



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2025 – 06:21 PM EDT

PDB ID : 9D0I / pdb\_00009d0i  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with Se-cresomycin, mRNA, deacylated A-site tRNA<sup>phe</sup>, aminoacylated P-site fMet-tRNA<sup>met</sup>, and deacylated E-site tRNA<sup>phe</sup> at 2.45Å resolution  
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Robinson, P.J.; Benedetto, A.E.; Yu, M.; Tresco, B.I.C.; See, D.N.Y.; Jiang, T.; Ramkissoon, A.; Dunand, C.F.; Svetlov, M.S.; Lee, J.; Myers, A.G.; Polikanov, Y.S.  
Deposited on : 2024-08-07  
Resolution : 2.45 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

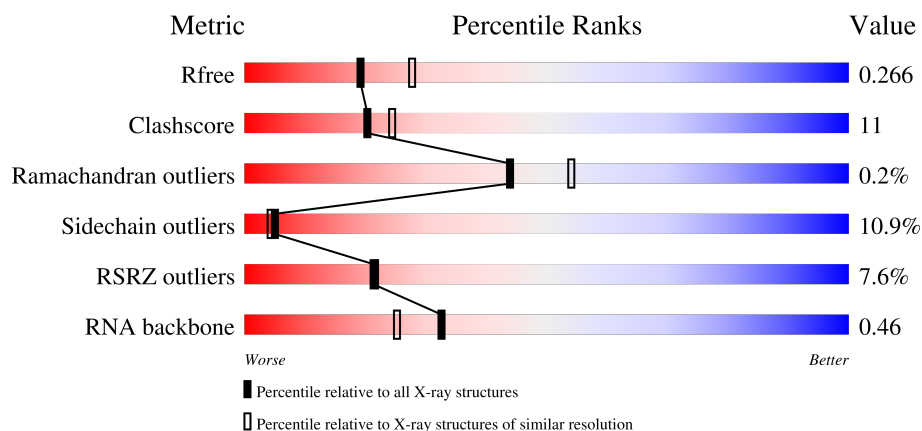
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)
RNA backbone	3690	1040 (2.76-2.16)




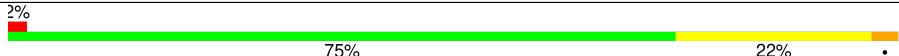
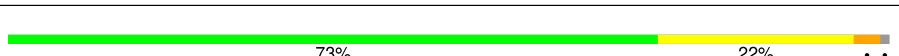
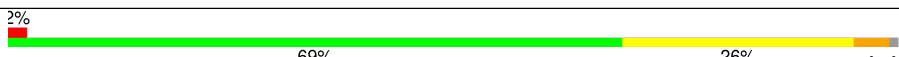
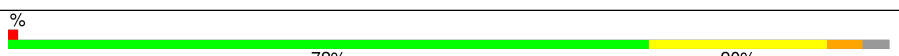
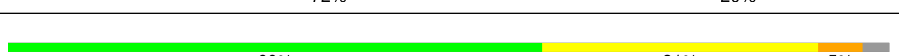
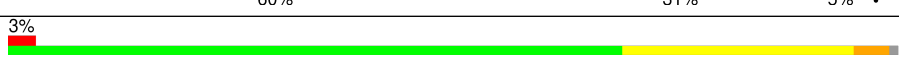

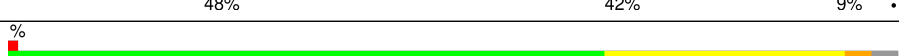


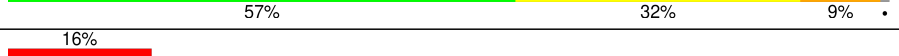
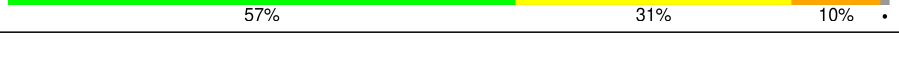




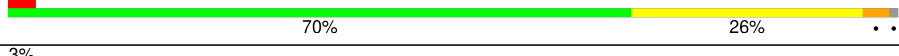

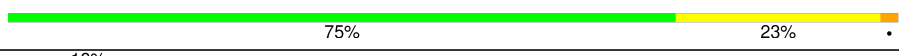



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>7%</div> <div></div> </div> </div>
1	2A	2915	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>9%</div> <div></div> </div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

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Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	

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

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Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

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

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	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
56	MG	1a	1641	-	-	-	X
56	MG	1a	1711	-	-	-	X
56	MG	1a	1713	-	-	-	X
56	MG	1n	101	-	-	-	X
56	MG	2A	3446	-	-	-	X
56	MG	2a	3008	-	-	-	X
56	MG	2a	3111	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-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 Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0	0
			1530	685	274	498	71	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	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 Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1103	Total	Mg	0	0
			1103	1103		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	17	Total	Mg	0	0
			17	17		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	5	Total 5	Mg 5	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	6	Total 6	Mg 6	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	4	Total 4	Mg 4	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	12	Total 12	Mg 12	0	0
56	1V	7	Total 7	Mg 7	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	7	Total 7	Mg 7	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	8	Total 8	Mg 8	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	4	Total 4	Mg 4	0	0
56	15	7	Total 7	Mg 7	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	4	Total 4	Mg 4	0	0
56	18	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	19	1	Total 1	Mg 1	0	0
56	1a	215	Total 215	Mg 215	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	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	8	Total 8	Mg 8	0	0
56	1x	14	Total 14	Mg 14	0	0
56	1y	1	Total 1	Mg 1	0	0
56	2A	885	Total 885	Mg 885	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	7	Total 7	Mg 7	0	0
56	2E	10	Total 10	Mg 10	0	0
56	2F	5	Total 5	Mg 5	0	0
56	2G	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	4	Total 4	Mg 4	0	0
56	21	2	Total 2	Mg 2	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	2	Total 2	Mg 2	0	0
56	28	3	Total 3	Mg 3	0	0
56	29	1	Total 1	Mg 1	0	0
56	2a	241	Total 241	Mg 241	0	0

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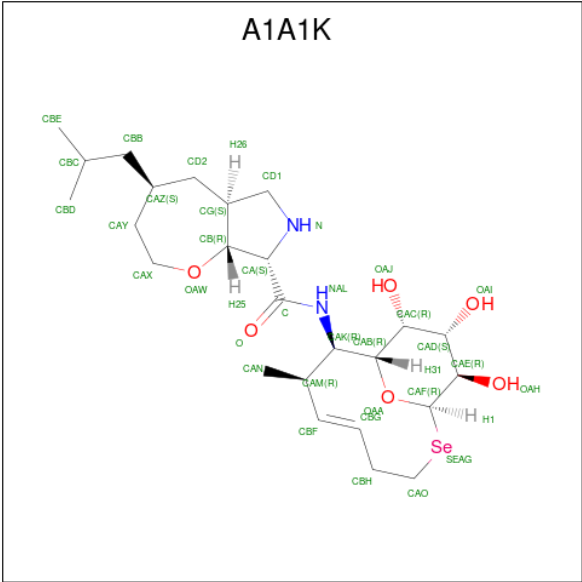
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	2	Total 2	Mg 2	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0
56	2w	7	Total 7	Mg 7	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	1	Total 1	K 1	0	0
57	2x	1	Total 1	K 1	0	0

- Molecule 58 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1R,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-13-oxa-2-selenabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: A1A1K) (formula: C<sub>25</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub>Se).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	1A	1	Total	C	N	O	Se	0	0
			34	25	2	6	1		
58	2A	1	Total	C	N	O	Se	0	0
			34	25	2	6	1		

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

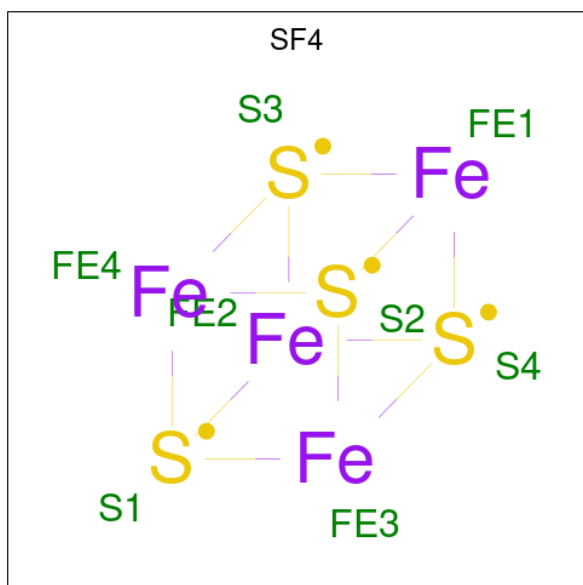
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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:  $\text{Fe}_4\text{S}_4$ ).



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	2018	Total	O	0	0
			2018	2018		
61	1B	62	Total	O	0	0
			62	62		
61	1D	26	Total	O	0	0
			26	26		
61	1E	27	Total	O	0	0
			27	27		
61	1F	17	Total	O	0	0
			17	17		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	3	Total 3	O 3	0	0
61	1H	2	Total 2	O 2	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	6	Total 6	O 6	0	0
61	1O	7	Total 7	O 7	0	0
61	1P	23	Total 23	O 23	0	0
61	1Q	7	Total 7	O 7	0	0
61	1R	13	Total 13	O 13	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	8	Total 8	O 8	0	0
61	1U	15	Total 15	O 15	0	0
61	1V	7	Total 7	O 7	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	5	Total 5	O 5	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	12	Total 12	O 12	0	0
61	11	12	Total 12	O 12	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	15	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	3	Total 3	O 3	0	0
61	17	7	Total 7	O 7	0	0
61	18	11	Total 11	O 11	0	0
61	1a	378	Total 378	O 378	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	1i	1	Total 1	O 1	0	0
61	1l	8	Total 8	O 8	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	4	Total 4	O 4	0	0
61	1w	10	Total 10	O 10	0	0
61	1x	16	Total 16	O 16	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1160	Total 1160	O 1160	0	0
61	2B	23	Total 23	O 23	0	0
61	2D	22	Total 22	O 22	0	0
61	2E	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2F	13	Total 13	O 13	0	0
61	2I	3	Total 3	O 3	0	0
61	2O	3	Total 3	O 3	0	0
61	2P	15	Total 15	O 15	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	5	Total 5	O 5	0	0
61	2U	4	Total 4	O 4	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	2	Total 2	O 2	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	6	Total 6	O 6	0	0
61	21	13	Total 13	O 13	0	0
61	23	1	Total 1	O 1	0	0
61	25	1	Total 1	O 1	0	0
61	26	1	Total 1	O 1	0	0
61	27	5	Total 5	O 5	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	264	Total 264	O 264	0	0
61	2d	2	Total 2	O 2	0	0

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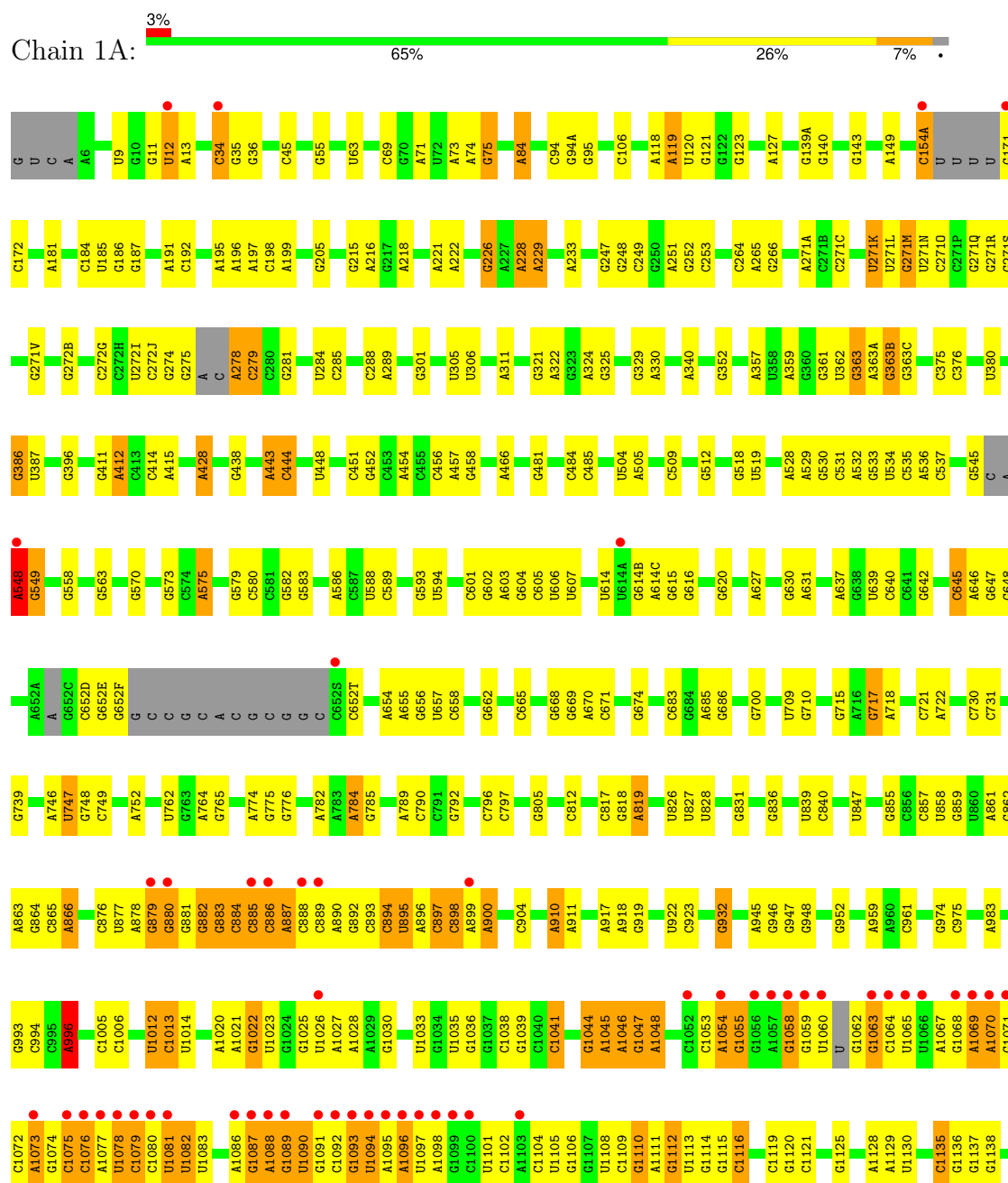
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2e	2	Total	O	0	0
			2	2		
61	2j	3	Total	O	0	0
			3	3		
61	2l	6	Total	O	0	0
			6	6		
61	2p	1	Total	O	0	0
			1	1		
61	2q	1	Total	O	0	0
			1	1		
61	2r	1	Total	O	0	0
			1	1		
61	2t	3	Total	O	0	0
			3	3		
61	2v	2	Total	O	0	0
			2	2		
61	2w	1	Total	O	0	0
			1	1		
61	2x	7	Total	O	0	0
			7	7		
61	2y	6	Total	O	0	0
			6	6		

