0.14	36,36,36,36	0
56	MG	1A	3041	1/1	0.96	0.20	32,32,32,32	0
56	MG	1A	3224	1/1	0.96	0.18	42,42,42,42	0
56	MG	1A	3155	1/1	0.96	0.08	29,29,29,29	0
56	MG	1A	4049	1/1	0.96	0.35	30,30,30,30	0
56	MG	1A	4051	1/1	0.96	0.09	13,13,13,13	0
56	MG	2A	3015	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3359	1/1	0.96	0.05	32,32,32,32	0
56	MG	1A	3864	1/1	0.96	0.12	20,20,20,20	0
56	MG	2A	3019	1/1	0.96	0.22	50,50,50,50	0
56	MG	1A	3290	1/1	0.96	0.22	46,46,46,46	0
56	MG	1A	3005	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	3054	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3453	1/1	0.96	0.21	41,41,41,41	0
56	MG	1a	3057	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	3571	1/1	0.96	0.09	17,17,17,17	0
56	MG	1A	3028	1/1	0.96	0.21	20,20,20,20	0
56	MG	1A	3110	1/1	0.96	0.06	27,27,27,27	0
56	MG	1A	3874	1/1	0.96	0.14	36,36,36,36	0
56	MG	2A	3282	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	4064	1/1	0.96	0.08	30,30,30,30	0
56	MG	2A	3034	1/1	0.96	0.07	56,56,56,56	0
56	MG	2A	3035	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3577	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3037	1/1	0.96	0.06	61,61,61,61	0
56	MG	2A	3039	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3578	1/1	0.96	0.08	23,23,23,23	0
56	MG	1A	3579	1/1	0.96	0.12	31,31,31,31	0
56	MG	2A	3579	1/1	0.96	0.05	51,51,51,51	0
56	MG	1A	3163	1/1	0.96	0.04	24,24,24,24	0
56	MG	1A	3368	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3880	1/1	0.96	0.19	23,23,23,23	0
56	MG	2A	3295	1/1	0.96	0.17	43,43,43,43	0
56	MG	1A	3582	1/1	0.96	0.08	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3111	1/1	0.96	0.10	30,30,30,30	0
56	MG	1A	3370	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3885	1/1	0.96	0.05	16,16,16,16	0
56	MG	1B	212	1/1	0.96	0.12	46,46,46,46	0
56	MG	2A	3301	1/1	0.96	0.05	40,40,40,40	0
56	MG	2A	3302	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3372	1/1	0.96	0.11	35,35,35,35	0
56	MG	1B	214	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3296	1/1	0.96	0.13	37,37,37,37	0
56	MG	2a	1654	1/1	0.96	0.14	58,58,58,58	0
56	MG	1a	3083	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3890	1/1	0.96	0.10	36,36,36,36	0
56	MG	2a	1657	1/1	0.96	0.08	36,36,36,36	0
56	MG	1a	3085	1/1	0.96	0.15	33,33,33,33	0
56	MG	2A	3060	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3724	1/1	0.96	0.05	44,44,44,44	0
56	MG	1a	3087	1/1	0.96	0.07	44,44,44,44	0
56	MG	1a	3088	1/1	0.96	0.25	57,57,57,57	0
56	MG	2A	3603	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3462	1/1	0.96	0.13	22,22,22,22	0
56	MG	1A	3591	1/1	0.96	0.09	30,30,30,30	0
56	MG	2A	3067	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3167	1/1	0.96	0.15	47,47,47,47	0
56	MG	1A	3079	1/1	0.96	0.16	32,32,32,32	0
56	MG	1A	3377	1/1	0.96	0.16	40,40,40,40	0
56	MG	2A	3610	1/1	0.96	0.05	47,47,47,47	0
56	MG	2A	3612	1/1	0.96	0.14	65,65,65,65	0
56	MG	1A	3235	1/1	0.96	0.04	22,22,22,22	0
56	MG	1A	3734	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3080	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3736	1/1	0.96	0.19	16,16,16,16	0
56	MG	2A	3330	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3331	1/1	0.96	0.06	47,47,47,47	0
56	MG	1a	3098	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3380	1/1	0.96	0.12	33,33,33,33	0
56	MG	2A	3080	1/1	0.96	0.07	28,28,28,28	0
56	MG	2a	1685	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3059	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3118	1/1	0.96	0.05	29,29,29,29	0
56	MG	1A	3119	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3084	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3743	1/1	0.96	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3240	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3045	1/1	0.96	0.12	13,13,13,13	0
56	MG	1D	302	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3912	1/1	0.96	0.08	25,25,25,25	0
56	MG	2A	3090	1/1	0.96	0.17	32,32,32,32	0
56	MG	2A	3092	1/1	0.96	0.10	38,38,38,38	0
56	MG	1a	3111	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3177	1/1	0.96	0.06	34,34,34,34	0
56	MG	1a	3113	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3124	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3084	1/1	0.96	0.07	35,35,35,35	0
56	MG	2a	1703	1/1	0.96	0.13	41,41,41,41	0
56	MG	1D	311	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3918	1/1	0.96	0.07	33,33,33,33	0
56	MG	1D	314	1/1	0.96	0.08	29,29,29,29	0
56	MG	2A	3101	1/1	0.96	0.04	30,30,30,30	0
56	MG	1A	3483	1/1	0.96	0.20	32,32,32,32	0
56	MG	2A	3645	1/1	0.96	0.06	33,33,33,33	0
56	MG	2A	3646	1/1	0.96	0.08	59,59,59,59	0
56	MG	1A	3484	1/1	0.96	0.12	22,22,22,22	0
56	MG	1E	306	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3309	1/1	0.96	0.05	32,32,32,32	0
56	MG	2A	3651	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3371	1/1	0.96	0.11	22,22,22,22	0