### 3 Residue-property plots [i](#)

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

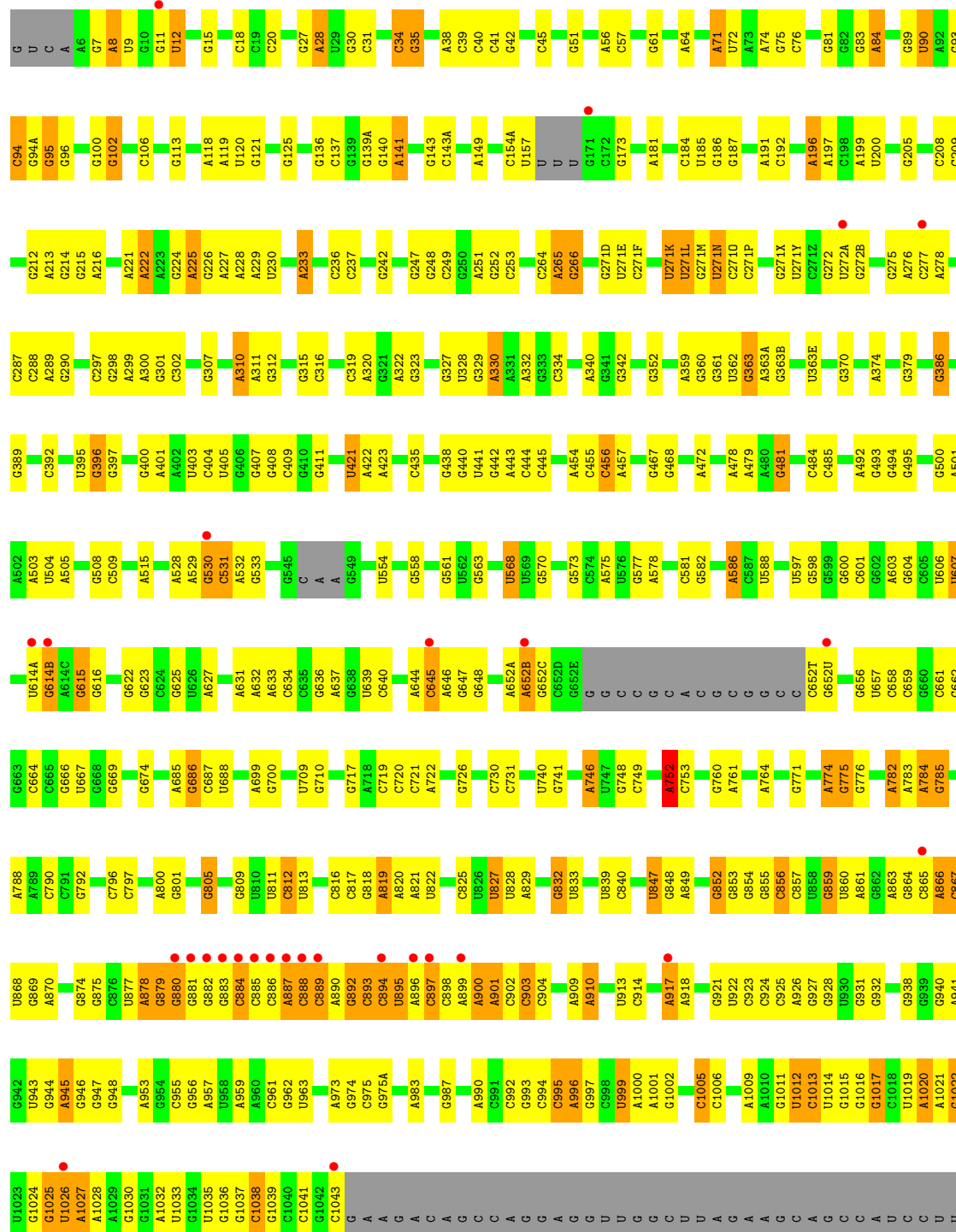
#### • Molecule 1: 23S Ribosomal RNA





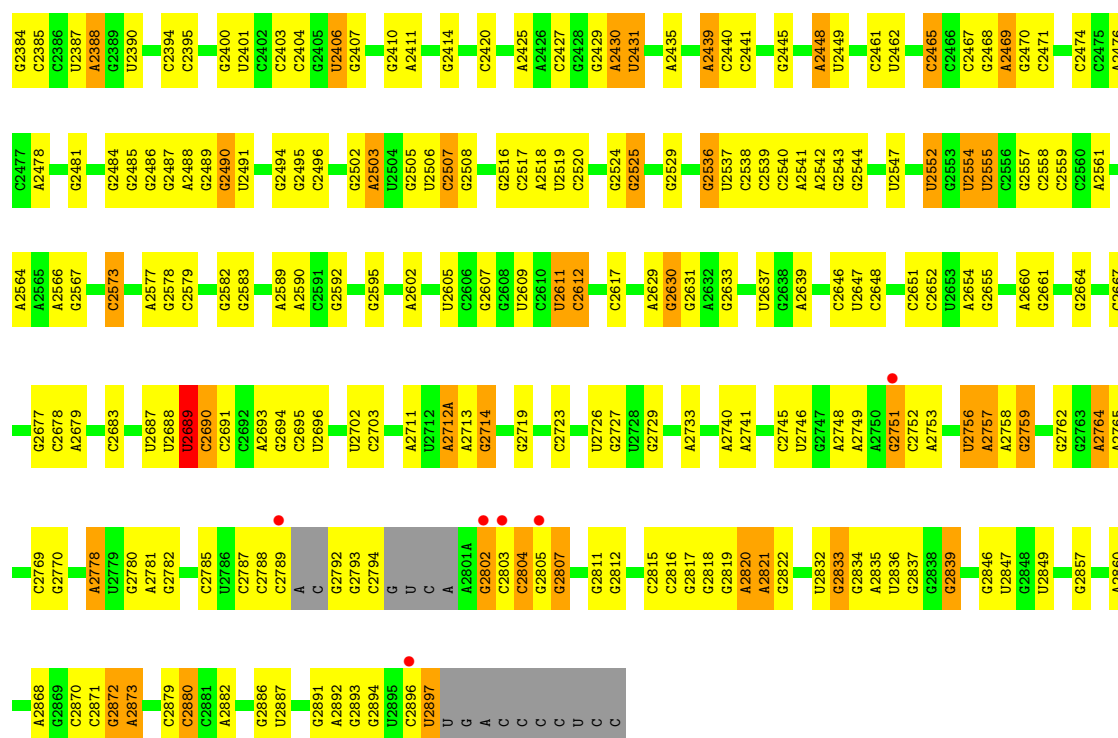


• Molecule 1: 23S Ribosomal RNA



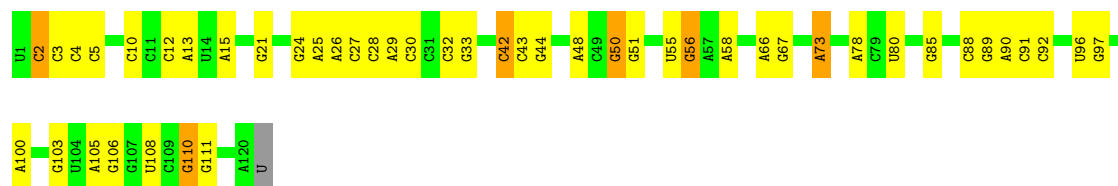






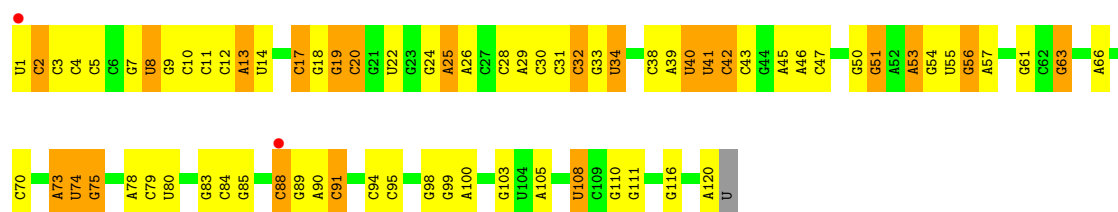
### • Molecule 2: 5S Ribosomal RNA

Chain 1B: 60% 34% 5%



### • Molecule 2: 5S Ribosomal RNA

Chain 2B: 39% 42% 18%



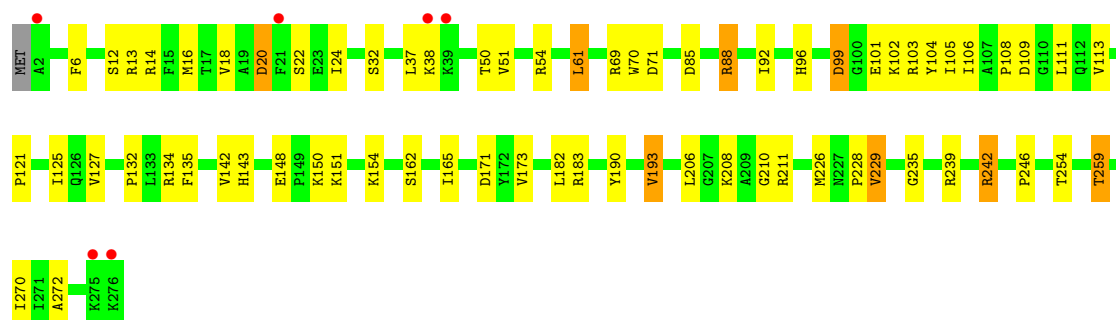
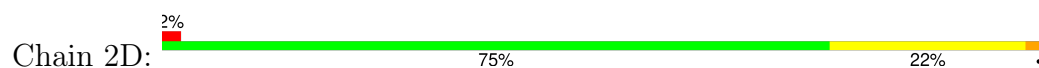
### • Molecule 3: 50S ribosomal protein L2

Chain 1D: 78% 20% 2%

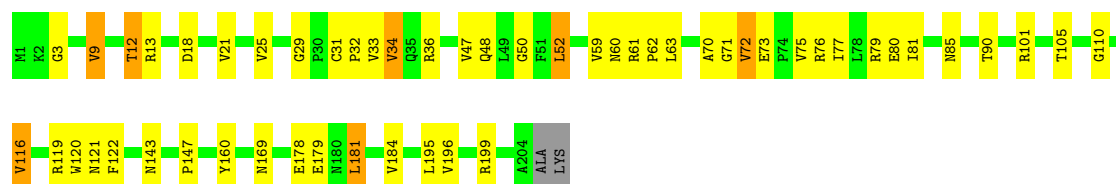




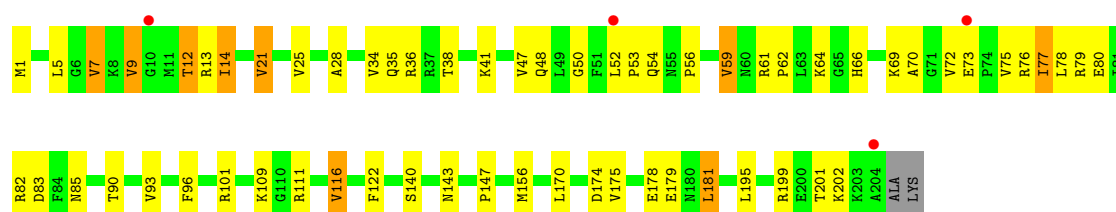
• Molecule 3: 50S ribosomal protein L2



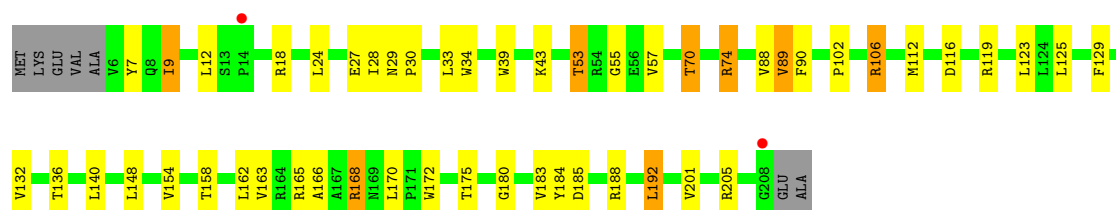
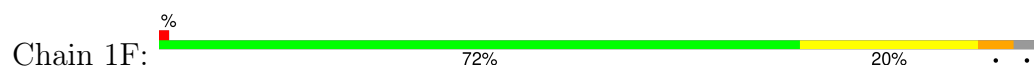
• Molecule 4: 50S ribosomal protein L3



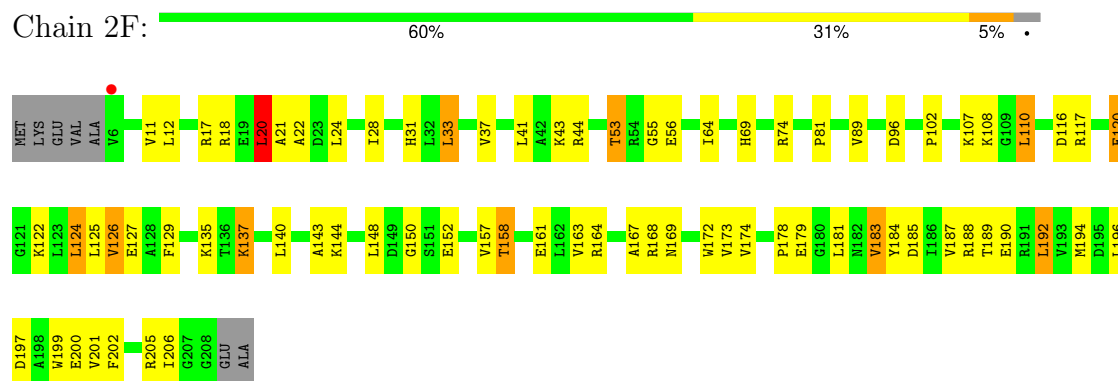
• Molecule 4: 50S ribosomal protein L3



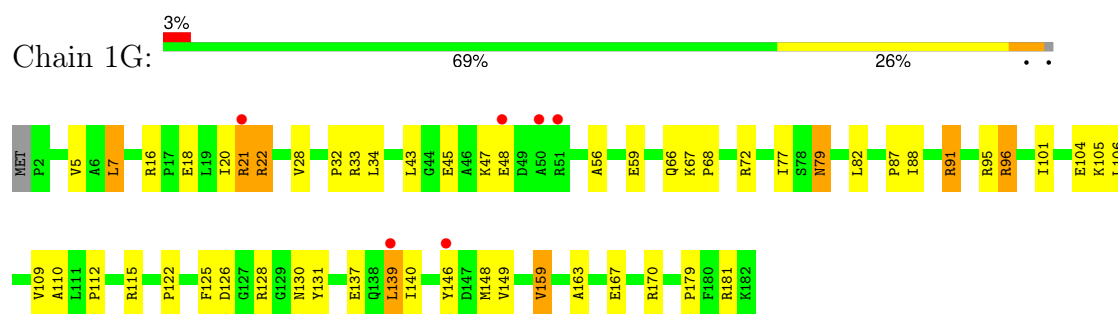
• Molecule 5: 50S ribosomal protein L4



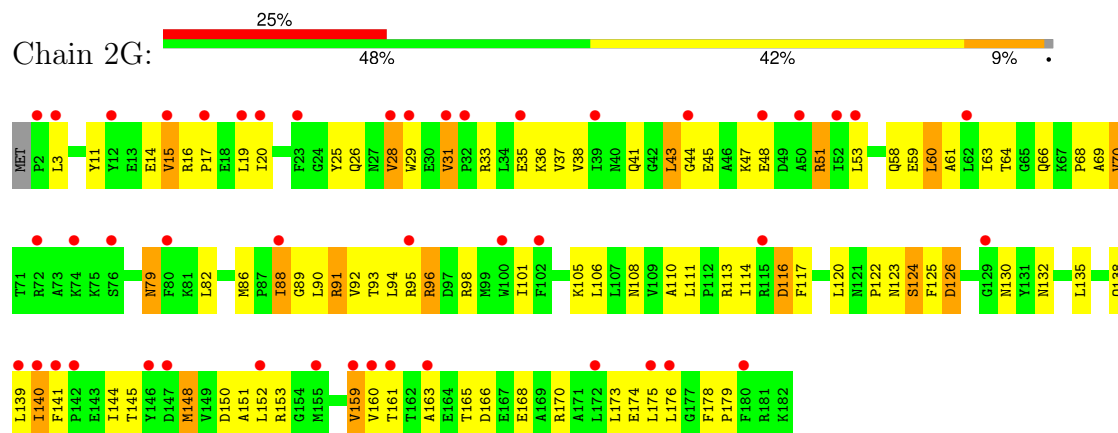
- Molecule 5: 50S ribosomal protein L4



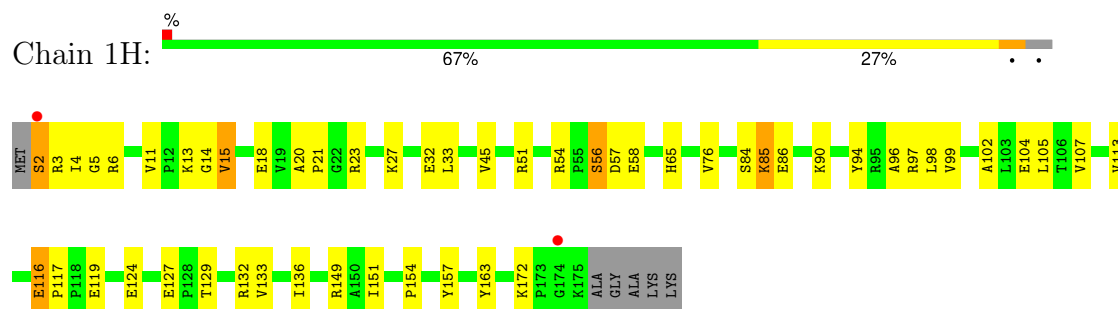
- Molecule 6: 50S ribosomal protein L5



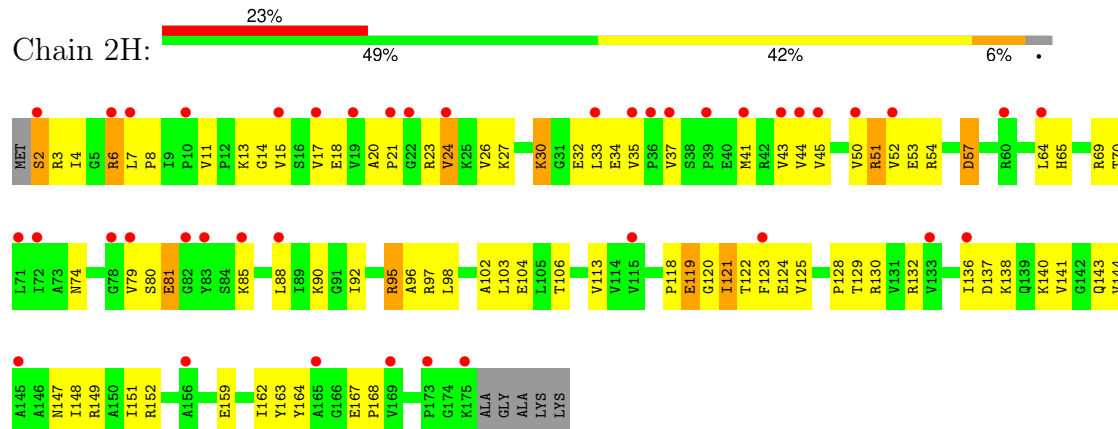
- Molecule 6: 50S ribosomal protein L5



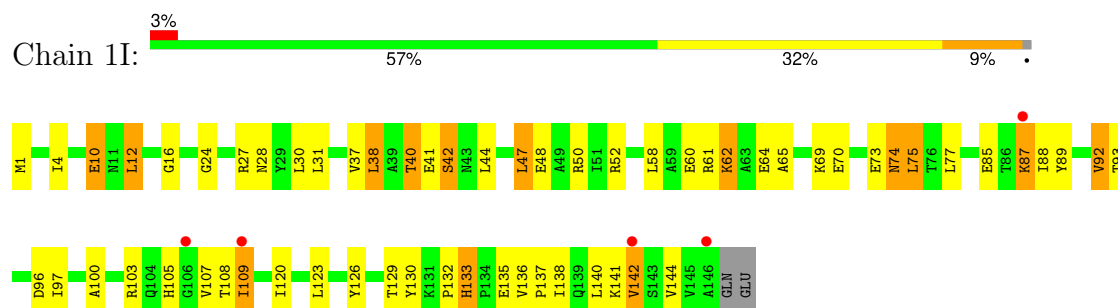
- Molecule 7: 50S ribosomal protein L6



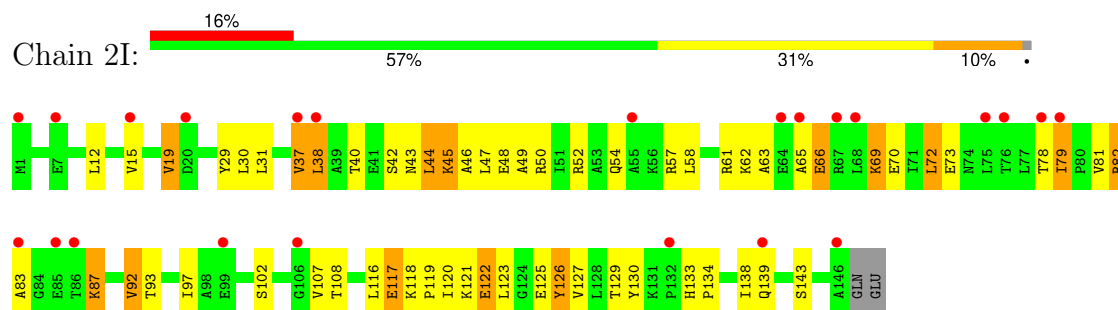
- Molecule 7: 50S ribosomal protein L6



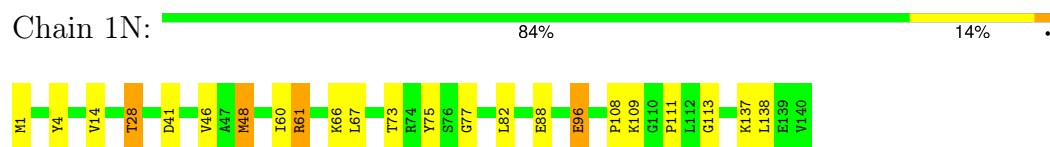
- Molecule 8: 50S ribosomal protein L9



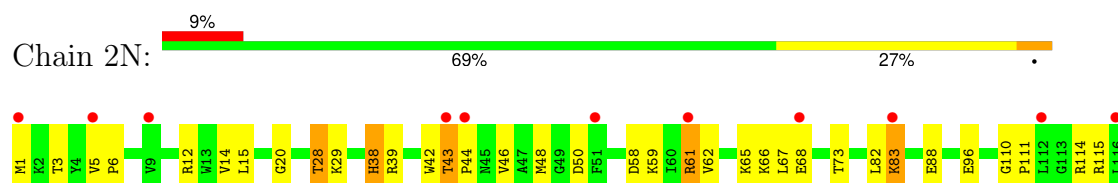
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

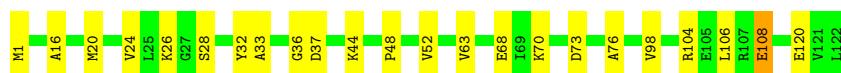
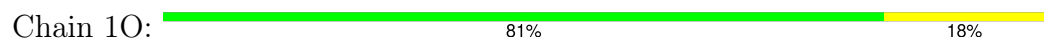


- Molecule 9: 50S ribosomal protein L13

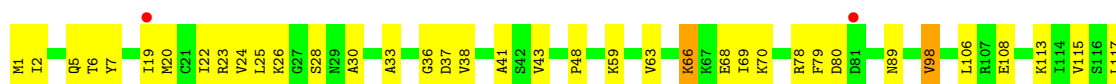




- Molecule 10: 50S ribosomal protein L14



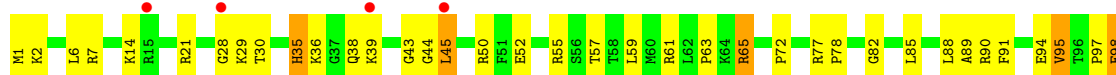
- Molecule 10: 50S ribosomal protein L14



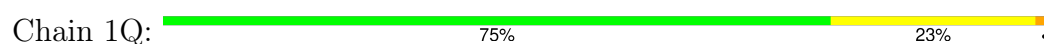
- Molecule 11: 50S ribosomal protein L15



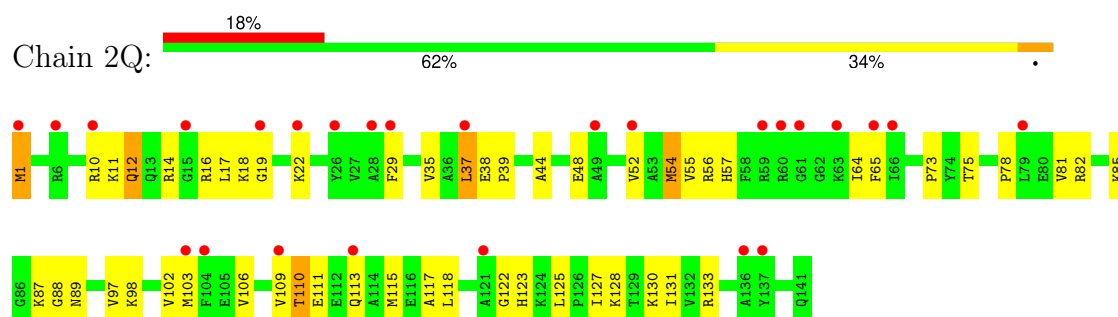
- Molecule 11: 50S ribosomal protein L15