56	MG	1A	3755	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3107	1/1	0.96	0.12	27,27,27,27	0
56	MG	1A	3245	1/1	0.96	0.21	28,28,28,28	0
56	MG	1a	3133	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3181	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3001	1/1	0.96	0.10	32,32,32,32	0
56	MG	1a	3136	1/1	0.96	0.11	49,49,49,49	0
56	MG	2A	3661	1/1	0.96	0.26	36,36,36,36	0
56	MG	1A	3009	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	3089	1/1	0.96	0.09	21,21,21,21	0
56	MG	2A	3385	1/1	0.96	0.08	27,27,27,27	0
56	MG	2A	3666	1/1	0.96	0.08	46,46,46,46	0
56	MG	1a	3140	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3400	1/1	0.96	0.07	33,33,33,33	0
56	MG	2a	1732	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3929	1/1	0.96	0.35	35,35,35,35	0
56	MG	2a	1735	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3123	1/1	0.96	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3402	1/1	0.96	0.12	28,28,28,28	0
56	MG	1A	3403	1/1	0.96	0.06	33,33,33,33	0
56	MG	2A	3674	1/1	0.96	0.13	23,23,23,23	0
56	MG	1A	3497	1/1	0.96	0.05	23,23,23,23	0
56	MG	2A	3398	1/1	0.96	0.12	26,26,26,26	0
56	MG	2A	3399	1/1	0.96	0.06	57,57,57,57	0
56	MG	1A	3498	1/1	0.96	0.10	39,39,39,39	0
56	MG	1G	3001	1/1	0.96	0.10	29,29,29,29	0
56	MG	2A	3681	1/1	0.96	0.16	49,49,49,49	0
56	MG	2A	3129	1/1	0.96	0.24	54,54,54,54	0
56	MG	1G	3002	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3771	1/1	0.96	0.09	17,17,17,17	0
56	MG	1A	3772	1/1	0.96	0.15	22,22,22,22	0
56	MG	2A	3686	1/1	0.96	0.12	40,40,40,40	0
56	MG	2a	1756	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3937	1/1	0.96	0.05	40,40,40,40	0
56	MG	2A	3134	1/1	0.96	0.12	51,51,51,51	0
56	MG	2A	3135	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3691	1/1	0.96	0.06	68,68,68,68	0
56	MG	1A	3627	1/1	0.96	0.07	26,26,26,26	0
56	MG	2A	3137	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3405	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3406	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3777	1/1	0.96	0.06	36,36,36,36	0
56	MG	2a	1768	1/1	0.96	0.06	55,55,55,55	0
56	MG	2A	3416	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3142	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3187	1/1	0.96	0.06	28,28,28,28	0
56	MG	1A	3253	1/1	0.96	0.38	24,24,24,24	0
56	MG	1A	3632	1/1	0.96	0.23	27,27,27,27	0
56	MG	1A	3255	1/1	0.96	0.05	36,36,36,36	0
56	MG	1A	3946	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3151	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3152	1/1	0.96	0.13	45,45,45,45	0
56	MG	2A	3153	1/1	0.96	0.16	49,49,49,49	0
56	MG	2A	3712	1/1	0.96	0.10	35,35,35,35	0
56	MG	2a	1782	1/1	0.96	0.14	58,58,58,58	0
56	MG	1A	3256	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3324	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3157	1/1	0.96	0.22	51,51,51,51	0
56	MG	1a	3166	1/1	0.96	0.07	49,49,49,49	0
56	MG	2a	1787	1/1	0.96	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3718	1/1	0.96	0.05	56,56,56,56	0
56	MG	1Q	201	1/1	0.96	0.24	33,33,33,33	0
56	MG	1Q	202	1/1	0.96	0.12	28,28,28,28	0
56	MG	1a	3171	1/1	0.96	0.09	55,55,55,55	0
56	MG	2A	3162	1/1	0.96	0.14	54,54,54,54	0
56	MG	1Q	203	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3724	1/1	0.96	0.11	66,66,66,66	0
56	MG	1A	3639	1/1	0.96	0.05	39,39,39,39	0
56	MG	2A	3165	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3727	1/1	0.96	0.14	49,49,49,49	0
56	MG	1R	202	1/1	0.96	0.10	30,30,30,30	0
56	MG	2A	3730	1/1	0.96	0.19	32,32,32,32	0
56	MG	1A	3325	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	3641	1/1	0.96	0.09	13,13,13,13	0
56	MG	2A	3734	1/1	0.96	0.10	25,25,25,25	0
56	MG	1A	3953	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3642	1/1	0.96	0.08	34,34,34,34	0
56	MG	1a	3184	1/1	0.96	0.05	49,49,49,49	0
56	MG	1A	3643	1/1	0.96	0.25	29,29,29,29	0
56	MG	1a	3188	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3747	1/1	0.96	0.07	35,35,35,35	0
56	MG	2a	1809	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3957	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3450	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3179	1/1	0.96	0.19	45,45,45,45	0
56	MG	2A	3452	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3133	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3415	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3090	1/1	0.96	0.20	18,18,18,18	0
56	MG	2A	3459	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3516	1/1	0.96	0.08	30,30,30,30	0
56	MG	2A	3462	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3962	1/1	0.96	0.07	23,23,23,23	0
56	MG	2B	3005	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3031	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3651	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	3519	1/1	0.96	0.15	21,21,21,21	0
56	MG	2A	3189	1/1	0.96	0.10	38,38,38,38	0
56	MG	1a	3198	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3049	1/1	0.96	0.07	21,21,21,21	0
56	MG	1A	3096	1/1	0.96	0.06	26,26,26,26	0
56	MG	1A	3807	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
56	MG	1A	3658	1/1	0.96	0.05	46,46,46,46	0
56	MG	1A	3422	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3199	1/1	0.96	0.17	32,32,32,32	0
56	MG	2d	502	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3663	1/1	0.96	0.13	43,43,43,43	0
56	MG	1a	3208	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3813	1/1	0.96	0.13	29,29,29,29	0
56	MG	1l	105	1/1	0.96	0.08	32,32,32,32	0
56	MG	12	3001	1/1	0.96	0.11	44,44,44,44	0
56	MG	1A	3665	1/1	0.96	0.05	12,12,12,12	0
56	MG	1A	3024	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3817	1/1	0.96	0.12	20,20,20,20	0
56	MG	15	102	1/1	0.96	0.07	22,22,22,22	0
56	MG	2D	306	1/1	0.96	0.24	43,43,43,43	0
56	MG	1A	3667	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3982	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	3270	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3271	1/1	0.96	0.19	53,53,53,53	0
56	MG	2E	304	1/1	0.96	0.05	49,49,49,49	0
56	MG	1A	3272	1/1	0.96	0.04	34,34,34,34	0
56	MG	1n	503	1/1	0.96	0.10	38,38,38,38	0
56	MG	17	102	1/1	0.96	0.17	31,31,31,31	0
56	MG	2E	308	1/1	0.96	0.09	49,49,49,49	0
56	MG	2E	309	1/1	0.96	0.08	41,41,41,41	0
56	MG	2v	3005	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3530	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3532	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3827	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3533	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3992	1/1	0.96	0.11	49,49,49,49	0
56	MG	1A	3428	1/1	0.96	0.10	26,26,26,26	0
56	MG	2A	3222	1/1	0.96	0.24	44,44,44,44	0
56	MG	1A	3830	1/1	0.96	0.20	39,39,39,39	0
56	MG	2Q	3002	1/1	0.96	0.06	41,41,41,41	0
56	MG	2x	101	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3535	1/1	0.96	0.06	23,23,23,23	0
56	MG	1A	3010	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3203	1/1	0.96	0.05	27,27,27,27	0
56	MG	2x	105	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	4002	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3539	1/1	0.96	0.07	20,20,20,20	0
56	MG	1A	3102	1/1	0.96	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3142	1/1	0.96	0.06	17,17,17,17	0
56	MG	1A	4008	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	3543	1/1	0.96	0.06	20,20,20,20	0
56	MG	1x	102	1/1	0.96	0.18	49,49,49,49	0
57	K	2A	3745	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3840	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3345	1/1	0.96	0.07	24,24,24,24	0
56	MG	1A	3688	1/1	0.96	0.14	21,21,21,21	0
56	MG	12	3002	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3215	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3098	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	4043	1/1	0.97	0.23	23,23,23,23	0
56	MG	1a	3174	1/1	0.97	0.05	51,51,51,51	0
56	MG	1a	3175	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	4044	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3501	1/1	0.97	0.14	30,30,30,30	0
56	MG	2A	3342	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3121	1/1	0.97	0.06	31,31,31,31	0
56	MG	15	106	1/1	0.97	0.12	19,19,19,19	0
56	MG	1a	3179	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3585	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3786	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3787	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3310	1/1	0.97	0.05	24,24,24,24	0
56	MG	17	101	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3587	1/1	0.97	0.05	12,12,12,12	0
56	MG	1a	3187	1/1	0.97	0.15	43,43,43,43	0
56	MG	17	103	1/1	0.97	0.20	33,33,33,33	0
56	MG	2A	3355	1/1	0.97	0.12	23,23,23,23	0
56	MG	2a	1635	1/1	0.97	0.08	39,39,39,39	0
56	MG	17	105	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3100	1/1	0.97	0.06	38,38,38,38	0
56	MG	18	102	1/1	0.97	0.05	29,29,29,29	0
56	MG	18	103	1/1	0.97	0.11	41,41,41,41	0
56	MG	19	502	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3792	1/1	0.97	0.08	19,19,19,19	0
56	MG	1A	4054	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3685	1/1	0.97	0.05	21,21,21,21	0
56	MG	1A	3915	1/1	0.97	0.06	34,34,34,34	0
56	MG	2A	3144	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3620	1/1	0.97	0.05	34,34,34,34	0
56	MG	1A	4057	1/1	0.97	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3589	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3371	1/1	0.97	0.09	39,39,39,39	0
56	MG	1a	3201	1/1	0.97	0.16	44,44,44,44	0
56	MG	1A	3011	1/1	0.97	0.06	20,20,20,20	0
56	MG	2A	3378	1/1	0.97	0.07	25,25,25,25	0
56	MG	2A	3379	1/1	0.97	0.08	41,41,41,41	0