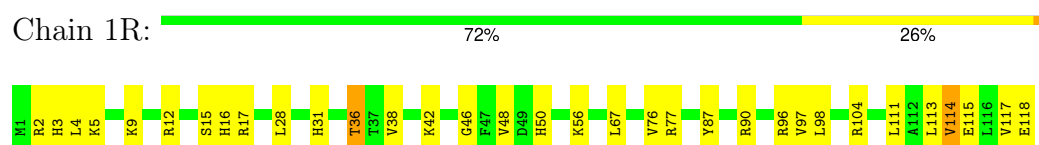
- Molecule 12: 50S ribosomal protein L16



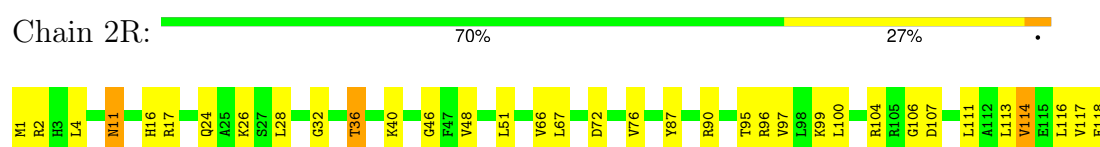
- Molecule 12: 50S ribosomal protein L16



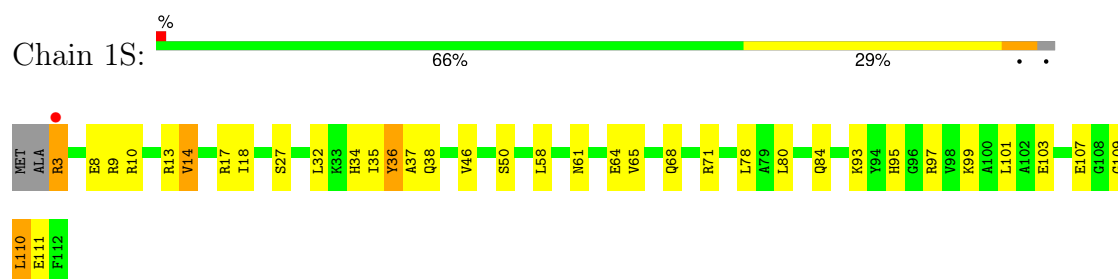
- Molecule 13: 50S ribosomal protein L17



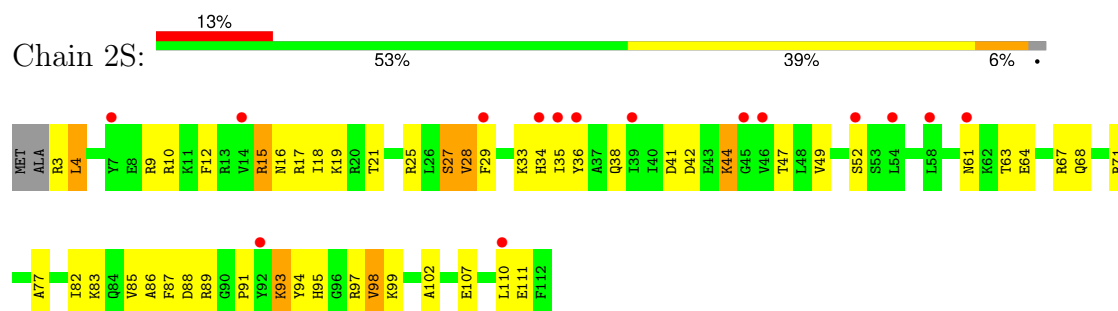
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

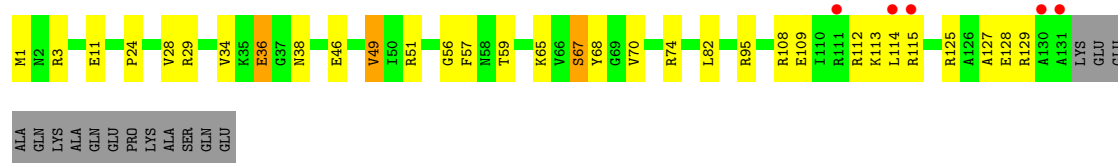


- Molecule 14: 50S ribosomal protein L18

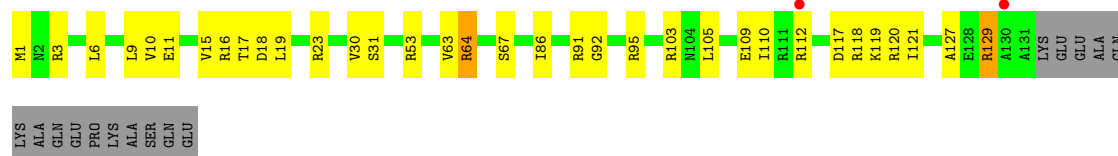


- Molecule 15: 50S ribosomal protein L19

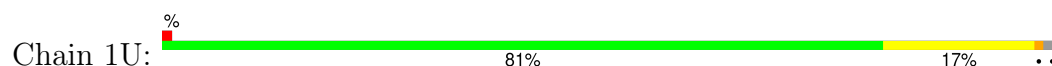




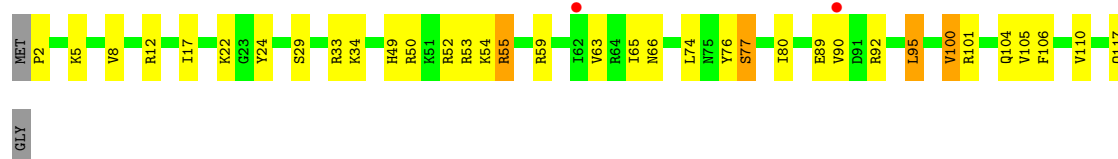
- Molecule 15: 50S ribosomal protein L19



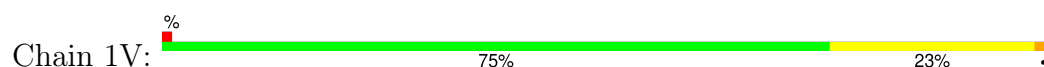
- Molecule 16: 50S ribosomal protein L20



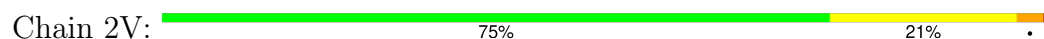
- Molecule 16: 50S ribosomal protein L20



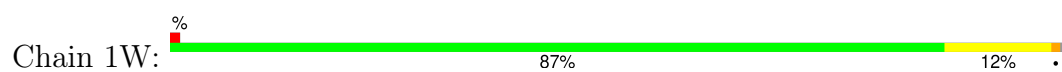
- Molecule 17: 50S ribosomal protein L21



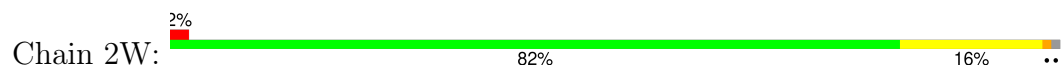
- Molecule 17: 50S ribosomal protein L21



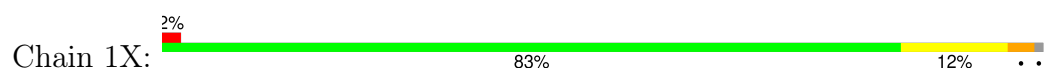
- Molecule 18: 50S ribosomal protein L22



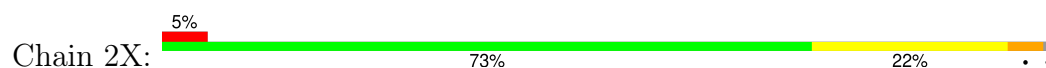
- Molecule 18: 50S ribosomal protein L22



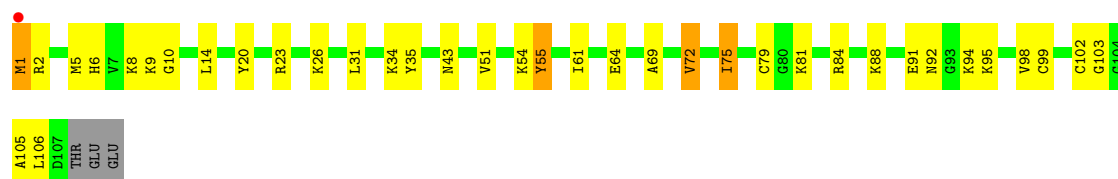
- Molecule 19: 50S ribosomal protein L23



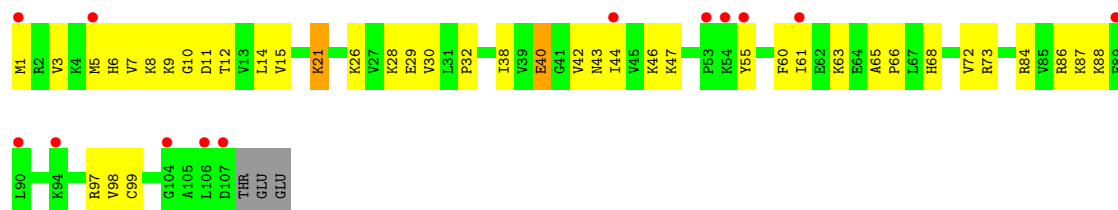
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

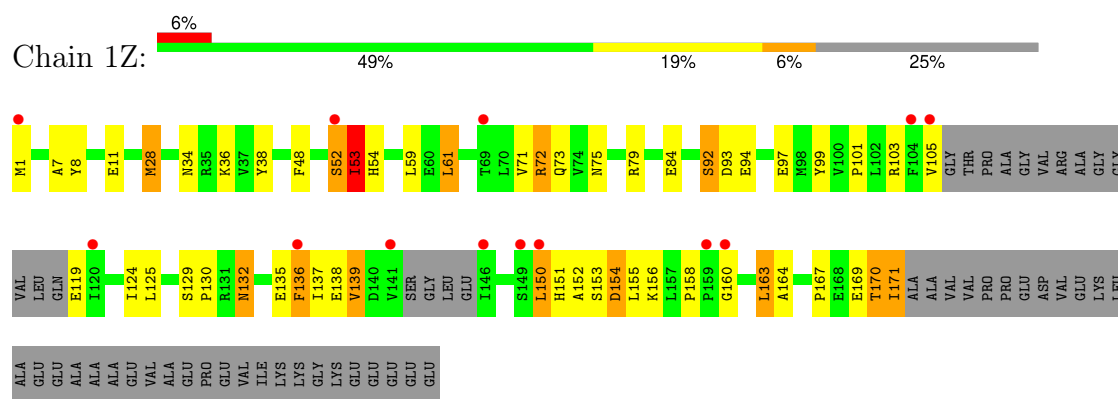


- Molecule 20: 50S ribosomal protein L24

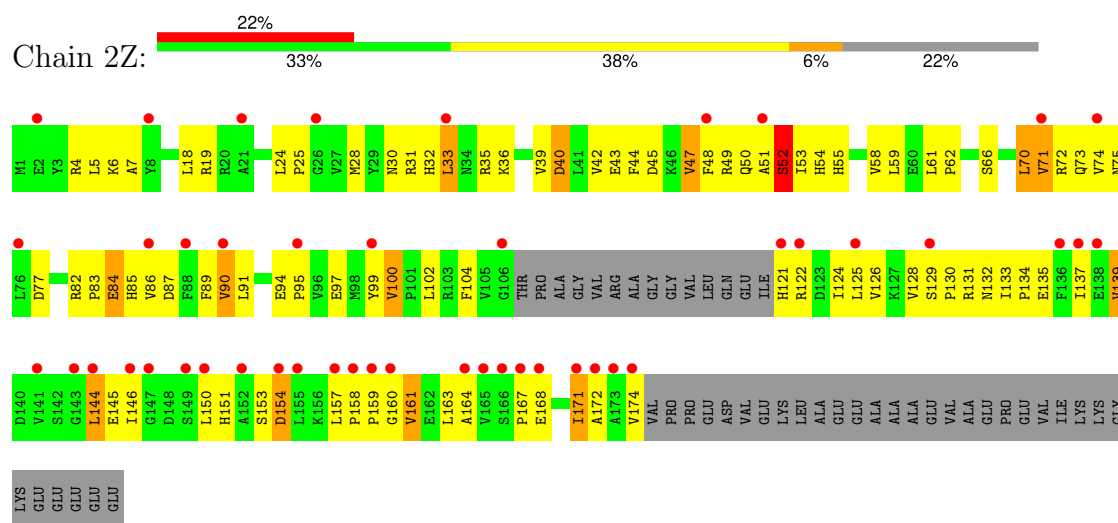


- Molecule 21: 50S ribosomal protein L25

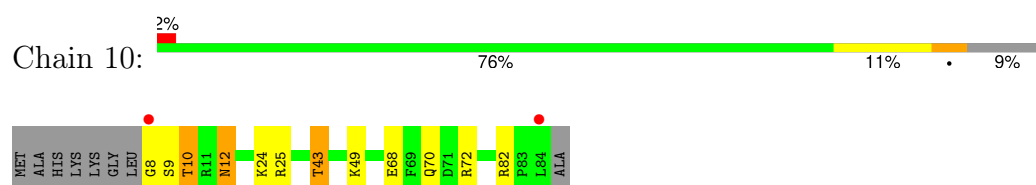




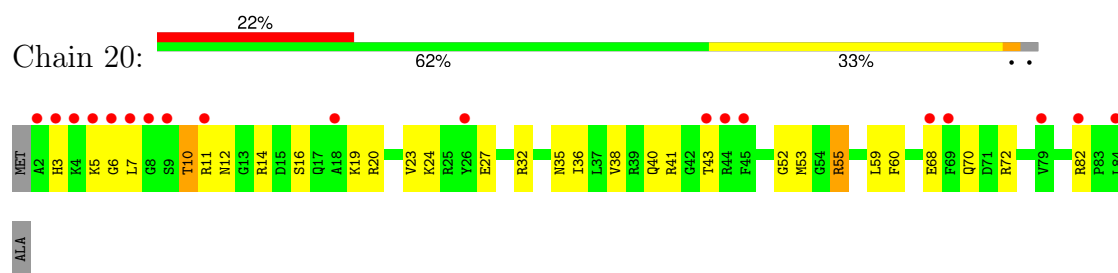
• Molecule 21: 50S ribosomal protein L25



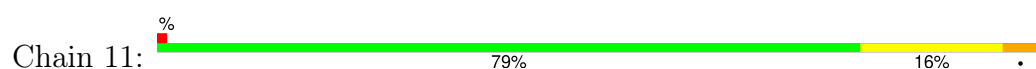
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

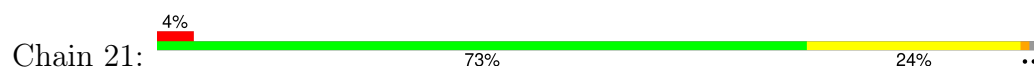


• Molecule 23: 50S ribosomal protein L28

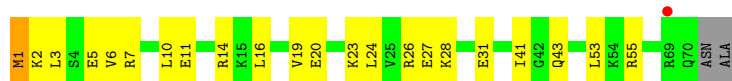




- Molecule 23: 50S ribosomal protein L28



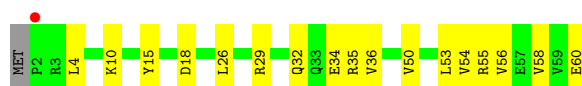
- Molecule 24: 50S ribosomal protein L29



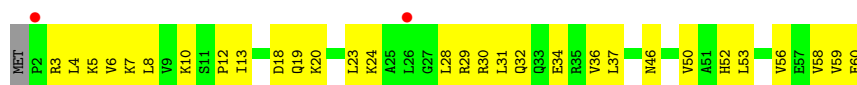
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



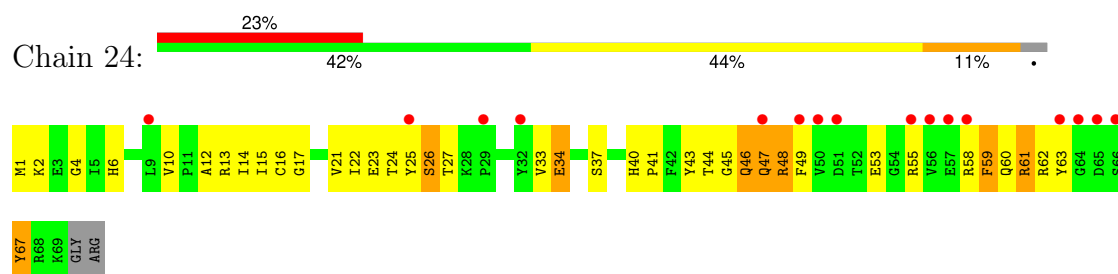
- Molecule 25: 50S ribosomal protein L30



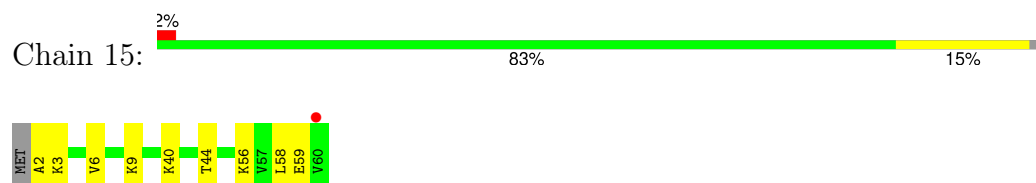
- Molecule 26: 50S ribosomal protein L31



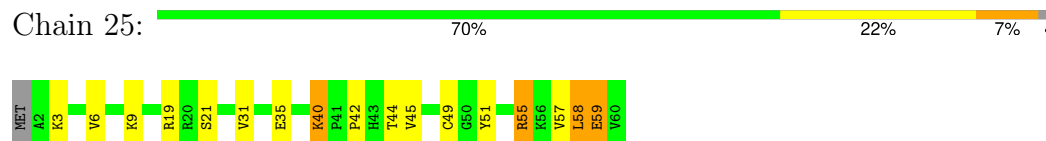
- Molecule 26: 50S ribosomal protein L31



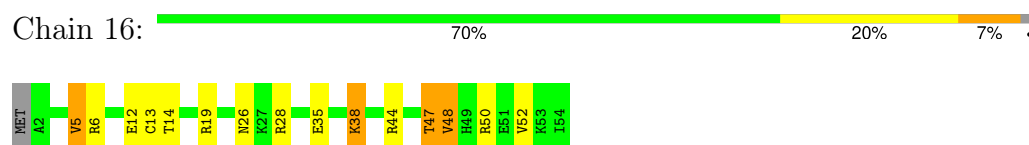
- Molecule 27: 50S ribosomal protein L32



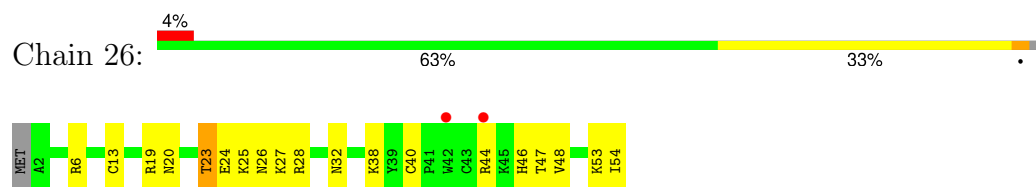
- Molecule 27: 50S ribosomal protein L32



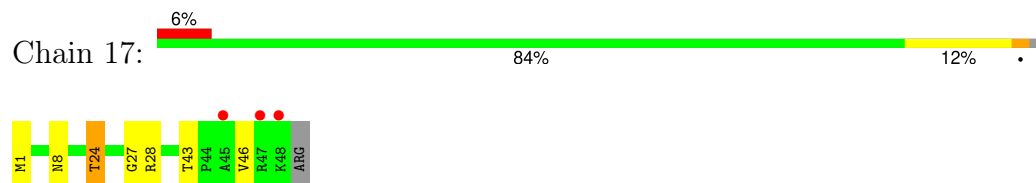
- Molecule 28: 50S ribosomal protein L33



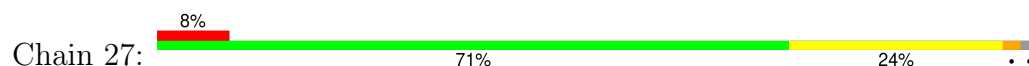
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34





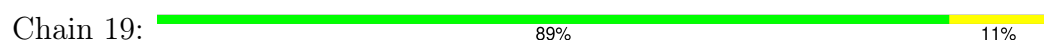
- Molecule 30: 50S ribosomal protein L35



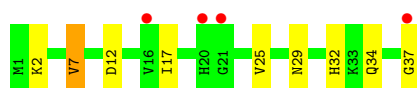
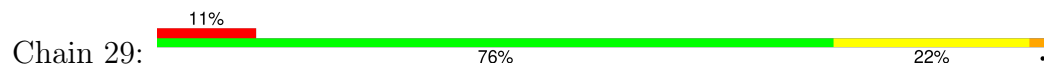
- Molecule 30: 50S ribosomal protein L35



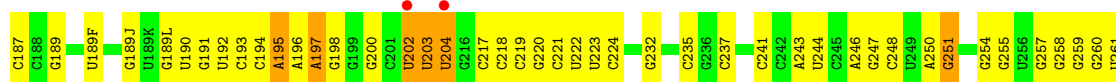
- Molecule 31: 50S ribosomal protein L36

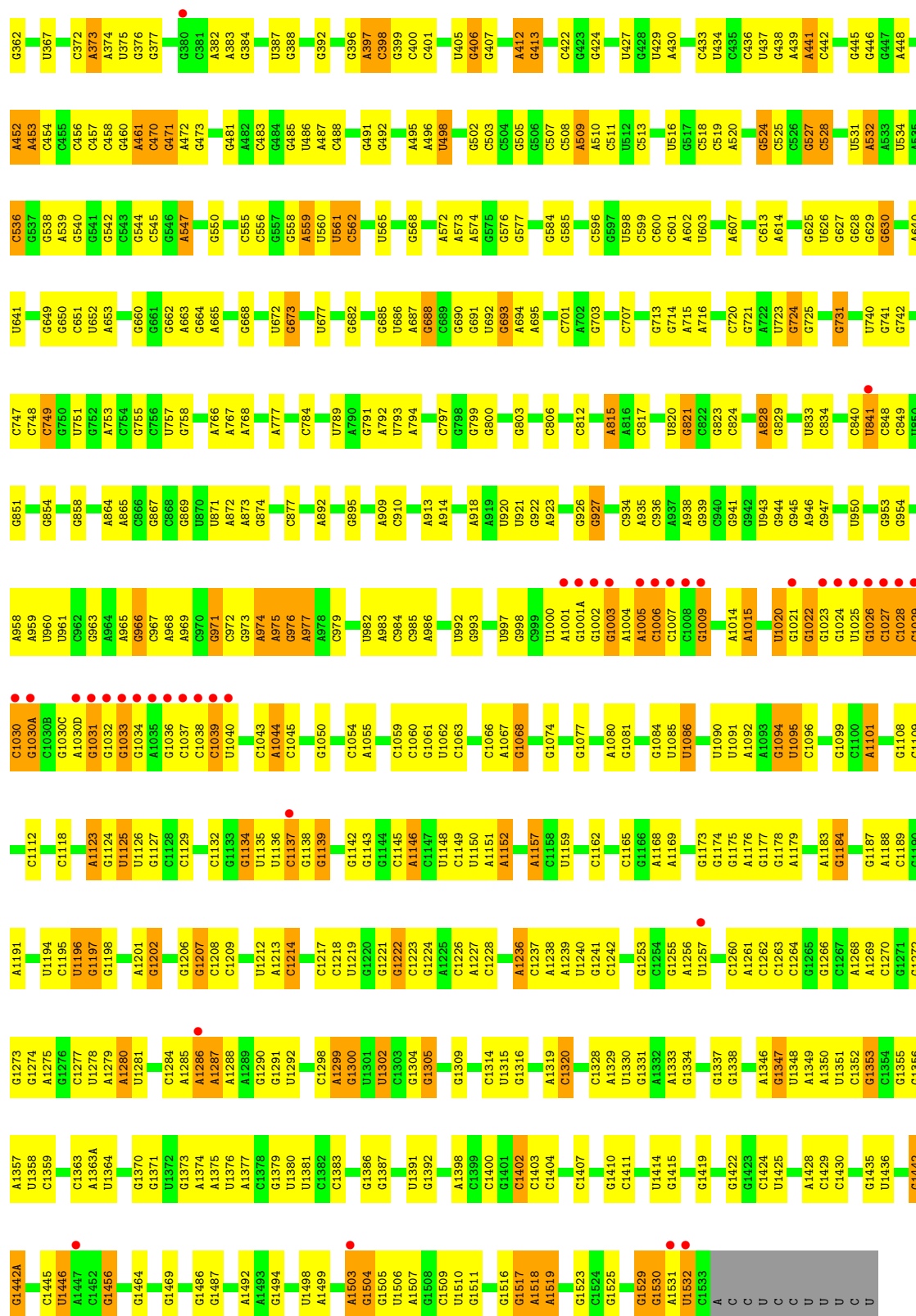


- Molecule 31: 50S ribosomal protein L36

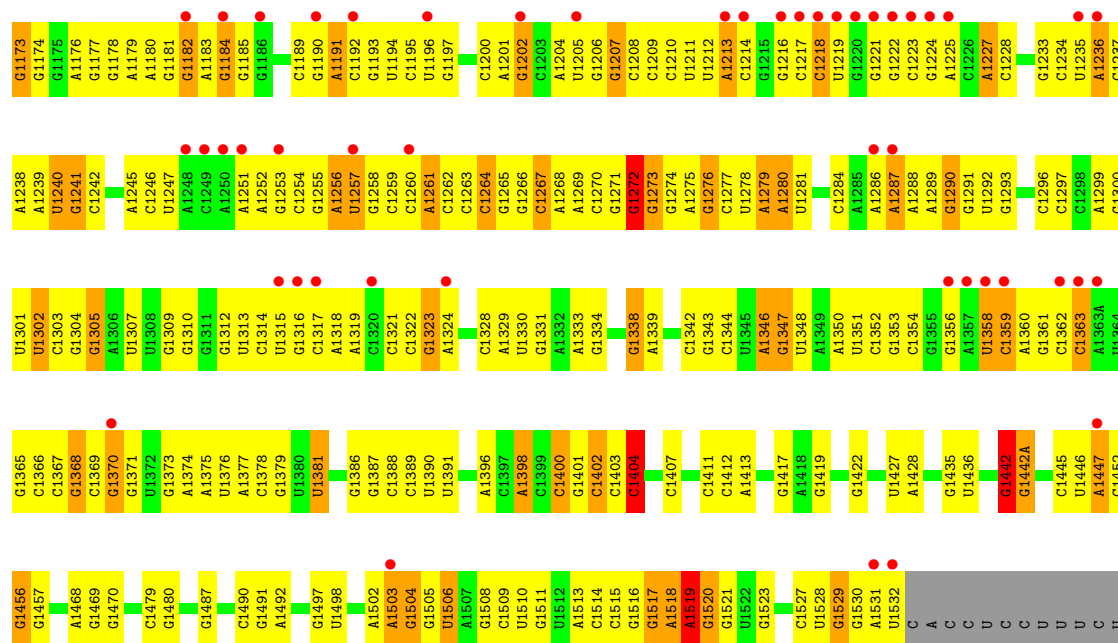


- Molecule 32: 16S Ribosomal RNA

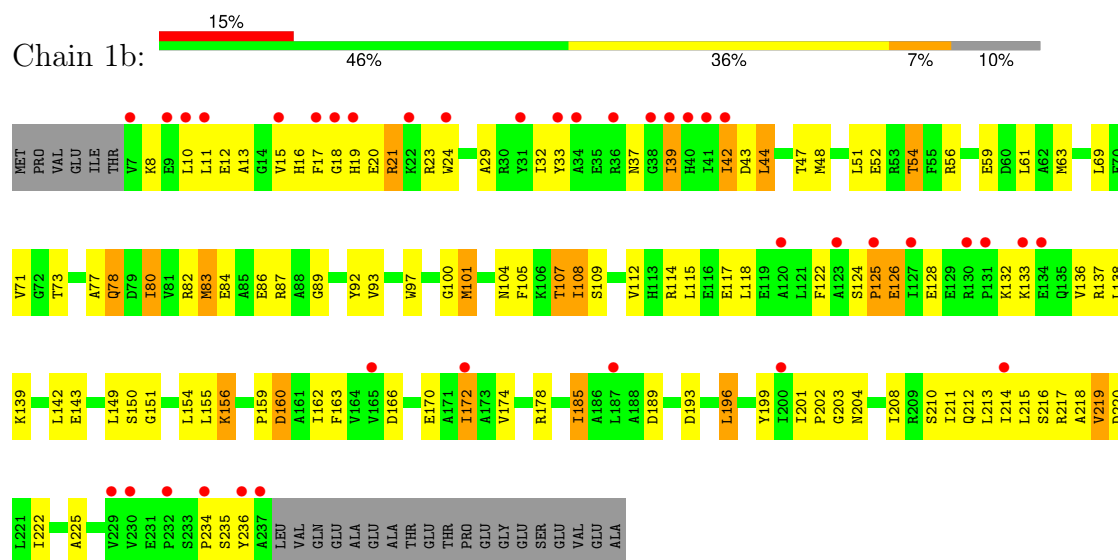




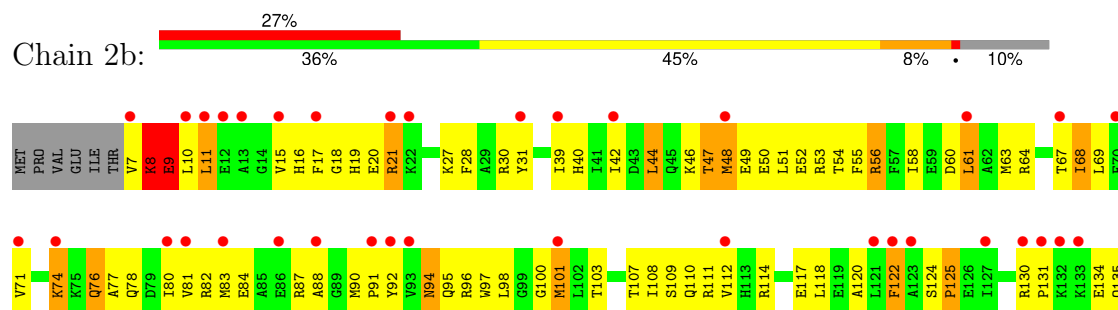
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A1111	G1050	C995	C934	U841	C736	C651	G557	G481	C398	G297	C177	U	U	U	U	U	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	U18	U19	U20	U21	U22	U23	U24	U25	U26	U27	U28	U29	U30	U31	U32	U33	U34	U35	U36	U37	U38	U39	U40	U41	U42	U43	U44	U45	U46	U47	U48	U49	U50	U51	U52	U53	U54	U55	U56	U57	U58	U59	U60	U61	U62	U63	U64	U65	U66	U67	U68	U69	U70	U71	U72	U73	U74	U75	U76	U77	U78	U79	U80	U81	U82	U83	U84	U85	U86	U87	U88	U89	U90	U91	U92	U93	U94	U95	U96	U97	U98	U99	U100	U101	U102	U103	U104	U105	U106	U107	U108	U109	U110	U111	U112	U113	U114	U115	U116	U117	U118	U119	U120	U121	U122	U123	U124	U125	U126	U127	U128	U129	U130	U131	U132	U133	U134	U135	U136	U137	U138	U139	U140	U141	U142	U143	U144	U145	U146	U147	U148	U149	U150	U151	U152	U153	U154	U155	U156	U157	U158	U159	U160	U161	U162	U163	U164	U165	U166	U167	U168	U169	U170	U171	U172	U173	U174	U175	U176	U177	U178	U179	U180	U181	U182	U183	U184	U185	U186	U187	U188	U189	U190	U191	U192	U193	U194	U195	U196	U197	U198	U199	U200	U201	U202	U203	U204	U205	U206	U207	U208	U209	U210	U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	U253	U254	U255	U256	U257	U258	U259	U260	U261	U262	U263	U264	U265	U266	U267	U268	U269	U270	U271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1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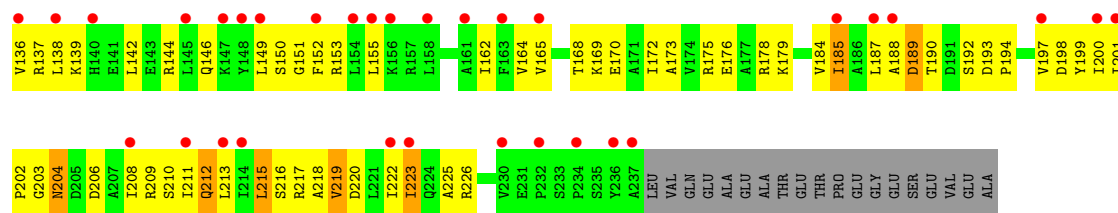


• Molecule 33: 30S ribosomal protein S2

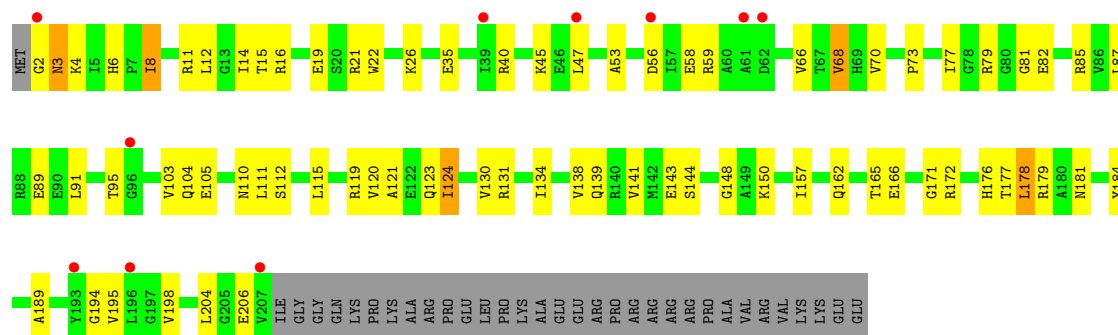


• Molecule 33: 30S ribosomal protein S2

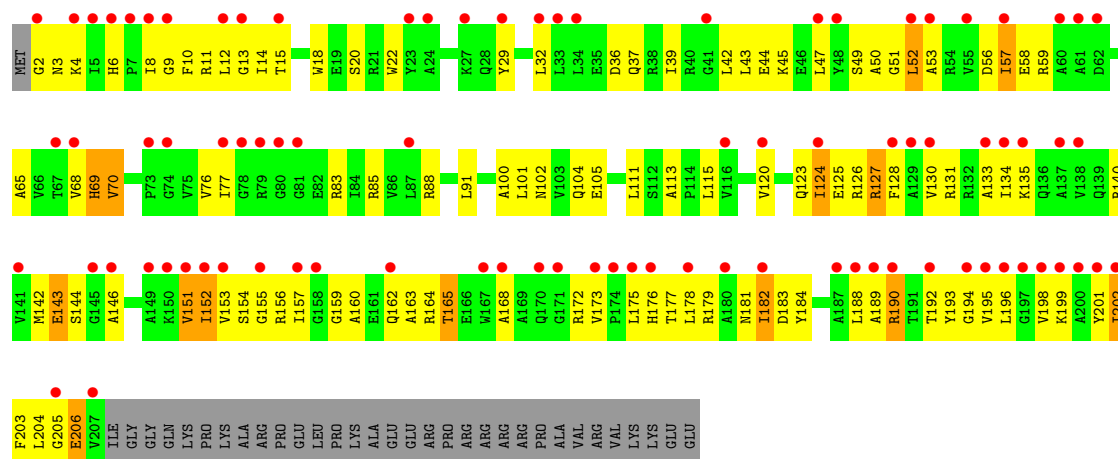




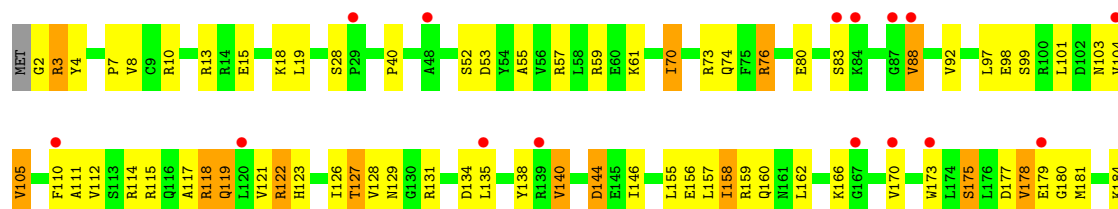
• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3



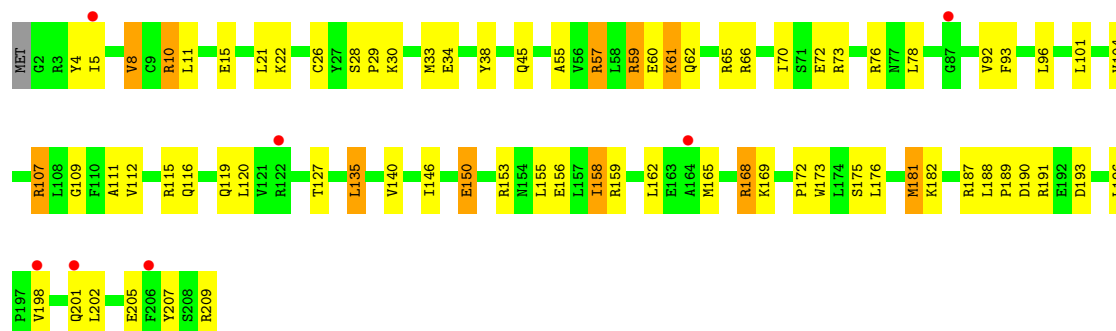
• Molecule 35: 30S ribosomal protein S4



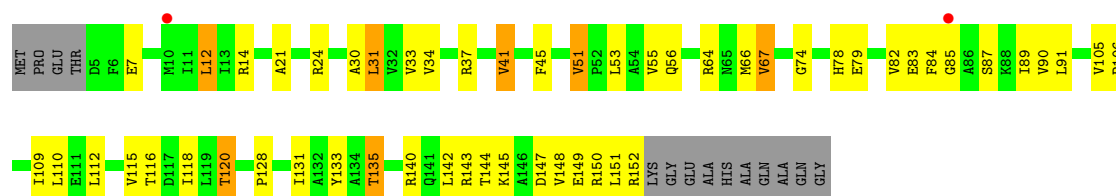




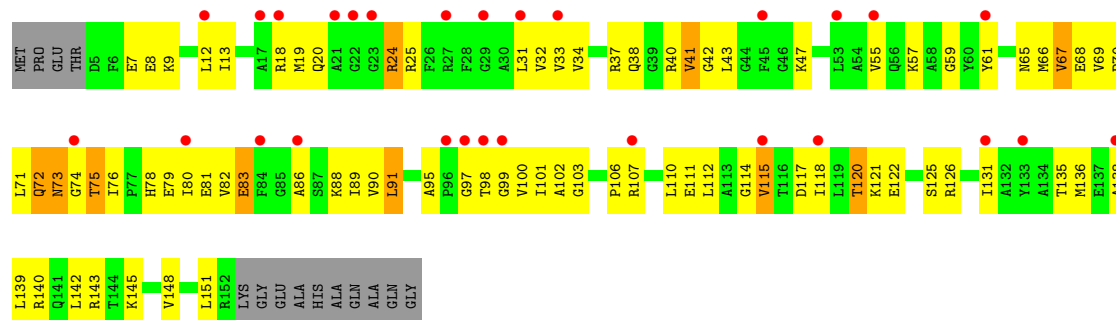
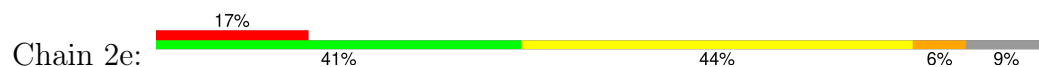
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