56	MG	2A	3381	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3268	1/1	0.97	0.11	31,31,31,31	0
56	MG	1a	3010	1/1	0.97	0.09	45,45,45,45	0
56	MG	1A	4062	1/1	0.97	0.06	21,21,21,21	0
56	MG	1a	3206	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3173	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3594	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3388	1/1	0.97	0.11	25,25,25,25	0
56	MG	1A	3037	1/1	0.97	0.20	22,22,22,22	0
56	MG	1A	3438	1/1	0.97	0.07	29,29,29,29	0
56	MG	2a	1664	1/1	0.97	0.29	56,56,56,56	0
56	MG	2a	1665	1/1	0.97	0.05	49,49,49,49	0
56	MG	2A	3392	1/1	0.97	0.04	33,33,33,33	0
56	MG	2A	3393	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3175	1/1	0.97	0.16	21,21,21,21	0
56	MG	1A	3512	1/1	0.97	0.04	40,40,40,40	0
56	MG	1a	3213	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3123	1/1	0.97	0.06	21,21,21,21	0
56	MG	1b	3001	1/1	0.97	0.07	69,69,69,69	0
56	MG	1A	3146	1/1	0.97	0.21	23,23,23,23	0
56	MG	1B	207	1/1	0.97	0.18	40,40,40,40	0
56	MG	1f	3001	1/1	0.97	0.08	31,31,31,31	0
56	MG	2A	3169	1/1	0.97	0.15	45,45,45,45	0
56	MG	2A	3404	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3442	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3038	1/1	0.97	0.14	25,25,25,25	0
56	MG	1A	3323	1/1	0.97	0.06	19,19,19,19	0
56	MG	1a	3025	1/1	0.97	0.11	24,24,24,24	0
56	MG	2A	3174	1/1	0.97	0.13	47,47,47,47	0
56	MG	1A	3607	1/1	0.97	0.09	19,19,19,19	0
56	MG	2a	1686	1/1	0.97	0.06	67,67,67,67	0
56	MG	1A	3520	1/1	0.97	0.08	11,11,11,11	0
56	MG	1A	3148	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3446	1/1	0.97	0.07	43,43,43,43	0
56	MG	1a	3030	1/1	0.97	0.16	43,43,43,43	0
56	MG	1B	215	1/1	0.97	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3149	1/1	0.97	0.25	28,28,28,28	0
56	MG	2A	3183	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3709	1/1	0.97	0.08	30,30,30,30	0
56	MG	1B	219	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3384	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3670	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3278	1/1	0.97	0.12	40,40,40,40	0
56	MG	2A	3425	1/1	0.97	0.05	59,59,59,59	0
56	MG	1A	3150	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3184	1/1	0.97	0.15	14,14,14,14	0
56	MG	1a	3040	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3232	1/1	0.97	0.08	17,17,17,17	0
56	MG	1A	3389	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3531	1/1	0.97	0.07	19,19,19,19	0
56	MG	2A	3679	1/1	0.97	0.27	49,49,49,49	0
56	MG	1A	3233	1/1	0.97	0.11	35,35,35,35	0
56	MG	1A	3185	1/1	0.97	0.08	26,26,26,26	0
56	MG	1A	3063	1/1	0.97	0.14	23,23,23,23	0
56	MG	1A	3393	1/1	0.97	0.11	24,24,24,24	0
56	MG	1A	3536	1/1	0.97	0.06	25,25,25,25	0
56	MG	1A	3015	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3835	1/1	0.97	0.21	42,42,42,42	0
56	MG	1a	3051	1/1	0.97	0.18	55,55,55,55	0
56	MG	2A	3688	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3154	1/1	0.97	0.14	31,31,31,31	0
56	MG	1A	3287	1/1	0.97	0.04	30,30,30,30	0
56	MG	1A	3838	1/1	0.97	0.12	53,53,53,53	0
56	MG	1A	3726	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3076	1/1	0.97	0.15	26,26,26,26	0
56	MG	2a	1721	1/1	0.97	0.05	73,73,73,73	0
56	MG	2A	3209	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3077	1/1	0.97	0.13	21,21,21,21	0
56	MG	2A	3447	1/1	0.97	0.13	27,27,27,27	0
56	MG	1D	305	1/1	0.97	0.08	28,28,28,28	0
56	MG	2A	3699	1/1	0.97	0.06	39,39,39,39	0
56	MG	1D	306	1/1	0.97	0.05	17,17,17,17	0
56	MG	1A	3842	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3729	1/1	0.97	0.07	49,49,49,49	0
56	MG	1D	310	1/1	0.97	0.04	33,33,33,33	0
56	MG	2A	3453	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3195	1/1	0.97	0.14	27,27,27,27	0
56	MG	2a	1734	1/1	0.97	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	3065	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3731	1/1	0.97	0.13	16,16,16,16	0
56	MG	2A	3709	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3633	1/1	0.97	0.05	52,52,52,52	0
56	MG	2A	3711	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3544	1/1	0.97	0.04	12,12,12,12	0
56	MG	2A	3461	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3005	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3020	1/1	0.97	0.05	18,18,18,18	0
56	MG	1a	3070	1/1	0.97	0.04	30,30,30,30	0
56	MG	2A	3717	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3344	1/1	0.97	0.17	31,31,31,31	0
56	MG	2a	1749	1/1	0.97	0.11	55,55,55,55	0
56	MG	2A	3467	1/1	0.97	0.14	28,28,28,28	0
56	MG	1A	3197	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3468	1/1	0.97	0.05	37,37,37,37	0
56	MG	1E	309	1/1	0.97	0.08	15,15,15,15	0
56	MG	1A	3159	1/1	0.97	0.21	36,36,36,36	0
56	MG	1A	3160	1/1	0.97	0.34	29,29,29,29	0
56	MG	1a	3078	1/1	0.97	0.44	48,48,48,48	0
56	MG	1a	3079	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3974	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3856	1/1	0.97	0.07	62,62,62,62	0