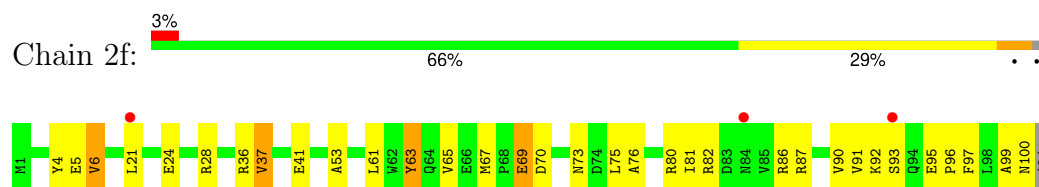
• Molecule 36: 30S ribosomal protein S5



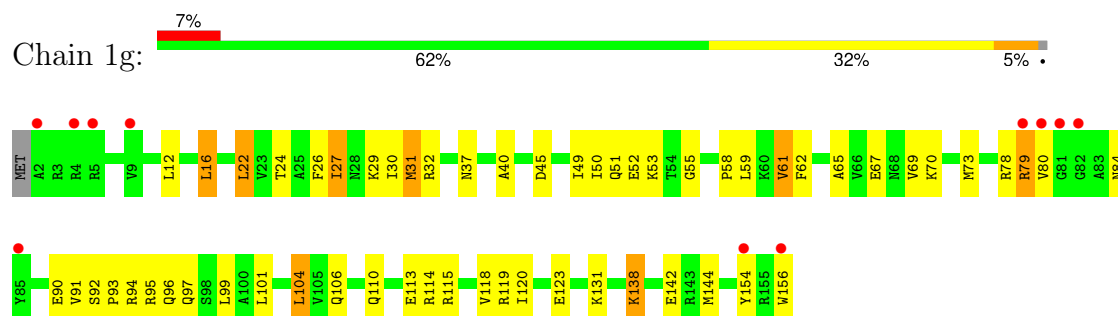
• Molecule 37: 30S ribosomal protein S6



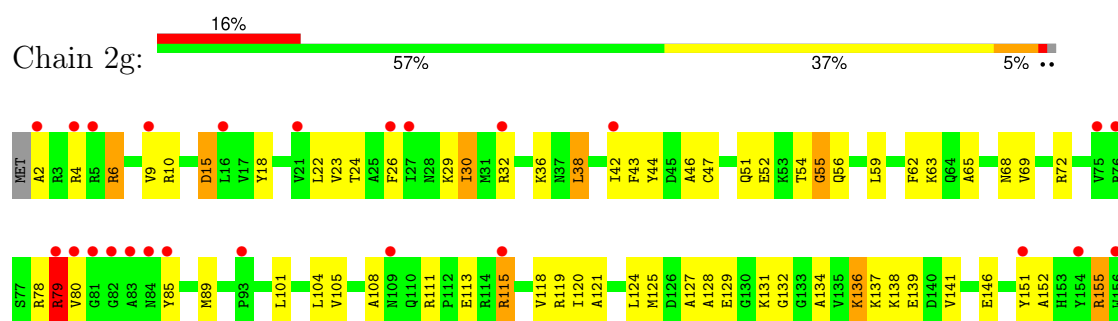
- Molecule 37: 30S ribosomal protein S6



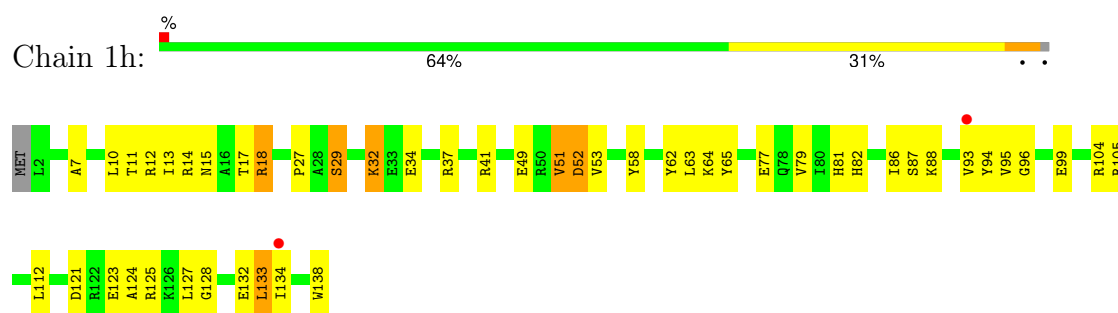
- Molecule 38: 30S ribosomal protein S7



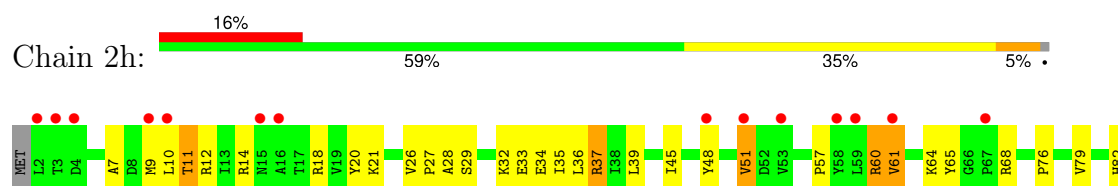
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

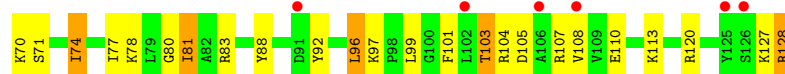


- Molecule 39: 30S ribosomal protein S8

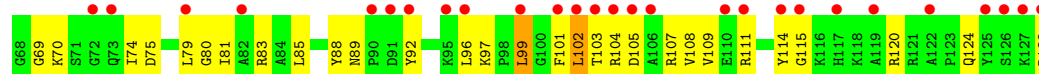
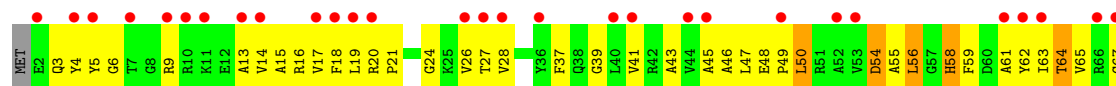
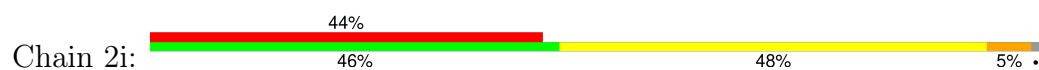




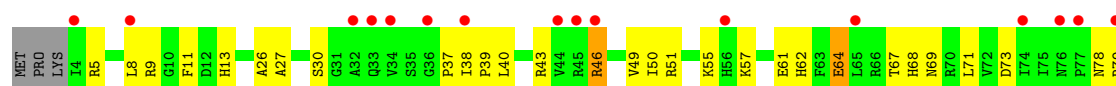
• Molecule 40: 30S ribosomal protein S9



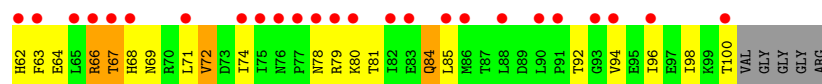
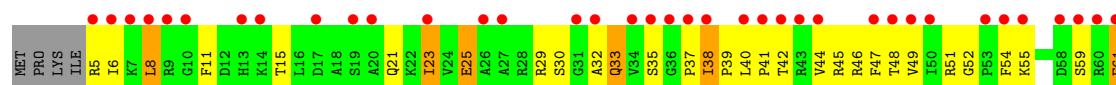
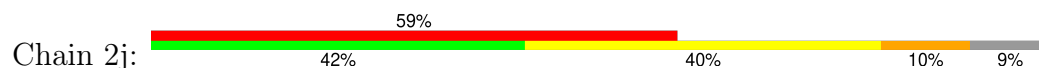
• Molecule 40: 30S ribosomal protein S9



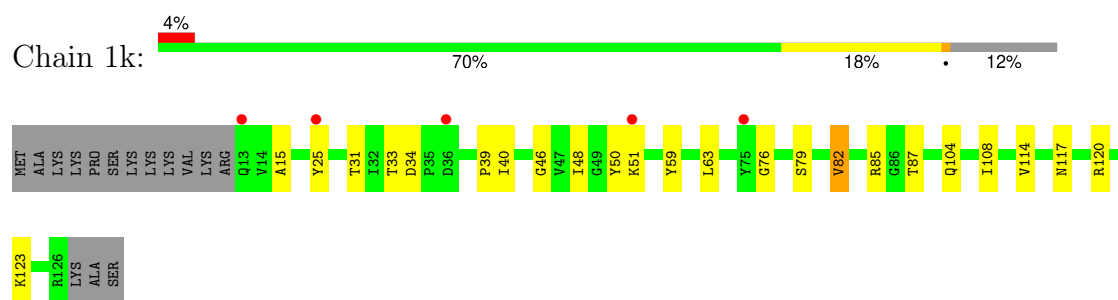
• Molecule 41: 30S ribosomal protein S10



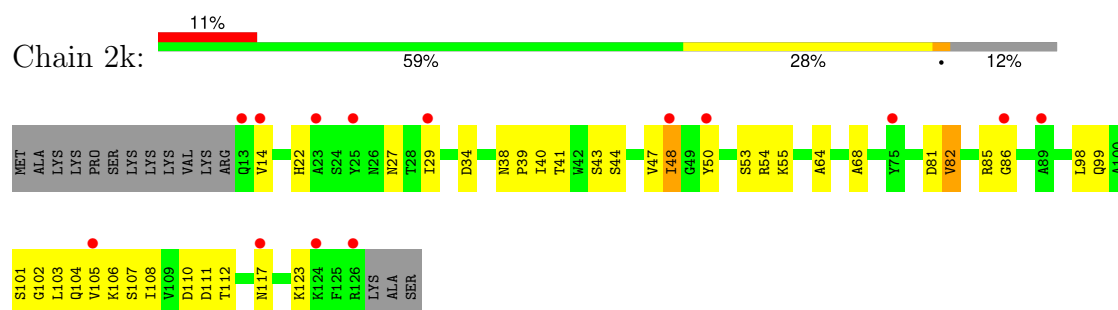
• Molecule 41: 30S ribosomal protein S10



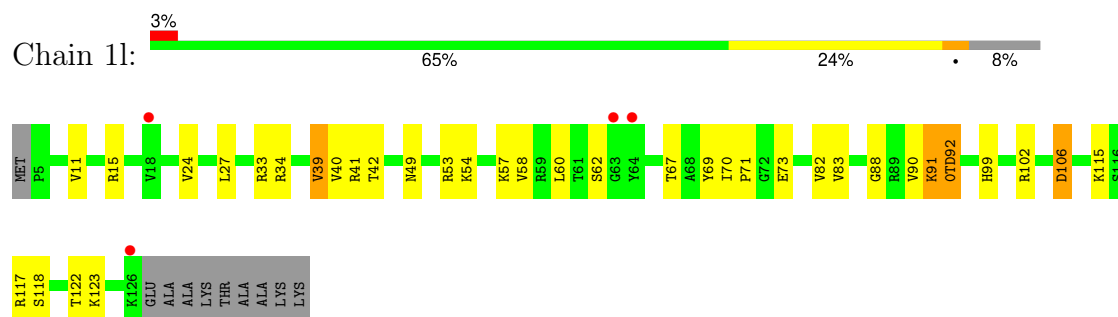
• Molecule 42: 30S ribosomal protein S11



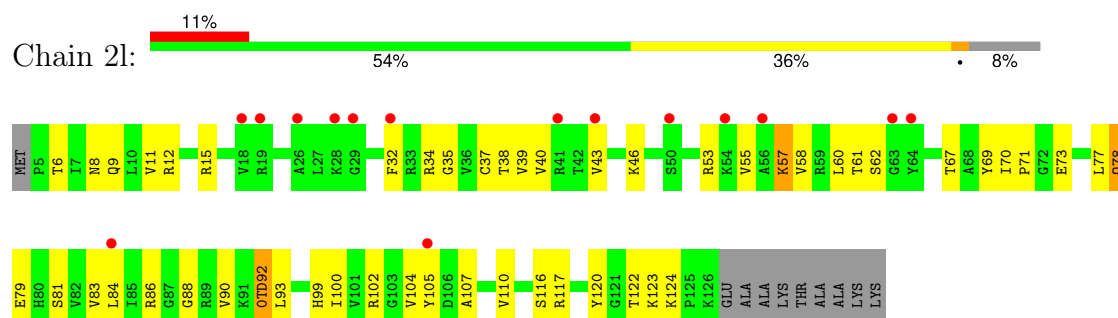
• Molecule 42: 30S ribosomal protein S11



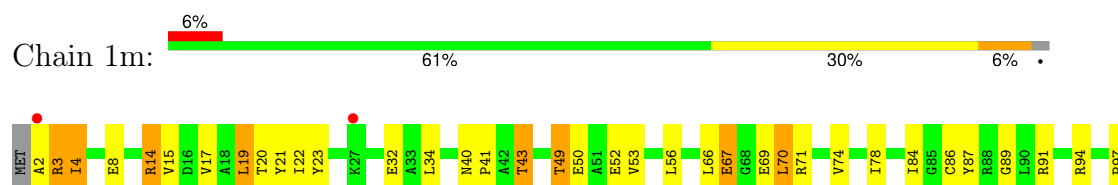
• Molecule 43: 30S ribosomal protein S12



• Molecule 43: 30S ribosomal protein S12

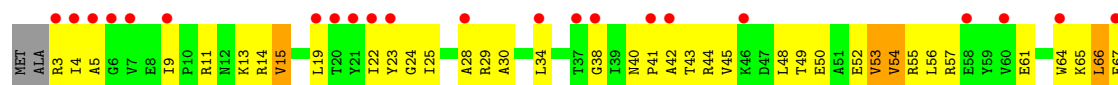
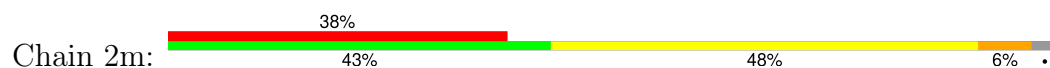


• Molecule 44: 30S ribosomal protein S13





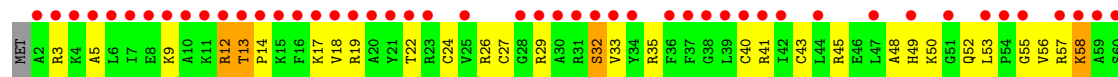
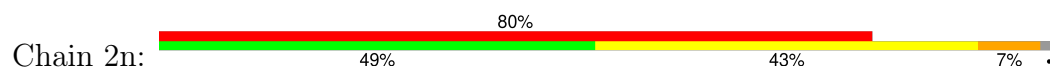
- Molecule 44: 30S ribosomal protein S13



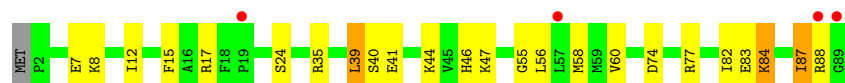
- Molecule 45: 30S ribosomal protein S14 type Z



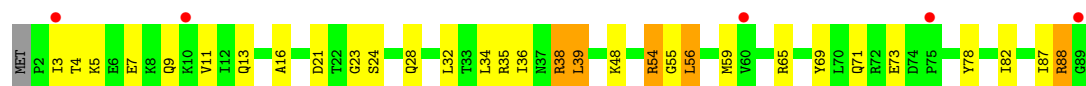
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

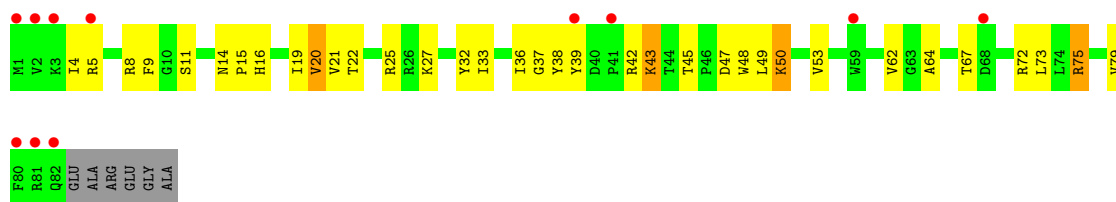


- Molecule 46: 30S ribosomal protein S15

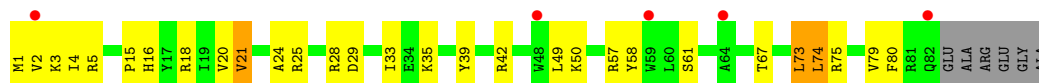


- Molecule 47: 30S ribosomal protein S16

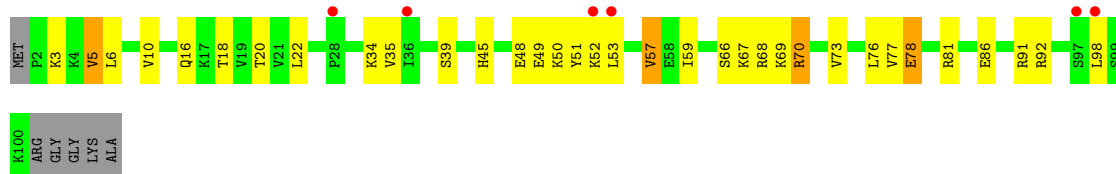




- Molecule 47: 30S ribosomal protein S16



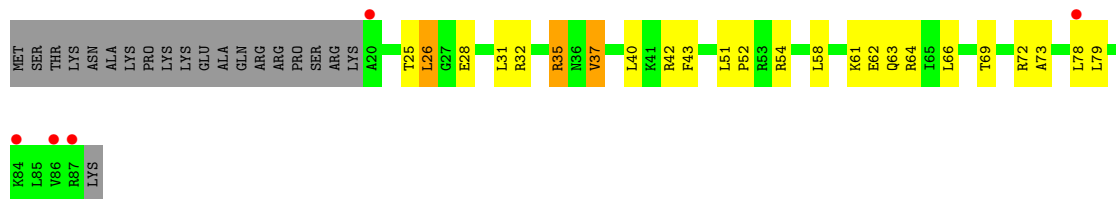
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

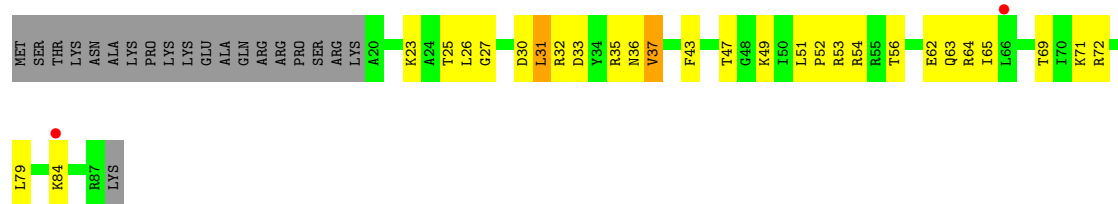


- Molecule 49: 30S ribosomal protein S18

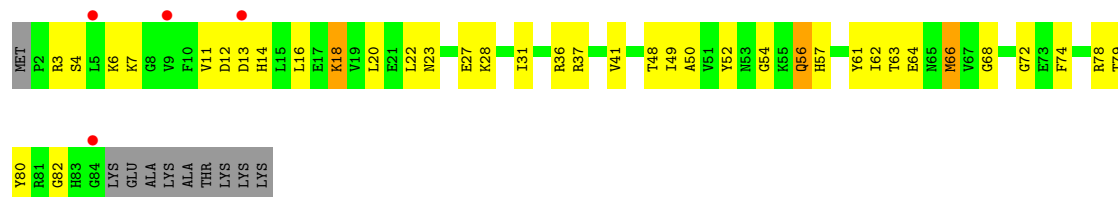


- Molecule 49: 30S ribosomal protein S18

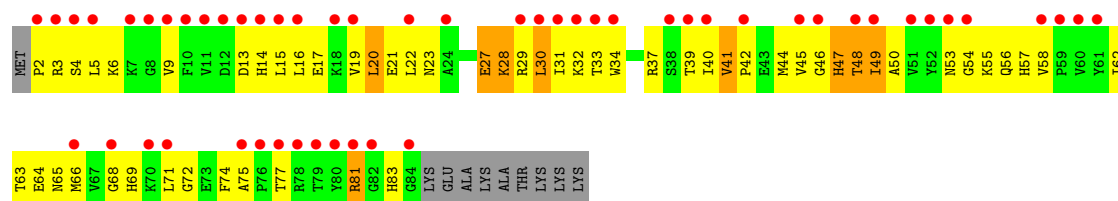




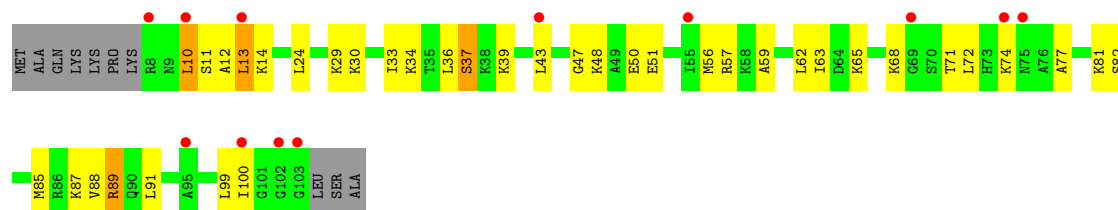
• Molecule 50: 30S ribosomal protein S19