56	MG	2A	3729	1/1	0.97	0.13	43,43,43,43	0
56	MG	1a	3082	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3348	1/1	0.97	0.14	44,44,44,44	0
56	MG	2a	1766	1/1	0.97	0.11	36,36,36,36	0
56	MG	1A	3742	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3553	1/1	0.97	0.09	10,10,10,10	0
56	MG	2A	3026	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3473	1/1	0.97	0.19	42,42,42,42	0
56	MG	2A	3485	1/1	0.97	0.17	56,56,56,56	0
56	MG	2A	3740	1/1	0.97	0.15	37,37,37,37	0
56	MG	1A	3002	1/1	0.97	0.13	46,46,46,46	0
56	MG	2A	3029	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3557	1/1	0.97	0.12	25,25,25,25	0
56	MG	2A	3243	1/1	0.97	0.15	49,49,49,49	0
56	MG	1A	3411	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3095	1/1	0.97	0.22	28,28,28,28	0
56	MG	1A	3202	1/1	0.97	0.17	27,27,27,27	0
56	MG	1A	3561	1/1	0.97	0.05	17,17,17,17	0
56	MG	1A	3751	1/1	0.97	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3756	1/1	0.97	0.08	33,33,33,33	0
56	MG	1G	3005	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3496	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3164	1/1	0.97	0.11	12,12,12,12	0
56	MG	1A	3753	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3754	1/1	0.97	0.14	22,22,22,22	0
56	MG	1N	203	1/1	0.97	0.11	51,51,51,51	0
56	MG	2A	3254	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3994	1/1	0.97	0.13	21,21,21,21	0
56	MG	2A	3043	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3504	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3657	1/1	0.97	0.10	23,23,23,23	0
56	MG	1a	3101	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3250	1/1	0.97	0.18	20,20,20,20	0
56	MG	1A	3416	1/1	0.97	0.04	17,17,17,17	0
56	MG	1A	4000	1/1	0.97	0.08	29,29,29,29	0
56	MG	1A	3661	1/1	0.97	0.09	18,18,18,18	0
56	MG	1A	3165	1/1	0.97	0.15	31,31,31,31	0
56	MG	2A	3264	1/1	0.97	0.04	47,47,47,47	0
56	MG	1a	3107	1/1	0.97	0.14	39,39,39,39	0
56	MG	1a	3108	1/1	0.97	0.17	40,40,40,40	0
56	MG	2B	3020	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	4003	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3035	1/1	0.97	0.10	24,24,24,24	0
56	MG	1A	3664	1/1	0.97	0.09	43,43,43,43	0
56	MG	2A	3056	1/1	0.97	0.07	52,52,52,52	0
56	MG	2A	3057	1/1	0.97	0.04	47,47,47,47	0
56	MG	2A	3272	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3763	1/1	0.97	0.10	22,22,22,22	0
56	MG	1A	3206	1/1	0.97	0.04	30,30,30,30	0
56	MG	2A	3061	1/1	0.97	0.17	30,30,30,30	0
56	MG	1A	3488	1/1	0.97	0.12	23,23,23,23	0
56	MG	1a	3115	1/1	0.97	0.08	48,48,48,48	0
56	MG	2a	1817	1/1	0.97	0.23	51,51,51,51	0
56	MG	1Q	205	1/1	0.97	0.06	28,28,28,28	0
56	MG	1a	3119	1/1	0.97	0.12	52,52,52,52	0
56	MG	1A	4011	1/1	0.97	0.11	37,37,37,37	0
56	MG	1R	203	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3884	1/1	0.97	0.06	30,30,30,30	0
56	MG	2A	3534	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3573	1/1	0.97	0.05	24,24,24,24	0
56	MG	1A	3886	1/1	0.97	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3072	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	4015	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3768	1/1	0.97	0.04	33,33,33,33	0
56	MG	2A	3540	1/1	0.97	0.05	37,37,37,37	0
56	MG	1a	3128	1/1	0.97	0.07	50,50,50,50	0
56	MG	2P	201	1/1	0.97	0.06	54,54,54,54	0
56	MG	1T	201	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3254	1/1	0.97	0.17	11,11,11,11	0
56	MG	1U	202	1/1	0.97	0.03	30,30,30,30	0
56	MG	1A	4018	1/1	0.97	0.05	24,24,24,24	0
56	MG	1U	204	1/1	0.97	0.07	23,23,23,23	0
56	MG	2f	3001	1/1	0.97	0.09	40,40,40,40	0
56	MG	2R	3003	1/1	0.97	0.28	48,48,48,48	0
56	MG	1A	4020	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3770	1/1	0.97	0.08	12,12,12,12	0
56	MG	1A	3891	1/1	0.97	0.05	33,33,33,33	0
56	MG	2T	3003	1/1	0.97	0.07	41,41,41,41	0
56	MG	1W	3004	1/1	0.97	0.07	21,21,21,21	0
56	MG	1W	3005	1/1	0.97	0.06	21,21,21,21	0
56	MG	1X	101	1/1	0.97	0.08	73,73,73,73	0
56	MG	2U	204	1/1	0.97	0.24	60,60,60,60	0
56	MG	2A	3554	1/1	0.97	0.08	24,24,24,24	0
56	MG	2U	206	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	4023	1/1	0.97	0.45	21,21,21,21	0
56	MG	2A	3557	1/1	0.97	0.18	27,27,27,27	0
56	MG	1X	104	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	4024	1/1	0.97	0.21	43,43,43,43	0
56	MG	2A	3305	1/1	0.97	0.14	51,51,51,51	0
56	MG	2A	3091	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3669	1/1	0.97	0.09	35,35,35,35	0
56	MG	1Y	503	1/1	0.97	0.17	42,42,42,42	0
56	MG	1Z	3001	1/1	0.97	0.05	42,42,42,42	0
56	MG	20	3002	1/1	0.97	0.05	52,52,52,52	0
56	MG	1A	3360	1/1	0.97	0.05	32,32,32,32	0
56	MG	1A	3894	1/1	0.97	0.07	37,37,37,37	0
56	MG	1a	3152	1/1	0.97	0.05	60,60,60,60	0
56	MG	2A	3313	1/1	0.97	0.19	41,41,41,41	0
56	MG	1A	3081	1/1	0.97	0.10	24,24,24,24	0
56	MG	10	101	1/1	0.97	0.06	41,41,41,41	0
56	MG	10	102	1/1	0.97	0.07	25,25,25,25	0
56	MG	2A	3317	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3114	1/1	0.97	0.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3574	1/1	0.97	0.11	46,46,46,46	0
56	MG	2A	3575	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3364	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3210	1/1	0.97	0.14	25,25,25,25	0
56	MG	11	101	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3323	1/1	0.97	0.18	31,31,31,31	0
56	MG	2y	3004	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3899	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3778	1/1	0.97	0.08	13,13,13,13	0
56	MG	1A	3115	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	4038	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3780	1/1	0.97	0.13	44,44,44,44	0
56	MG	2A	3585	1/1	0.97	0.07	34,34,34,34	0
56	MG	2A	3110	1/1	0.97	0.09	37,37,37,37	0
56	MG	2a	1613	1/1	0.97	0.24	60,60,60,60	0
59	ZN	2n	501	1/1	0.97	0.05	93,93,93,93	0
56	MG	2A	3380	1/1	0.98	0.08	25,25,25,25	0
56	MG	2A	3741	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3647	1/1	0.98	0.08	16,16,16,16	0
56	MG	2A	3743	1/1	0.98	0.06	51,51,51,51	0
56	MG	2A	3059	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3122	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3572	1/1	0.98	0.09	12,12,12,12	0
56	MG	1A	3917	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3820	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3751	1/1	0.98	0.29	44,44,44,44	0
56	MG	1A	3249	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3211	1/1	0.98	0.10	30,30,30,30	0
56	MG	2A	3754	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	3085	1/1	0.98	0.06	13,13,13,13	0
56	MG	1A	4031	1/1	0.98	0.17	35,35,35,35	0
56	MG	1a	3185	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3576	1/1	0.98	0.07	15,15,15,15	0
56	MG	1A	3655	1/1	0.98	0.08	11,11,11,11	0
56	MG	2A	3395	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3343	1/1	0.98	0.11	30,30,30,30	0
56	MG	1A	3214	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3021	1/1	0.98	0.05	29,29,29,29	0
56	MG	1O	203	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3738	1/1	0.98	0.04	32,32,32,32	0
56	MG	2A	3077	1/1	0.98	0.13	41,41,41,41	0
56	MG	1A	3125	1/1	0.98	0.24	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3660	1/1	0.98	0.05	26,26,26,26	0
56	MG	1A	4040	1/1	0.98	0.09	34,34,34,34	0
56	MG	1P	202	1/1	0.98	0.06	23,23,23,23	0
56	MG	1a	3056	1/1	0.98	0.12	50,50,50,50	0
56	MG	1A	3032	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3452	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	3514	1/1	0.98	0.06	21,21,21,21	0
56	MG	1A	3218	1/1	0.98	0.04	23,23,23,23	0
56	MG	1A	3219	1/1	0.98	0.12	19,19,19,19	0
56	MG	1A	3517	1/1	0.98	0.07	28,28,28,28	0
56	MG	1R	201	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	3259	1/1	0.98	0.11	45,45,45,45	0
56	MG	1A	3260	1/1	0.98	0.17	18,18,18,18	0
56	MG	1A	3220	1/1	0.98	0.08	24,24,24,24	0
56	MG	1A	4050	1/1	0.98	0.14	26,26,26,26	0
56	MG	1A	3353	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3127	1/1	0.98	0.05	37,37,37,37	0
56	MG	2A	3596	1/1	0.98	0.08	32,32,32,32	0
56	MG	1A	3153	1/1	0.98	0.07	29,29,29,29	0
56	MG	1a	3071	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	3088	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3050	1/1	0.98	0.04	45,45,45,45	0
56	MG	1a	3215	1/1	0.98	0.07	39,39,39,39	0
56	MG	1U	201	1/1	0.98	0.04	20,20,20,20	0
56	MG	1A	3358	1/1	0.98	0.07	44,44,44,44	0
56	MG	2a	1742	1/1	0.98	0.04	70,70,70,70	0
56	MG	1A	3848	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	3676	1/1	0.98	0.15	31,31,31,31	0
56	MG	1U	205	1/1	0.98	0.06	23,23,23,23	0
56	MG	2a	1746	1/1	0.98	0.06	67,67,67,67	0
56	MG	1U	206	1/1	0.98	0.07	16,16,16,16	0
56	MG	1A	3948	1/1	0.98	0.05	14,14,14,14	0
56	MG	1A	3757	1/1	0.98	0.08	22,22,22,22	0
56	MG	1W	3001	1/1	0.98	0.08	34,34,34,34	0
56	MG	2A	3611	1/1	0.98	0.06	47,47,47,47	0
56	MG	1W	3002	1/1	0.98	0.11	29,29,29,29	0
56	MG	2O	8002	1/1	0.98	0.12	52,52,52,52	0
56	MG	2a	1754	1/1	0.98	0.11	61,61,61,61	0
56	MG	2a	1755	1/1	0.98	0.07	70,70,70,70	0
56	MG	1A	3851	1/1	0.98	0.12	44,44,44,44	0
56	MG	1A	3156	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3051	1/1	0.98	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3114	1/1	0.98	0.17	29,29,29,29	0
56	MG	1A	3529	1/1	0.98	0.14	34,34,34,34	0
56	MG	1A	3312	1/1	0.98	0.04	42,42,42,42	0
56	MG	1X	103	1/1	0.98	0.09	29,29,29,29	0
56	MG	1A	3131	1/1	0.98	0.09	35,35,35,35	0
56	MG	1A	3601	1/1	0.98	0.05	24,24,24,24	0
56	MG	2A	3274	1/1	0.98	0.14	45,45,45,45	0
56	MG	2A	3120	1/1	0.98	0.23	38,38,38,38	0
56	MG	1A	3764	1/1	0.98	0.07	24,24,24,24	0
56	MG	1A	3363	1/1	0.98	0.05	32,32,32,32	0
56	MG	1B	204	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3684	1/1	0.98	0.04	44,44,44,44	0