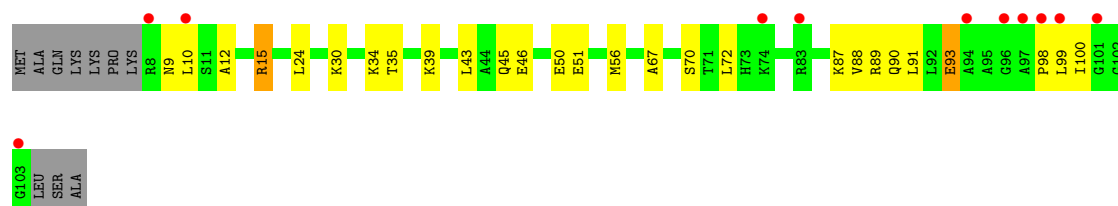
• Molecule 50: 30S ribosomal protein S19



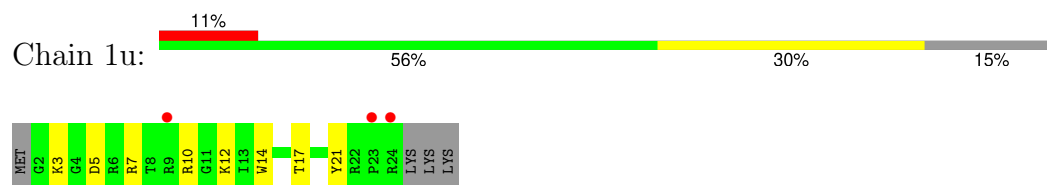
• Molecule 51: 30S ribosomal protein S20



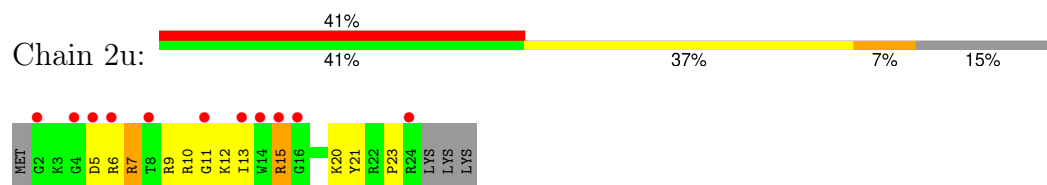
• Molecule 51: 30S ribosomal protein S20



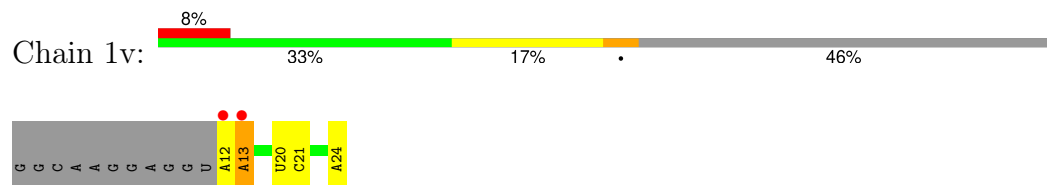
- Molecule 52: 30S ribosomal protein Thx



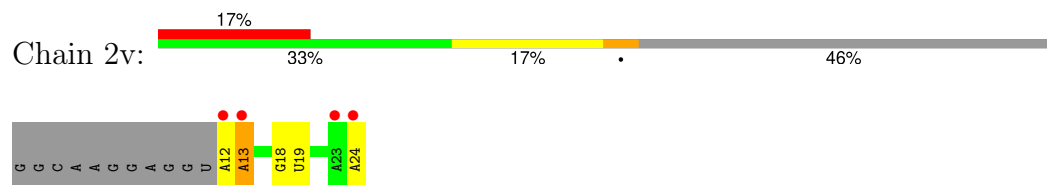
- Molecule 52: 30S ribosomal protein Thx



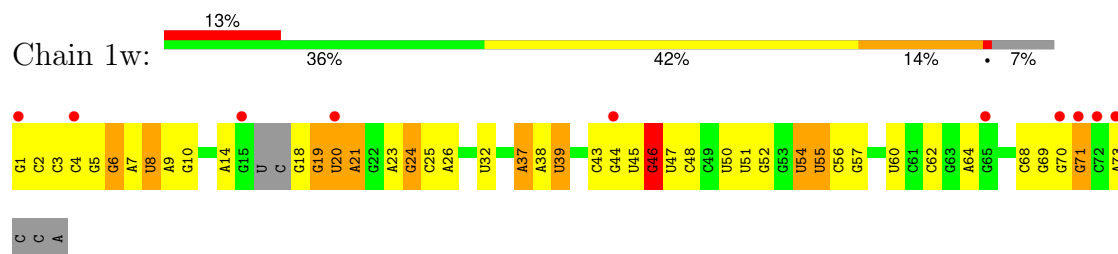
- Molecule 53: MF-mRNA



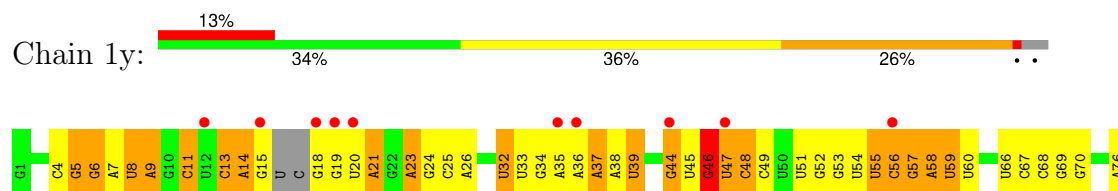
- Molecule 53: MF-mRNA



- Molecule 54: A-site and E-site Deacylated tRNAphe



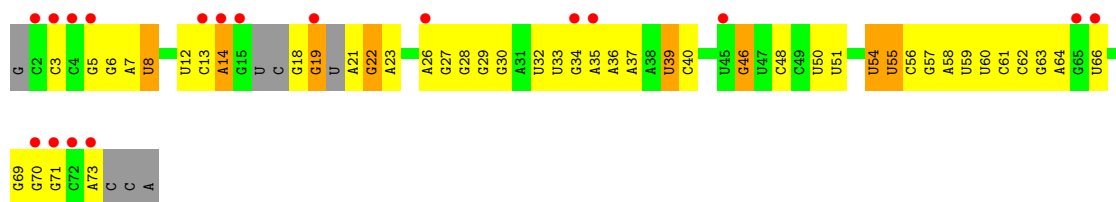
- Molecule 54: A-site and E-site Deacylated tRNAphe



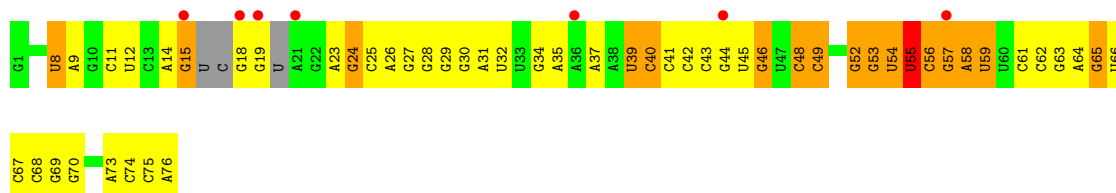
- Molecule 54: A-site and E-site Deacylated tRNAphe



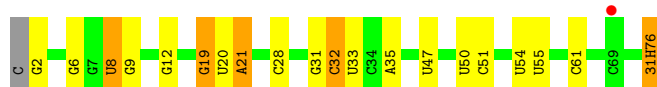
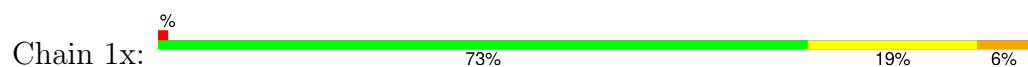




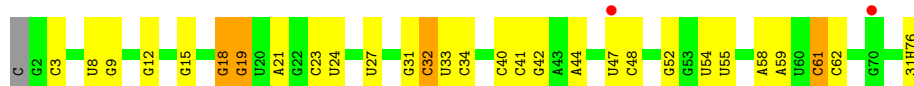
- Molecule 54: A-site and E-site Deacylated tRNA<sup>phe</sup>



- Molecule 55: P-site Aminoacylated fMet-tRNA<sup>met</sup>



- Molecule 55: P-site Aminoacylated fMet-tRNA<sup>met</sup>



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.79Å 449.98Å 627.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.69 – 2.45 123.69 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (123.69-2.45) 99.7 (123.69-2.45)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.217 , 0.265 0.219 , 0.266	Depositor DCC
$R_{free}$ test set	107260 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	300078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PSU, K, OMU, 5MC, 4SU, M2G, 4OC, 2MA, SF4, MIA, 31H, 5MU, A1A1K, OMC, UR3, ZN, OMG, 0TD, MA6, G7M, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1A	0.56	0/69011	0.74	15/107720 (0.0%)
1	2A	0.41	0/67295	0.62	6/105042 (0.0%)
2	1B	0.45	0/2882	0.70	0/4494
2	2B	0.40	0/2879	0.59	0/4487
3	1D	0.53	0/2186	0.73	0/2944
3	2D	0.42	0/2186	0.67	0/2944
4	1E	0.53	0/1592	0.75	0/2149
4	2E	0.38	0/1592	0.64	0/2149
5	1F	0.54	0/1619	0.79	2/2193 (0.1%)
5	2F	0.39	0/1615	0.64	0/2188
6	1G	0.41	0/1448	0.62	0/1957
6	2G	0.38	0/1453	0.59	0/1963
7	1H	0.41	0/1356	0.60	0/1834
7	2H	0.37	0/1356	0.51	0/1834
8	1I	0.38	0/1112	0.63	0/1514
8	2I	0.37	0/1079	0.63	0/1475
9	1N	0.52	0/1144	0.72	0/1543
9	2N	0.37	0/1144	0.59	0/1543
10	1O	0.51	0/943	0.70	0/1269
10	2O	0.40	0/943	0.59	0/1269
11	1P	0.56	0/1152	0.80	0/1533
11	2P	0.40	0/1152	0.64	0/1533
12	1Q	0.57	0/1143	0.73	0/1527
12	2Q	0.38	0/1143	0.60	0/1527
13	1R	0.58	0/982	0.77	1/1312 (0.1%)
13	2R	0.39	0/982	0.61	0/1312
14	1S	0.44	0/883	0.71	0/1176
14	2S	0.42	0/880	0.63	0/1172
15	1T	0.48	0/1105	0.69	0/1477
15	2T	0.38	0/1097	0.62	0/1468
16	1U	0.58	0/977	0.78	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.39	0/977	0.58	0/1301
17	1V	0.54	0/782	0.74	0/1049
17	2V	0.34	0/782	0.58	0/1049
18	1W	0.58	0/897	0.72	0/1205
18	2W	0.42	0/897	0.60	0/1205
19	1X	0.53	0/764	0.78	2/1025 (0.2%)
19	2X	0.38	0/764	0.67	2/1025 (0.2%)
20	1Y	0.44	0/819	0.75	0/1095
20	2Y	0.38	0/819	0.62	0/1095
21	1Z	0.44	0/1267	0.68	1/1717 (0.1%)
21	2Z	0.40	0/1299	0.61	0/1763
22	10	0.58	0/616	0.83	2/821 (0.2%)
22	20	0.42	0/662	0.60	0/881
23	11	0.49	0/762	0.70	0/1014
23	21	0.44	0/762	0.67	0/1014
24	12	0.50	0/590	0.62	0/781
24	22	0.34	0/590	0.52	0/781
25	13	0.56	0/474	0.68	0/635
25	23	0.35	0/469	0.62	0/630
26	14	0.45	0/565	0.82	0/761
26	24	0.44	0/545	0.64	0/737
27	15	0.59	0/469	0.77	0/635
27	25	0.42	0/469	0.54	0/635
28	16	0.54	0/460	0.72	0/613
28	26	0.40	0/456	0.59	0/608
29	17	0.63	0/426	0.82	0/561
29	27	0.50	0/426	0.69	0/561
30	18	0.53	0/525	0.73	0/691
30	28	0.38	0/525	0.60	0/691
31	19	0.55	0/310	0.72	0/407
31	29	0.34	0/310	0.62	0/407
32	1a	0.38	1/35795 (0.0%)	0.59	1/55864 (0.0%)
32	2a	0.38	0/35886	0.57	3/56005 (0.0%)
33	1b	0.39	0/1881	0.68	0/2542
33	2b	0.44	0/1860	0.68	2/2518 (0.1%)
34	1c	0.36	0/1572	0.57	0/2126
34	2c	0.43	0/1566	0.63	0/2119
35	1d	0.33	0/1685	0.60	0/2262
35	2d	0.36	0/1704	0.58	0/2284
36	1e	0.35	0/1145	0.57	0/1543
36	2e	0.41	0/1149	0.61	0/1548
37	1f	0.36	0/823	0.54	0/1115
37	2f	0.36	0/829	0.53	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.33	0/1250	0.53	0/1679
38	2g	0.35	0/1254	0.52	0/1683
39	1h	0.33	0/1108	0.56	0/1494
39	2h	0.33	0/1108	0.59	0/1494
40	1i	0.33	0/1002	0.62	0/1346
40	2i	0.40	0/997	0.63	0/1343
41	1j	0.38	0/722	0.56	0/982
41	2j	0.44	0/727	0.62	0/988
42	1k	0.37	0/844	0.60	0/1145
42	2k	0.34	0/848	0.51	0/1149
43	1l	0.41	0/937	0.66	0/1260
43	2l	0.36	0/937	0.62	2/1260 (0.2%)
44	1m	0.38	0/969	0.61	0/1302
44	2m	0.41	0/961	0.60	0/1291
45	1n	0.34	0/501	0.64	0/664
45	2n	0.45	0/501	0.66	0/664
46	1o	0.39	0/739	0.55	0/985
46	2o	0.34	0/739	0.54	0/985
47	1p	0.36	0/697	0.64	0/939
47	2p	0.37	0/693	0.63	0/935
48	1q	0.39	0/836	0.60	0/1117
48	2q	0.36	0/836	0.55	0/1117
49	1r	0.38	0/560	0.61	0/746
49	2r	0.34	0/560	0.58	0/746
50	1s	0.36	0/667	0.65	0/900
50	2s	0.47	0/661	0.80	2/893 (0.2%)
51	1t	0.35	0/730	0.62	0/965
51	2t	0.38	0/729	0.60	0/965
52	1u	0.32	0/203	0.57	0/266
52	2u	0.40	0/203	0.58	0/266
53	1v	0.41	0/310	0.52	0/480
53	2v	0.43	0/310	0.54	0/480
54	1w	0.51	2/1537 (0.1%)	0.55	0/2390
54	1y	0.46	2/1606 (0.1%)	0.56	0/2497
54	2w	0.55	2/1487 (0.1%)	0.59	0/2311
54	2y	0.47	2/1583 (0.1%)	0.53	0/2459
55	1x	0.46	1/1700 (0.1%)	0.64	0/2650
55	2x	0.40	1/1700 (0.1%)	0.58	0/2650
All	All	0.45	11/316456 (0.0%)	0.65	41/473777 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	1E	0	1
4	2E	0	1
5	2F	0	1
6	1G	0	1
6	2G	0	1
11	1P	0	3
11	2P	0	3
21	1Z	0	1
21	2Z	0	1
23	1I	0	1
26	14	0	1
33	1b	0	1
33	2b	0	2
38	2g	0	1
44	1m	0	1
44	2m	0	1
All	All	0	21

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	46	G7M	O3'-P	5.94	1.62	1.56
54	1y	8	4SU	O3'-P	5.68	1.61	1.56
54	1w	46	G7M	O3'-P	5.47	1.61	1.56
54	1y	46	G7M	O3'-P	5.39	1.61	1.56
54	1w	8	4SU	O3'-P	5.35	1.61	1.56

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	11.11	126.17	109.50
1	1A	2689	U	P-O3'-C3'	8.45	132.87	120.20
1	1A	2689	U	C2'-C3'-O3'	8.23	121.85	109.50
1	2A	1992	G	C2'-C3'-O3'	8.13	121.70	109.50
22	10	12	ASN	CA-C-N	-7.59	106.54	121.41

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1E	70	ALA	Peptide

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Mol	Chain	Res	Type	Group
6	1G	95	ARG	Peptide
11	1P	28	GLY	Peptide
11	1P	35	HIS	Peptide
11	1P	43	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	633	0
1	2A	60322	0	30428	886	0
2	1B	2577	0	1305	31	0
2	2B	2575	0	1303	68	0
3	1D	2136	0	2218	38	0
3	2D	2136	0	2218	46	0
4	1E	1559	0	1618	36	0
4	2E	1559	0	1618	45	0
5	1F	1584	0	1625	31	0
5	2F	1580	0	1619	51	0
6	1G	1423	0	1436	34	0
6	2G	1428	0	1438	79	0
7	1H	1330	0	1407	29	0
7	2H	1330	0	1407	50	0
8	1I	1097	0	1140	41	0
8	2I	1064	0	1082	41	0
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	28	0
10	1O	933	0	996	17	0
10	2O	933	0	996	27	0
11	1P	1135	0	1212	36	0
11	2P	1135	0	1212	49	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1179	37	0
13	1R	968	0	1033	22	0
13	2R	968	0	1033	28	0
14	1S	873	0	927	25	0
14	2S	870	0	923	46	0
15	1T	1091	0	1151	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	23	0
17	1V	771	0	830	17	0
17	2V	771	0	830	17	0
18	1W	886	0	940	9	0
18	2W	886	0	940	10	0
19	1X	750	0	814	14	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	22	0
21	1Z	1240	0	1240	46	0
21	2Z	1271	0	1273	75	0
22	10	608	0	622	11	0
22	20	653	0	674	29	0
23	11	755	0	826	18	0
23	21	755	0	826	19	0
24	12	588	0	643	15	0
24	22	588	0	643	12	0
25	13	469	0	518	8	0
25	23	464	0	514	26	0
26	14	552	0	533	32	0
26	24	532	0	503	37	0
27	15	455	0	465	5	0
27	25	455	0	465	11	0
28	16	453	0	473	8	0
28	26	449	0	469	11	0
29	17	418	0	467	5	0
29	27	418	0	467	9	0
30	18	517	0	582	12	0
30	28	517	0	582	16	0
31	19	307	0	335	1	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	514	0
32	2a	32327	0	16338	742	0
33	1b	1846	0	1867	93	0
33	2b	1825	0	1828	124	0
34	1c	1548	0	1535	45	0
34	2c	1542	0	1517	84	0
35	1d	1655	0	1672	60	0
35	2d	1674	0	1714	60	0
36	1e	1129	0	1185	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	2e	1133	0	1191	64	0
37	1f	810	0	804	16	0
37	2f	816	0	808	29	0
38	1g	1231	0	1238	36	0
38	2g	1235	0	1249	51	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	39	0
40	1i	983	0	986	48	0
40	2i	978	0	966	61	0
41	1j	709	0	650	35	0
41	2j	714	0	672	47	0
42	1k	829	0	825	13	0
42	2k	833	0	836	25	0
43	1l	932	0	981	20	0
43	2l	932	0	981	31	0
44	1m	958	0	1002	30	0
44	2m	950	0	988	69	0
45	1n	492	0	529	22	0
45	2n	492	0	529	30	0
46	1o	728	0	760	17	0
46	2o	728	0	760	24	0
47	1p	681	0	697	32	0
47	2p	677	0	686	22	0
48	1q	823	0	891	22	0
48	2q	823	0	891	24	0
49	1r	555	0	618	16	0
49	2r	555	0	618	24	0
50	1s	652	0	662	26	0
50	2s	646	0	644	50	0
51	1t	728	0	798	30	0
51	2t	727	0	796	18	0
52	1u	199	0	208	6	0
52	2u	199	0	208	10	0
53	1v	277	0	140	4	0
53	2v	277	0	140	9	0
54	1w	1530	0	785	28	0
54	1y	1585	0	803	29	0
54	2w	1482	0	754	25	0
54	2y	1565	0	794	42	0
55	1x	1635	0	838	11	0
55	2x	1635	0	839	17	0
56	10	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	4	0	0	0	0
56	15	7	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	7	0	0	0	0
56	19	1	0	0	0	0
56	1A	1103	0	0	0	0
56	1B	37	0	0	0	0
56	1D	12	0	0	0	0
56	1E	17	0	0	0	0
56	1F	13	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	6	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	4	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	12	0	0	0	0
56	1V	7	0	0	0	0
56	1W	7	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	215	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	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	8	0	0	0	0
56	1x	14	0	0	0	0
56	1y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	20	4	0	0	0	0
56	21	2	0	0	0	0
56	23	1	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	2	0	0	0	0
56	28	3	0	0	0	0
56	29	1	0	0	0	0
56	2A	885	0	0	0	0
56	2B	20	0	0	0	0
56	2D	7	0	0	0	0
56	2E	10	0	0	0	0
56	2F	5	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	3	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	1	0	0	0	0
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	241	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
56	2j	1	0	0	0	0
56	2l	4	0	0	0	0
56	2p	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	7	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2x	1	0	0	0	0
58	1A	34	0	0	1	0
58	2A	34	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	1	0
60	2d	8	0	0	1	0
61	10	12	0	0	2	0
61	11	12	0	0	0	0
61	12	4	0	0	1	0
61	13	4	0	0	0	0
61	15	5	0	0	0	0
61	16	3	0	0	0	0
61	17	7	0	0	0	0
61	18	11	0	0	1	0
61	1A	2018	0	0	79	0
61	1B	62	0	0	2	0
61	1D	26	0	0	0	0
61	1E	27	0	0	2	0
61	1F	17	0	0	0	0
61	1G	3	0	0	1	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	6	0	0	1	0
61	1O	7	0	0	1	0
61	1P	23	0	0	1	0
61	1Q	7	0	0	0	0
61	1R	13	0	0	5	0
61	1S	5	0	0	0	0
61	1T	8	0	0	0	0
61	1U	15	0	0	0	0
61	1V	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1W	8	0	0	2	0
6l	1X	5	0	0	0	0
6l	1Y	2	0	0	1	0
6l	1Z	1	0	0	0	0
6l	1a	378	0	0	29	0
6l	1b	1	0	0	0	0
6l	1e	1	0	0	0	0
6l	1f	1	0	0	0	0
6l	1i	1	0	0	0	0
6l	1l	8	0	0	1	0
6l	1o	1	0	0	0	0
6l	1p	1	0	0	0	0
6l	1q	2	0	0	0	0
6l	1u	1	0	0	1	0
6l	1v	4	0	0	0	0
6l	1w	10	0	0	1	0
6l	1x	16	0	0	0	0
6l	1y	2	0	0	0	0
6l	20	6	0	0	0	0
6l	21	13	0	0	0	0
6l	23	1	0	0	1	0
6l	25	1	0	0	0	0
6l	26	1	0	0	1	0
6l	27	5	0	0	0	0
6l	28	3	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	1160	0	0	82	0
6l	2B	23	0	0	0	0
6l	2D	22	0	0	0	0
6l	2E	12	0	0	0	0
6l	2F	13	0	0	1	0
6l	2I	3	0	0	1	0
6l	2O	3	0	0	0	0
6l	2P	15	0	0	2	0
6l	2Q	1	0	0	0	0
6l	2R	4	0	0	0	0
6l	2T	5	0	0	0	0
6l	2U	4	0	0	0	0
6l	2W	3	0	0	0	0
6l	2X	2	0	0	0	0
6l	2Z	1	0	0	0	0
6l	2a	264	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	2d	2	0	0	0	0
6l	2e	2	0	0	0	0
6l	2j	3	0	0	2	0
6l	2l	6	0	0	1	0
6l	2p	1	0	0	0	0
6l	2q	1	0	0	0	0
6l	2r	1	0	0	0	0
6l	2t	3	0	0	0	0
6l	2v	2	0	0	0	0
6l	2w	1	0	0	0	0
6l	2x	7	0	0	0	0
6l	2y	6	0	0	0	0
All	All	300078	0	196592	5320	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 11.