56	MG	1B	206	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3189	1/1	0.98	0.07	23,23,23,23	0
56	MG	2A	3455	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3456	1/1	0.98	0.06	26,26,26,26	0
56	MG	2a	1776	1/1	0.98	0.12	47,47,47,47	0
56	MG	1w	109	1/1	0.98	0.22	37,37,37,37	0
56	MG	1A	3686	1/1	0.98	0.07	18,18,18,18	0
56	MG	2A	3634	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3470	1/1	0.98	0.12	33,33,33,33	0
56	MG	2a	1781	1/1	0.98	0.06	67,67,67,67	0
56	MG	1A	3132	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3865	1/1	0.98	0.10	18,18,18,18	0
56	MG	1A	3689	1/1	0.98	0.33	20,20,20,20	0
56	MG	2A	3463	1/1	0.98	0.12	27,27,27,27	0
56	MG	2A	3288	1/1	0.98	0.11	30,30,30,30	0
56	MG	1A	3316	1/1	0.98	0.24	34,34,34,34	0
56	MG	1A	3191	1/1	0.98	0.07	24,24,24,24	0
56	MG	1A	3421	1/1	0.98	0.10	37,37,37,37	0
56	MG	1B	216	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3138	1/1	0.98	0.13	34,34,34,34	0
56	MG	1A	3475	1/1	0.98	0.13	28,28,28,28	0
56	MG	1A	3872	1/1	0.98	0.05	27,27,27,27	0
56	MG	1A	3776	1/1	0.98	0.14	25,25,25,25	0
56	MG	2A	3649	1/1	0.98	0.04	21,21,21,21	0
56	MG	2A	3473	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3108	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3143	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3615	1/1	0.98	0.05	12,12,12,12	0
56	MG	1A	3976	1/1	0.98	0.08	50,50,50,50	0
56	MG	1A	3541	1/1	0.98	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3479	1/1	0.98	0.07	34,34,34,34	0
56	MG	15	103	1/1	0.98	0.23	25,25,25,25	0
56	MG	2A	3148	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3978	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3660	1/1	0.98	0.05	37,37,37,37	0
56	MG	1a	3116	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3275	1/1	0.98	0.07	25,25,25,25	0
56	MG	1A	3478	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3782	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3665	1/1	0.98	0.03	36,36,36,36	0
56	MG	1A	3194	1/1	0.98	0.07	35,35,35,35	0
56	MG	2A	3155	1/1	0.98	0.05	34,34,34,34	0
56	MG	1a	3122	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	3983	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3161	1/1	0.98	0.23	20,20,20,20	0
56	MG	1A	3701	1/1	0.98	0.03	15,15,15,15	0
56	MG	1A	3481	1/1	0.98	0.03	28,28,28,28	0
56	MG	17	104	1/1	0.98	0.04	27,27,27,27	0
56	MG	1B	234	1/1	0.98	0.10	41,41,41,41	0
56	MG	2A	3010	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3091	1/1	0.98	0.04	31,31,31,31	0
56	MG	2A	3320	1/1	0.98	0.12	17,17,17,17	0
56	MG	1A	3788	1/1	0.98	0.06	25,25,25,25	0
56	MG	1a	3132	1/1	0.98	0.09	34,34,34,34	0
56	MG	2A	3167	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3033	1/1	0.98	0.04	21,21,21,21	0
56	MG	1B	238	1/1	0.98	0.04	23,23,23,23	0
56	MG	2A	3326	1/1	0.98	0.10	48,48,48,48	0
56	MG	2A	3505	1/1	0.98	0.07	42,42,42,42	0
56	MG	2A	3016	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3093	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3375	1/1	0.98	0.22	34,34,34,34	0
56	MG	1a	3137	1/1	0.98	0.05	51,51,51,51	0
56	MG	2A	3020	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3430	1/1	0.98	0.20	40,40,40,40	0
56	MG	2A	3176	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	3042	1/1	0.98	0.04	19,19,19,19	0
56	MG	1A	3554	1/1	0.98	0.09	14,14,14,14	0
56	MG	1A	3066	1/1	0.98	0.03	22,22,22,22	0
56	MG	1A	3328	1/1	0.98	0.09	25,25,25,25	0
56	MG	2A	3696	1/1	0.98	0.03	39,39,39,39	0
56	MG	1D	308	1/1	0.98	0.05	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3999	1/1	0.98	0.05	25,25,25,25	0
56	MG	2A	3519	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3797	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3344	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3139	1/1	0.98	0.11	21,21,21,21	0
56	MG	1a	3147	1/1	0.98	0.05	58,58,58,58	0
56	MG	1A	3034	1/1	0.98	0.17	12,12,12,12	0
56	MG	1A	3800	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3022	1/1	0.98	0.03	22,22,22,22	0
56	MG	2A	3527	1/1	0.98	0.10	52,52,52,52	0
56	MG	1E	302	1/1	0.98	0.12	16,16,16,16	0
56	MG	1a	3016	1/1	0.98	0.07	38,38,38,38	0
56	MG	1E	304	1/1	0.98	0.15	22,22,22,22	0
56	MG	2A	3192	1/1	0.98	0.07	54,54,54,54	0
56	MG	1A	4005	1/1	0.98	0.17	10,10,10,10	0
56	MG	1A	3014	1/1	0.98	0.10	27,27,27,27	0
56	MG	2A	3356	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3099	1/1	0.98	0.08	23,23,23,23	0
56	MG	1a	3157	1/1	0.98	0.08	58,58,58,58	0
56	MG	1A	3007	1/1	0.98	0.05	12,12,12,12	0
56	MG	2A	3361	1/1	0.98	0.06	46,46,46,46	0
56	MG	1A	3120	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3564	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3541	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3500	1/1	0.98	0.10	20,20,20,20	0
56	MG	2A	3367	1/1	0.98	0.07	28,28,28,28	0
56	MG	2A	3368	1/1	0.98	0.04	36,36,36,36	0
56	MG	1A	3208	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3809	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3502	1/1	0.98	0.24	20,20,20,20	0
56	MG	1A	3723	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3569	1/1	0.98	0.06	17,17,17,17	0
56	MG	1F	304	1/1	0.98	0.10	20,20,20,20	0
56	MG	2a	1683	1/1	0.98	0.16	33,33,33,33	0
57	K	1A	3486	1/1	0.98	0.03	19,19,19,19	0
56	MG	2A	3732	1/1	0.98	0.15	24,24,24,24	0
56	MG	1A	3645	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	4019	1/1	0.98	0.13	26,26,26,26	0
56	MG	1a	3173	1/1	0.98	0.06	39,39,39,39	0
59	ZN	1n	501	1/1	0.98	0.03	51,51,51,51	0
59	ZN	2Y	501	1/1	0.98	0.04	79,79,79,79	0
56	MG	1A	3013	1/1	0.98	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1F	308	1/1	0.98	0.04	42,42,42,42	0
60	SF4	1d	501	8/8	0.98	0.05	52,54,61,66	0
60	SF4	2d	501	8/8	0.98	0.05	58,60,69,79	0
56	MG	2A	3122	1/1	0.99	0.04	26,26,26,26	0
56	MG	2a	1669	1/1	0.99	0.25	56,56,56,56	0
56	MG	2A	3357	1/1	0.99	0.06	21,21,21,21	0
56	MG	2A	3423	1/1	0.99	0.04	22,22,22,22	0
56	MG	2A	3424	1/1	0.99	0.02	24,24,24,24	0
56	MG	1A	3338	1/1	0.99	0.14	19,19,19,19	0
56	MG	1a	3167	1/1	0.99	0.06	42,42,42,42	0
56	MG	2A	3068	1/1	0.99	0.03	35,35,35,35	0
56	MG	1a	3117	1/1	0.99	0.03	27,27,27,27	0
56	MG	1a	3169	1/1	0.99	0.06	38,38,38,38	0
56	MG	2A	3363	1/1	0.99	0.05	43,43,43,43	0
56	MG	1D	312	1/1	0.99	0.19	27,27,27,27	0
56	MG	2A	3365	1/1	0.99	0.07	38,38,38,38	0
56	MG	2A	3704	1/1	0.99	0.07	37,37,37,37	0
56	MG	1A	3003	1/1	0.99	0.15	19,19,19,19	0
56	MG	1a	3172	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3258	1/1	0.99	0.13	33,33,33,33	0
56	MG	1A	3604	1/1	0.99	0.05	28,28,28,28	0
56	MG	1A	3605	1/1	0.99	0.03	14,14,14,14	0
56	MG	1E	303	1/1	0.99	0.04	22,22,22,22	0
56	MG	2a	1761	1/1	0.99	0.09	34,34,34,34	0
56	MG	1A	3490	1/1	0.99	0.06	26,26,26,26	0
56	MG	2A	3023	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	3954	1/1	0.99	0.10	53,53,53,53	0
56	MG	1A	3995	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3814	1/1	0.99	0.07	8,8,8,8	0
56	MG	2A	3197	1/1	0.99	0.05	39,39,39,39	0
56	MG	1A	3634	1/1	0.99	0.05	28,28,28,28	0
56	MG	1A	3635	1/1	0.99	0.10	25,25,25,25	0
56	MG	1A	3311	1/1	0.99	0.03	37,37,37,37	0
56	MG	1a	3131	1/1	0.99	0.07	38,38,38,38	0
56	MG	1A	3818	1/1	0.99	0.04	21,21,21,21	0
56	MG	1A	3064	1/1	0.99	0.05	12,12,12,12	0
56	MG	1A	3327	1/1	0.99	0.05	10,10,10,10	0
56	MG	1A	3888	1/1	0.99	0.08	15,15,15,15	0
56	MG	1A	3821	1/1	0.99	0.06	32,32,32,32	0
56	MG	1a	3039	1/1	0.99	0.03	47,47,47,47	0
56	MG	1A	3012	1/1	0.99	0.07	13,13,13,13	0
56	MG	2A	3038	1/1	0.99	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3176	1/1	0.99	0.19	25,25,25,25	0
56	MG	2A	3391	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	3612	1/1	0.99	0.04	24,24,24,24	0
56	MG	1B	227	1/1	0.99	0.05	36,36,36,36	0
56	MG	1V	201	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3394	1/1	0.99	0.12	37,37,37,37	0
56	MG	1A	3614	1/1	0.99	0.06	15,15,15,15	0
56	MG	2A	3736	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	3395	1/1	0.99	0.03	33,33,33,33	0
56	MG	1A	3932	1/1	0.99	0.12	13,13,13,13	0
56	MG	2A	3739	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3193	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3499	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3973	1/1	0.99	0.06	47,47,47,47	0
56	MG	1A	3116	1/1	0.99	0.15	26,26,26,26	0
56	MG	1A	3213	1/1	0.99	0.07	36,36,36,36	0
56	MG	2A	3340	1/1	0.99	0.10	30,30,30,30	0
56	MG	2A	3341	1/1	0.99	0.07	39,39,39,39	0
56	MG	1A	3178	1/1	0.99	0.10	21,21,21,21	0
56	MG	2A	3407	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3866	1/1	0.99	0.12	20,20,20,20	0
56	MG	1A	3266	1/1	0.99	0.08	24,24,24,24	0
56	MG	2a	1728	1/1	0.99	0.05	46,46,46,46	0
56	MG	1X	106	1/1	0.99	0.04	21,21,21,21	0
56	MG	1A	3401	1/1	0.99	0.11	38,38,38,38	0
56	MG	1A	3652	1/1	0.99	0.08	23,23,23,23	0
57	K	2A	3327	1/1	0.99	0.03	29,29,29,29	0
56	MG	1A	3267	1/1	0.99	0.02	24,24,24,24	0
56	MG	1A	3008	1/1	0.99	0.10	18,18,18,18	0
56	MG	1A	3404	1/1	0.99	0.10	28,28,28,28	0
59	ZN	1Y	501	1/1	0.99	0.02	58,58,58,58	0
59	ZN	14	501	1/1	0.99	0.03	70,70,70,70	0
59	ZN	19	501	1/1	0.99	0.07	42,42,42,42	0
56	MG	1O	204	1/1	0.99	0.06	45,45,45,45	0
56	MG	1A	3908	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	3552	1/1	0.99	0.08	23,23,23,23	0
59	ZN	25	501	1/1	0.99	0.05	45,45,45,45	0
59	ZN	26	501	1/1	0.99	0.03	59,59,59,59	0
59	ZN	29	501	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3067	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3987	1/1	0.99	0.06	36,36,36,36	0
56	MG	2A	3555	1/1	0.99	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
56	MG	1A	4010	1/1	1.00	0.06	23,23,23,23	0
56	MG	1A	3017	1/1	1.00	0.07	19,19,19,19	0
56	MG	1A	3567	1/1	1.00	0.09	13,13,13,13	0
59	ZN	15	104	1/1	1.00	0.07	42,42,42,42	0
59	ZN	16	102	1/1	1.00	0.05	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.