The worst 5 of 5320 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.30	1.28
1:1A:1054:A:N6	1:1A:1105:U:H3	1.52	1.06
1:1A:2499:C:OP1	61:1A:4203:HOH:O	1.75	1.04
1:2A:2714:G:OP2	61:2A:3901:HOH:O	1.78	1.02
1:1A:1082:U:O4	1:1A:1086:A:N1	1.93	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	13	14
4	2E	202/206 (98%)	190 (94%)	12 (6%)	0	100	100
5	1F	201/210 (96%)	194 (96%)	7 (4%)	0	100	100
5	2F	201/210 (96%)	184 (92%)	17 (8%)	0	100	100
6	1G	179/182 (98%)	165 (92%)	13 (7%)	1 (1%)	22	28
6	2G	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	22	28
7	1H	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
7	2H	172/180 (96%)	160 (93%)	12 (7%)	0	100	100
8	1I	144/148 (97%)	123 (85%)	21 (15%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	21 (15%)	0	100	100
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
11	1P	147/150 (98%)	133 (90%)	13 (9%)	1 (1%)	19	24
11	2P	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	19	24
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	91 (84%)	17 (16%)	0	100	100
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
17	2V	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	13	14
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	13	14
21	1Z	148/206 (72%)	129 (87%)	17 (12%)	2 (1%)	9	9
21	2Z	156/206 (76%)	128 (82%)	26 (17%)	2 (1%)	10	10
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
23	11	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	47 (70%)	20 (30%)	0	100	100
26	24	67/71 (94%)	47 (70%)	19 (28%)	1 (2%)	8	8
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	186 (81%)	41 (18%)	2 (1%)	14	18
33	2b	229/256 (90%)	181 (79%)	44 (19%)	4 (2%)	7	6
34	1c	204/239 (85%)	188 (92%)	16 (8%)	0	100	100
34	2c	204/239 (85%)	160 (78%)	44 (22%)	0	100	100
35	1d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	13 (9%)	0	100	100
36	2e	146/162 (90%)	124 (85%)	22 (15%)	0	100	100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
38	2g	153/156 (98%)	135 (88%)	17 (11%)	1 (1%)	19	24
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	119 (88%)	16 (12%)	0	100	100
40	1i	125/128 (98%)	104 (83%)	21 (17%)	0	100	100
40	2i	125/128 (98%)	103 (82%)	22 (18%)	0	100	100
41	1j	95/105 (90%)	78 (82%)	16 (17%)	1 (1%)	12	13
41	2j	94/105 (90%)	78 (83%)	15 (16%)	1 (1%)	12	13
42	1k	112/129 (87%)	101 (90%)	11 (10%)	0	100	100
42	2k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
43	1l	119/132 (90%)	111 (93%)	6 (5%)	2 (2%)	7	6
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	121/126 (96%)	103 (85%)	18 (15%)	0	100	100
44	2m	120/126 (95%)	99 (82%)	21 (18%)	0	100	100
45	1n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	6
45	2n	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	1
46	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	57 (86%)	9 (14%)	0	100	100
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
50	2s	81/93 (87%)	64 (79%)	17 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	81 (86%)	13 (14%)	0	100	100
51	2t	94/106 (89%)	82 (87%)	12 (13%)	0	100	100
52	1u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11364/12128 (94%)	10319 (91%)	1018 (9%)	27 (0%)	44	54

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	36	LYS
21	1Z	53	ILE
21	2Z	52	SER
33	2b	10	LEU
6	1G	96	ARG

### 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%)	198 (92%)	17 (8%)	10	11
3	2D	215/218 (99%)	193 (90%)	22 (10%)	6	5
4	1E	164/166 (99%)	153 (93%)	11 (7%)	13	17
4	2E	164/166 (99%)	146 (89%)	18 (11%)	5	4
5	1F	160/166 (96%)	139 (87%)	21 (13%)	3	2
5	2F	159/166 (96%)	135 (85%)	24 (15%)	2	1
6	1G	143/156 (92%)	128 (90%)	15 (10%)	5	5
6	2G	143/156 (92%)	117 (82%)	26 (18%)	1	0
7	1H	144/148 (97%)	128 (89%)	16 (11%)	5	4
7	2H	144/148 (97%)	119 (83%)	25 (17%)	1	0
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	0
8	2I	105/124 (85%)	78 (74%)	27 (26%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	110 (93%)	8 (7%)	13	16
9	2N	118/119 (99%)	104 (88%)	14 (12%)	4	3
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	51
10	2O	100/100 (100%)	93 (93%)	7 (7%)	12	15
11	1P	115/116 (99%)	109 (95%)	6 (5%)	19	27
11	2P	115/116 (99%)	108 (94%)	7 (6%)	15	21
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	18	26
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	15	20
13	1R	101/101 (100%)	97 (96%)	4 (4%)	27	39
13	2R	101/101 (100%)	94 (93%)	7 (7%)	13	16
14	1S	86/88 (98%)	77 (90%)	9 (10%)	5	5
14	2S	85/88 (97%)	72 (85%)	13 (15%)	2	1
15	1T	115/127 (91%)	106 (92%)	9 (8%)	10	12
15	2T	113/127 (89%)	107 (95%)	6 (5%)	19	27
16	1U	93/94 (99%)	86 (92%)	7 (8%)	11	13
16	2U	93/94 (99%)	84 (90%)	9 (10%)	6	6
17	1V	80/82 (98%)	73 (91%)	7 (9%)	8	8
17	2V	80/82 (98%)	74 (92%)	6 (8%)	11	13
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	47
18	2W	90/92 (98%)	84 (93%)	6 (7%)	13	17
19	1X	77/78 (99%)	72 (94%)	5 (6%)	14	18
19	2X	77/78 (99%)	70 (91%)	7 (9%)	7	7
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	3	2
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	2	1
21	1Z	135/179 (75%)	121 (90%)	14 (10%)	5	5
21	2Z	137/179 (76%)	118 (86%)	19 (14%)	3	2
22	10	61/67 (91%)	58 (95%)	3 (5%)	21	30
22	20	65/67 (97%)	62 (95%)	3 (5%)	23	33
23	11	80/83 (96%)	77 (96%)	3 (4%)	28	41
23	21	80/83 (96%)	76 (95%)	4 (5%)	20	29
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	58 (89%)	7 (11%)	5	4
25	13	51/52 (98%)	45 (88%)	6 (12%)	4	3
25	23	50/52 (96%)	46 (92%)	4 (8%)	10	11
26	14	59/63 (94%)	52 (88%)	7 (12%)	4	3
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	0
27	15	50/52 (96%)	48 (96%)	2 (4%)	27	39
27	25	50/52 (96%)	44 (88%)	6 (12%)	4	3
28	16	51/52 (98%)	45 (88%)	6 (12%)	4	3
28	26	50/52 (96%)	44 (88%)	6 (12%)	4	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	11	14
29	27	41/42 (98%)	38 (93%)	3 (7%)	11	14
30	18	54/55 (98%)	51 (94%)	3 (6%)	17	24
30	28	54/55 (98%)	50 (93%)	4 (7%)	11	13
31	19	34/34 (100%)	32 (94%)	2 (6%)	16	23
31	29	34/34 (100%)	32 (94%)	2 (6%)	16	23
33	1b	192/220 (87%)	167 (87%)	25 (13%)	3	2
33	2b	187/220 (85%)	153 (82%)	34 (18%)	1	0
34	1c	142/188 (76%)	121 (85%)	21 (15%)	2	1
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2	1
35	1d	169/181 (93%)	139 (82%)	30 (18%)	1	0
35	2d	173/181 (96%)	153 (88%)	20 (12%)	4	3
36	1e	113/123 (92%)	97 (86%)	16 (14%)	2	2
36	2e	114/123 (93%)	93 (82%)	21 (18%)	1	0
37	1f	84/90 (93%)	74 (88%)	10 (12%)	4	3
37	2f	85/90 (94%)	79 (93%)	6 (7%)	12	15
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	1
38	2g	120/127 (94%)	106 (88%)	14 (12%)	4	3
39	1h	114/119 (96%)	106 (93%)	8 (7%)	12	15
39	2h	114/119 (96%)	101 (89%)	13 (11%)	4	4
40	1i	90/99 (91%)	79 (88%)	11 (12%)	4	3
40	2i	89/99 (90%)	77 (86%)	12 (14%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	61 (92%)	5 (8%)	11	13
41	2j	69/92 (75%)	56 (81%)	13 (19%)	1	0
42	1k	82/99 (83%)	75 (92%)	7 (8%)	8	9
42	2k	83/99 (84%)	76 (92%)	7 (8%)	9	9
43	1l	96/108 (89%)	88 (92%)	8 (8%)	9	10
43	2l	96/108 (89%)	89 (93%)	7 (7%)	11	14
44	1m	93/101 (92%)	78 (84%)	15 (16%)	2	1
44	2m	92/101 (91%)	81 (88%)	11 (12%)	4	3
45	1n	49/50 (98%)	42 (86%)	7 (14%)	2	2
45	2n	49/50 (98%)	39 (80%)	10 (20%)	1	0
46	1o	78/80 (98%)	71 (91%)	7 (9%)	8	8
46	2o	78/80 (98%)	72 (92%)	6 (8%)	10	12
47	1p	69/74 (93%)	61 (88%)	8 (12%)	4	3
47	2p	68/74 (92%)	60 (88%)	8 (12%)	4	3
48	1q	94/97 (97%)	83 (88%)	11 (12%)	4	3
48	2q	94/97 (97%)	82 (87%)	12 (13%)	3	2
49	1r	59/77 (77%)	52 (88%)	7 (12%)	4	3
49	2r	59/77 (77%)	53 (90%)	6 (10%)	6	5
50	1s	69/80 (86%)	61 (88%)	8 (12%)	4	3
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	0
51	1t	70/82 (85%)	64 (91%)	6 (9%)	8	9
51	2t	70/82 (85%)	65 (93%)	5 (7%)	12	15
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2	1
All	All	9299/10064 (92%)	8282 (89%)	1017 (11%)	5	4

5 of 1017 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2D	32	SER
38	2g	115	ARG
7	2H	141	VAL
38	2g	6	ARG
44	2m	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	162	GLN
49	2r	63	GLN
35	2d	123	HIS
40	2i	3	GLN
37	1f	100	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	439 (15%)	40 (1%)
1	2A	2791/2915 (95%)	499 (17%)	39 (1%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	29 (24%)	0
32	1a	1497/1521 (98%)	239 (15%)	0
32	2a	1501/1521 (98%)	313 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	69/76 (90%)	23 (33%)	0
54	1y	72/76 (94%)	24 (33%)	0
54	2w	66/76 (86%)	16 (24%)	0
54	2y	70/76 (92%)	20 (28%)	0
55	1x	74/77 (96%)	6 (8%)	0
55	2x	74/77 (96%)	8 (10%)	0
All	All	9339/9620 (97%)	1632 (17%)	79 (0%)

5 of 1632 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	36	G
1	1A	45	C

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	856	C
1	2A	2119	A
1	2A	974	G

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Mol	Chain	Res	Type
1	2A	1530	C
1	2A	2439	A

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

86 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
54	4SU	1w	8	54	18,21,22	1.70	5 (27%)	25,30,33	1.95	5 (20%)
54	PSU	1w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.89	3 (14%)
43	0TD	1l	92	43	8,9,10	4.23	3 (37%)	6,11,13	6.30	2 (33%)
54	G7M	1y	46	54	20,26,27	1.32	1 (5%)	16,39,42	0.69	0
1	2MA	1A	2503	56,1	18,25,26	0.73	0	20,37,40	1.80	1 (5%)
1	5MU	1A	1939	56,1	19,22,23	1.49	4 (21%)	27,32,35	2.62	6 (22%)
55	PSU	1x	55	55	18,21,22	1.31	1 (5%)	21,30,33	1.87	4 (19%)
32	MA6	2a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	2.09	4 (22%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	1.91	4 (19%)
1	OMU	2A	2552	56,1	19,22,23	1.18	3 (15%)	25,31,34	1.66	5 (20%)
1	5MC	1A	1942	1	19,22,23	1.43	3 (15%)	26,32,35	1.31	4 (15%)
54	PSU	2y	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.03	5 (23%)
32	UR3	1a	1498	32	19,22,23	1.16	2 (10%)	26,32,35	1.76	5 (19%)
54	MIA	2y	37	54	17,24,32	1.03	1 (5%)	16,35,47	1.32	2 (12%)
54	MIA	1y	37	54	17,24,32	1.03	1 (5%)	16,35,47	1.37	2 (12%)
54	PSU	1y	55	54	18,21,22	1.44	1 (5%)	21,30,33	2.08	4 (19%)
32	4OC	2a	1402	32,56	20,23,24	0.80	1 (5%)	25,32,35	1.06	2 (8%)
54	PSU	2y	39	54	18,21,22	1.30	2 (11%)	21,30,33	1.84	4 (19%)
32	G7M	2a	527	32,56	20,26,27	1.36	2 (10%)	16,39,42	0.66	0
32	5MC	2a	1407	32	19,22,23	1.43	3 (15%)	26,32,35	1.36	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.84	3 (15%)	26,32,35	1.32	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	PSU	1w	55	54	18,21,22	1.45	2 (11%)	21,30,33	1.99	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.96	3 (14%)
32	MA6	1a	1519	32	19,26,27	1.06	1 (5%)	18,38,41	1.75	3 (16%)
32	4OC	1a	1402	32	20,23,24	0.84	1 (5%)	25,32,35	1.10	2 (8%)
1	PSU	2A	2605	1	18,21,22	1.27	3 (16%)	21,30,33	2.21	5 (23%)
54	PSU	1w	39	54	18,21,22	1.28	2 (11%)	21,30,33	2.23	4 (19%)
54	G7M	2w	46	54	20,26,27	1.29	1 (5%)	16,39,42	1.04	2 (12%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	0.92	0
32	PSU	2a	516	32	18,21,22	1.30	1 (5%)	21,30,33	1.88	4 (19%)
32	5MC	1a	1400	32	19,22,23	1.50	3 (15%)	26,32,35	1.36	4 (15%)
54	PSU	1y	32	54	18,21,22	1.37	3 (16%)	21,30,33	1.81	3 (14%)
54	PSU	2y	32	54	18,21,22	1.40	1 (5%)	21,30,33	1.98	3 (14%)
32	M2G	2a	966	32	20,27,28	1.28	3 (15%)	19,40,43	1.22	2 (10%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
55	5MU	2x	54	55	19,22,23	1.45	5 (26%)	27,32,35	2.25	7 (25%)
1	5MU	2A	1939	56,1	19,22,23	1.52	4 (21%)	27,32,35	2.57	6 (22%)
54	G7M	1w	46	54	20,26,27	1.33	1 (5%)	16,39,42	0.76	1 (6%)
1	PSU	1A	2605	56,1	18,21,22	1.66	3 (16%)	21,30,33	2.24	5 (23%)
32	MA6	1a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.93	4 (22%)
1	PSU	1A	1917	1	18,21,22	1.38	3 (16%)	21,30,33	2.14	4 (19%)
32	UR3	2a	1498	32,56	19,22,23	1.05	2 (10%)	26,32,35	1.96	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.72	0	25,31,34	0.88	1 (4%)
43	0TD	2l	92	43	8,9,10	4.69	1 (12%)	6,11,13	4.41	2 (33%)
54	4SU	2y	8	54	18,21,22	1.64	5 (27%)	25,30,33	2.35	6 (24%)
32	PSU	1a	516	32,56	18,21,22	1.42	3 (16%)	21,30,33	1.85	6 (28%)
1	5MC	2A	1962	56,1	19,22,23	1.72	3 (15%)	26,32,35	1.25	4 (15%)
54	5MU	2w	54	54	19,22,23	1.27	3 (15%)	27,32,35	1.76	6 (22%)
54	5MU	1w	54	54	19,22,23	1.32	4 (21%)	27,32,35	2.26	6 (22%)
55	5MU	1x	54	56,55	19,22,23	1.44	5 (26%)	27,32,35	2.27	6 (22%)
32	5MC	1a	1407	32	19,22,23	1.50	2 (10%)	26,32,35	1.25	3 (11%)
54	4SU	2w	8	54	18,21,22	1.52	3 (16%)	25,30,33	2.24	5 (20%)
54	MIA	2w	37	54	19,27,32	1.85	3 (15%)	18,39,47	1.67	5 (27%)
32	5MC	2a	1404	32	19,22,23	1.79	3 (15%)	26,32,35	1.36	4 (15%)
32	M2G	1a	966	32	20,27,28	1.36	3 (15%)	19,40,43	1.10	2 (10%)
54	5MU	2y	54	54	19,22,23	1.59	5 (26%)	27,32,35	2.09	9 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	1A	2251	56,1,55	19,26,27	1.06	1 (5%)	21,38,41	0.98	1 (4%)
55	31H	1x	76	56,55	27,34,35	1.13	2 (7%)	22,47,50	2.89	5 (22%)
1	5MU	2A	1915	1	19,22,23	1.48	3 (15%)	27,32,35	2.05	5 (18%)
54	PSU	2w	55	56,54	18,21,22	1.51	3 (16%)	21,30,33	1.99	4 (19%)
32	5MC	2a	967	32	19,22,23	1.68	2 (10%)	26,32,35	1.21	2 (7%)
54	5MU	1y	54	54	19,22,23	1.55	5 (26%)	27,32,35	1.80	7 (25%)
54	G7M	2y	46	54	20,26,27	1.39	2 (10%)	16,39,42	0.78	1 (6%)
32	5MC	2a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.36	3 (11%)
54	4SU	1y	8	54	18,21,22	1.60	4 (22%)	25,30,33	1.68	5 (20%)
32	5MC	1a	967	32	19,22,23	1.85	2 (10%)	26,32,35	1.13	2 (7%)
32	G7M	1a	527	32,56	20,26,27	1.27	2 (10%)	16,39,42	0.55	0
54	PSU	1y	39	54	18,21,22	1.44	2 (11%)	21,30,33	1.87	4 (19%)
55	5MC	2x	32	55	19,22,23	1.63	2 (10%)	26,32,35	1.43	4 (15%)
55	4SU	1x	8	55	18,21,22	2.26	5 (27%)	25,30,33	2.40	8 (32%)
55	PSU	2x	55	55	18,21,22	1.43	2 (11%)	21,30,33	2.15	5 (23%)
1	5MC	1A	1962	56,1	19,22,23	1.53	2 (10%)	26,32,35	1.28	4 (15%)
32	MA6	2a	1519	32	19,26,27	1.00	2 (10%)	18,38,41	2.08	3 (16%)
1	2MA	2A	2503	56,1	18,25,26	0.82	0	20,37,40	1.66	3 (15%)
1	OMG	2A	2251	56,1,55	19,26,27	0.95	1 (5%)	21,38,41	1.19	3 (14%)
55	4SU	2x	8	55	18,21,22	2.03	5 (27%)	25,30,33	1.60	8 (32%)
32	2MG	2a	1207	32	18,26,27	0.99	2 (11%)	16,38,41	1.24	1 (6%)
1	5MU	1A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.12	8 (29%)
55	31H	2x	76	56,55	27,34,35	1.25	3 (11%)	22,47,50	2.53	5 (22%)
54	MIA	1w	37	54	24,31,32	2.01	4 (16%)	22,44,47	2.69	7 (31%)
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.72	4 (25%)
55	5MC	1x	32	55	19,22,23	1.54	3 (15%)	26,32,35	1.48	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.55	3 (15%)	26,32,35	1.21	3 (11%)
1	OMU	1A	2552	56,1	19,22,23	1.11	2 (10%)	25,31,34	2.29	5 (20%)
1	PSU	1A	1911	1	18,21,22	1.44	3 (16%)	21,30,33	1.99	3 (14%)
54	PSU	2w	32	54	18,21,22	1.38	3 (16%)	21,30,33	1.98	4 (19%)

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
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	5/7/12/14	-
54	G7M	1y	46	54	-	1/3/25/26	0/3/3/3
1	2MA	1A	2503	56,1	-	0/3/25/26	0/3/3/3
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	6/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	3/9/29/30	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	3/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/3/25/26	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	56,1	-	1/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32,56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
1	OMG	1A	2251	56,1,55	-	0/5/27/28	0/3/3/3
55	31H	1x	76	56,55	-	4/18/40/41	0/3/3/3
1	5MU	2A	1915	1	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	56,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	1/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	0/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	2/3/25/26	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	2MA	2A	2503	56,1	-	1/3/25/26	0/3/3/3
1	OMG	2A	2251	56,1,55	-	0/5/27/28	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
55	31H	2x	76	56,55	-	4/18/40/41	0/3/3/3
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2

The worst 5 of 209 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.90	1.69	1.82
43	1l	92	0TD	CB-SB	-10.73	1.71	1.82
32	1a	967	5MC	C5-C4	6.86	1.49	1.44
32	1a	1404	5MC	C5-C4	6.81	1.49	1.44
54	1w	37	MIA	C13-C14	6.77	1.52	1.32

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-15.08	75.26	102.36
43	2l	92	0TD	CSB-SB-CB	-10.39	83.69	102.36
54	1w	37	MIA	C12-C13-C14	-9.66	109.68	127.01
55	1x	76	31H	O4'-C1'-N9	-8.53	97.44	108.75
32	2a	1498	UR3	C4-N3-C2	-7.94	118.19	124.58

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB

There are no ring outliers.

48 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	2	0
54	1y	46	G7M	1	0
1	1A	2503	2MA	1	0
1	1A	1939	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1518	MA6	4	0
1	2A	1911	PSU	1	0
1	2A	2552	OMU	1	0
54	2y	55	PSU	6	0
54	1y	37	MIA	1	0
54	1y	55	PSU	1	0
54	2y	39	PSU	1	0
54	1w	55	PSU	1	0
1	2A	1917	PSU	1	0
32	1a	1519	MA6	1	0
32	1a	1402	4OC	1	0
54	1w	39	PSU	1	0
54	1y	32	PSU	1	0
32	2a	966	M2G	1	0
54	2w	39	PSU	2	0
1	2A	1939	5MU	1	0
54	1w	46	G7M	1	0
32	1a	1518	MA6	3	0
43	2l	92	0TD	2	0
54	2y	8	4SU	1	0
54	2w	54	5MU	1	0
54	1w	54	5MU	1	0
54	2w	8	4SU	2	0
32	2a	1404	5MC	2	0
32	1a	966	M2G	1	0
1	1A	2251	OMG	1	0
55	1x	76	31H	1	0
54	2w	55	PSU	1	0
32	2a	967	5MC	1	0
54	2y	46	G7M	2	0
32	2a	1400	5MC	1	0
54	1y	8	4SU	2	0
32	1a	527	G7M	1	0
54	1y	39	PSU	1	0
55	2x	32	5MC	1	0
55	1x	8	4SU	2	0
32	2a	1519	MA6	4	0
1	2A	2503	2MA	2	0
1	2A	2251	OMG	1	0
32	2a	1207	2MG	4	0
54	1w	37	MIA	1	0
32	1a	1207	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1x	32	5MC	1	0
1	1A	2552	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2813 ligands modelled in this entry, 2809 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	A1A1K	1A	4105	56	31,37,37	1.76	7 (22%)	28,53,53	1.11	3 (10%)
60	SF4	1d	302	35	0,12,12	-	-	-		
60	SF4	2d	303	35	0,12,12	-	-	-		
58	A1A1K	2A	3886	-	31,37,37	1.45	4 (12%)	28,53,53	0.93	1 (3%)

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	A1A1K	1A	4105	56	-	2/26/71/71	0/3/4/4
60	SF4	1d	302	35	-	-	0/6/5/5
60	SF4	2d	303	35	-	-	0/6/5/5
58	A1A1K	2A	3886	-	-	3/26/71/71	0/3/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4105	A1A1K	CAM-CBF	-5.10	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3886	A1A1K	CAM-CBF	-4.82	1.39	1.51
58	2A	3886	A1A1K	OAW-CB	3.04	1.45	1.42
58	1A	4105	A1A1K	CAB-CAK	3.01	1.57	1.53
58	1A	4105	A1A1K	OAW-CB	2.77	1.45	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4105	A1A1K	CBC-CBB-CAZ	-3.13	110.61	116.68
58	2A	3886	A1A1K	CD2-CAZ-CAY	-2.31	110.33	113.78
58	1A	4105	A1A1K	CD2-CAZ-CAY	-2.31	110.34	113.78
58	1A	4105	A1A1K	CB-CA-C	2.14	114.68	110.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	2A	3886	A1A1K	O-C-CA-CB
58	2A	3886	A1A1K	NAL-C-CA-CB
58	1A	4105	A1A1K	O-C-CA-CB
58	1A	4105	A1A1K	NAL-C-CA-CB
58	2A	3886	A1A1K	O-C-CA-N

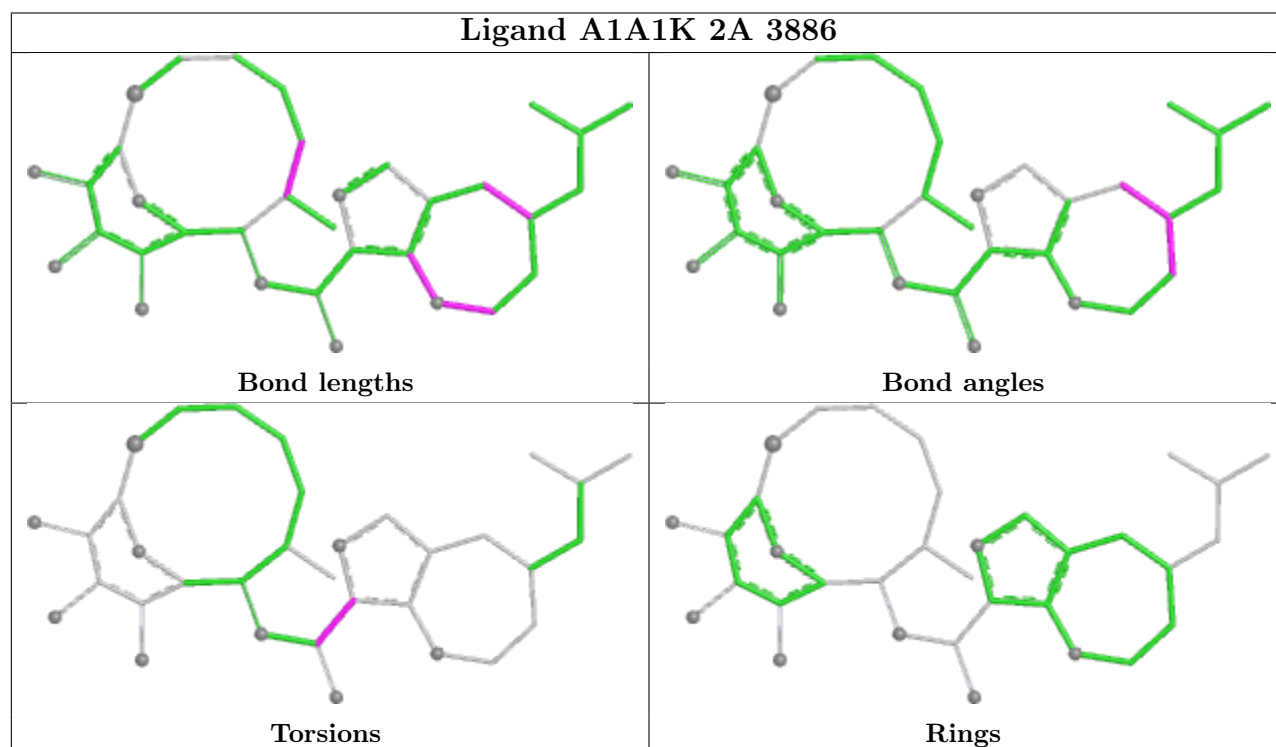
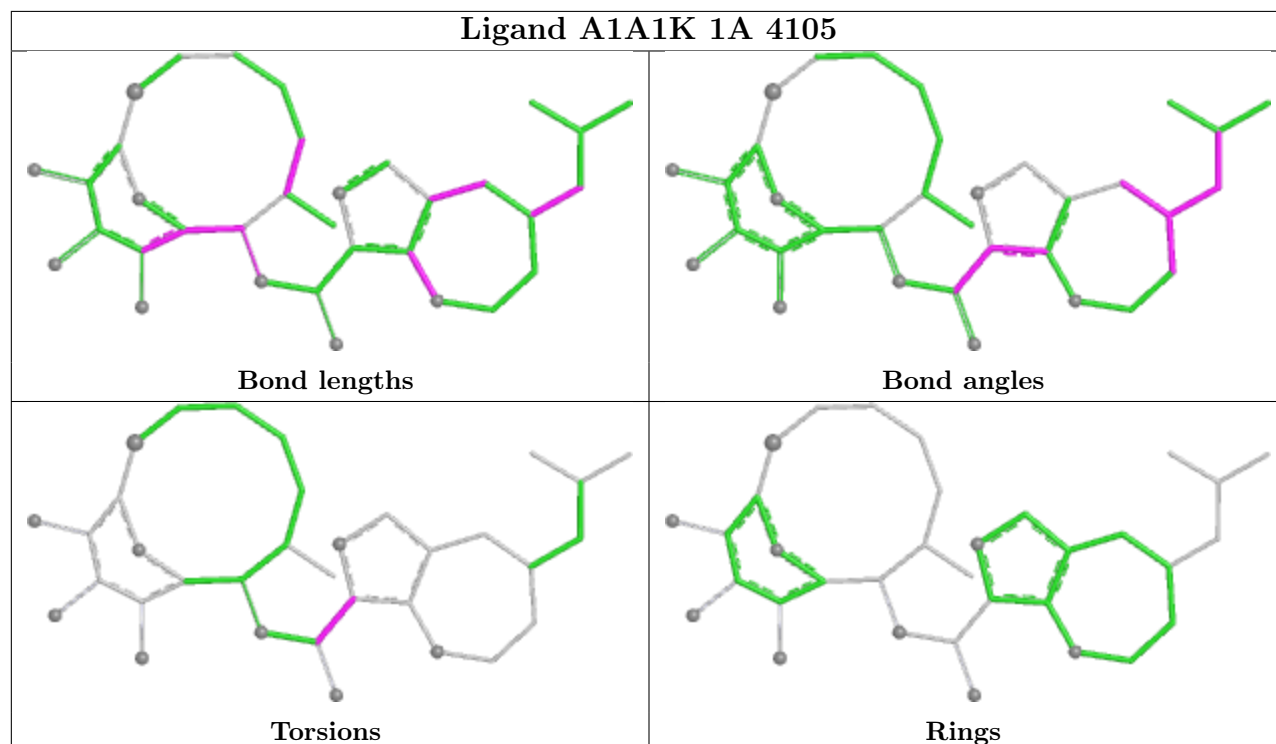
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4105	A1A1K	1	0
60	1d	302	SF4	1	0
60	2d	303	SF4	1	0
58	2A	3886	A1A1K	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	-0.60	92 (3%)	50	53	24, 41, 91, 106	0
1	2A	2789/2915 (95%)	-0.04	97 (3%)	47	49	37, 62, 92, 103	0
2	1B	120/121 (99%)	-0.41	0	100	100	34, 54, 67, 86	0
2	2B	120/121 (99%)	0.73	2 (1%)	69	70	65, 82, 87, 97	0
3	1D	275/276 (99%)	-0.22	3 (1%)	77	79	25, 42, 55, 79	0
3	2D	275/276 (99%)	0.28	6 (2%)	62	65	38, 55, 67, 82	0
4	1E	204/206 (99%)	-0.25	0	100	100	23, 43, 62, 79	0
4	2E	204/206 (99%)	0.45	4 (1%)	64	67	41, 63, 75, 87	0
5	1F	203/210 (96%)	-0.09	2 (0%)	79	80	22, 46, 72, 84	0
5	2F	203/210 (96%)	0.45	1 (0%)	87	88	40, 71, 81, 85	0
6	1G	181/182 (99%)	0.43	6 (3%)	49	51	45, 62, 73, 85	0
6	2G	181/182 (99%)	1.45	46 (25%)	2	2	72, 81, 86, 92	0
7	1H	174/180 (96%)	0.26	2 (1%)	77	79	41, 58, 69, 76	0
7	2H	174/180 (96%)	1.36	41 (23%)	2	2	72, 83, 90, 95	0
8	1I	146/148 (98%)	0.73	5 (3%)	48	50	48, 74, 80, 85	0
8	2I	146/148 (98%)	1.25	23 (15%)	6	5	59, 78, 86, 94	0
9	1N	140/140 (100%)	-0.17	0	100	100	32, 43, 62, 74	0
9	2N	140/140 (100%)	0.92	13 (9%)	16	16	51, 68, 80, 87	0
10	1O	122/122 (100%)	0.05	0	100	100	35, 45, 61, 67	0
10	2O	122/122 (100%)	0.47	2 (1%)	70	72	52, 63, 74, 76	0
11	1P	149/150 (99%)	0.10	4 (2%)	56	59	26, 49, 69, 75	0
11	2P	149/150 (99%)	0.67	5 (3%)	48	50	45, 71, 83, 91	0
12	1Q	141/141 (100%)	-0.15	0	100	100	33, 46, 62, 74	0
12	2Q	141/141 (100%)	1.24	26 (18%)	4	4	57, 70, 80, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.36	0 100 100	30, 38, 50, 58	0
13	2R	118/118 (100%)	0.09	0 100 100	45, 55, 66, 73	0
14	1S	110/112 (98%)	0.11	1 (0%) 81 81	43, 54, 64, 70	0
14	2S	110/112 (98%)	1.22	15 (13%) 8 7	67, 76, 83, 87	0
15	1T	131/146 (89%)	0.05	5 (3%) 44 46	37, 48, 69, 75	0
15	2T	131/146 (89%)	0.64	2 (1%) 71 73	56, 65, 76, 79	0
16	1U	116/118 (98%)	-0.49	1 (0%) 81 81	25, 35, 51, 66	0
16	2U	116/118 (98%)	0.53	2 (1%) 69 70	51, 65, 79, 84	0
17	1V	101/101 (100%)	-0.35	1 (0%) 79 80	26, 43, 59, 71	0
17	2V	101/101 (100%)	0.65	0 100 100	47, 74, 80, 86	0
18	1W	112/113 (99%)	-0.33	1 (0%) 81 81	26, 36, 55, 78	0
18	2W	112/113 (99%)	0.33	2 (1%) 67 69	43, 56, 70, 91	0
19	1X	95/96 (98%)	-0.10	2 (2%) 63 65	31, 42, 63, 81	0
19	2X	95/96 (98%)	0.69	5 (5%) 33 33	49, 63, 78, 87	0
20	1Y	107/110 (97%)	0.31	1 (0%) 81 81	41, 53, 70, 80	0
20	2Y	107/110 (97%)	1.17	13 (12%) 10 10	60, 75, 84, 90	0
21	1Z	154/206 (74%)	0.78	13 (8%) 18 18	46, 66, 84, 88	0
21	2Z	160/206 (77%)	1.69	46 (28%) 1 1	73, 83, 91, 94	0
22	10	77/85 (90%)	0.07	2 (2%) 57 60	31, 42, 57, 66	0
22	20	83/85 (97%)	1.42	19 (22%) 2 2	54, 69, 77, 90	0
23	11	97/98 (98%)	0.15	1 (1%) 79 80	34, 48, 71, 75	0
23	21	97/98 (98%)	0.57	4 (4%) 42 43	45, 59, 77, 83	0
24	12	70/72 (97%)	0.01	1 (1%) 73 75	39, 52, 64, 74	0
24	22	70/72 (97%)	0.82	6 (8%) 18 17	61, 74, 81, 83	0
25	13	59/60 (98%)	-0.27	1 (1%) 69 70	29, 40, 62, 74	0
25	23	59/60 (98%)	0.65	2 (3%) 48 50	58, 68, 77, 86	0
26	14	69/71 (97%)	0.68	3 (4%) 40 41	56, 74, 86, 88	0
26	24	69/71 (97%)	1.48	16 (23%) 2 2	80, 86, 90, 93	0
27	15	59/60 (98%)	-0.30	1 (1%) 69 70	26, 36, 52, 64	0
27	25	59/60 (98%)	0.18	0 100 100	40, 55, 69, 79	0
28	16	53/54 (98%)	-0.16	0 100 100	36, 45, 59, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.65	2 (3%) 44 46	54, 65, 73, 74	0
29	17	48/49 (97%)	-0.31	3 (6%) 27 28	25, 32, 60, 67	0
29	27	48/49 (97%)	0.19	4 (8%) 19 18	36, 45, 65, 74	0
30	18	64/65 (98%)	-0.27	0 100 100	31, 39, 46, 58	0
30	28	64/65 (98%)	0.68	0 100 100	51, 61, 66, 70	0
31	19	37/37 (100%)	-0.07	0 100 100	35, 44, 61, 64	0
31	29	37/37 (100%)	1.11	4 (10%) 12 12	62, 71, 79, 83	0
32	1a	1488/1521 (97%)	0.20	47 (3%) 50 53	40, 71, 92, 106	0
32	2a	1491/1521 (98%)	0.72	158 (10%) 13 13	53, 79, 95, 106	0
33	1b	231/256 (90%)	1.06	38 (16%) 5 5	70, 79, 88, 94	0
33	2b	231/256 (90%)	1.63	68 (29%) 1 1	76, 85, 89, 91	0
34	1c	206/239 (86%)	0.89	10 (4%) 36 36	66, 76, 83, 85	0
34	2c	206/239 (86%)	1.87	87 (42%) 1 0	73, 85, 89, 94	0
35	1d	208/209 (99%)	1.01	18 (8%) 17 17	59, 74, 82, 89	0
35	2d	208/209 (99%)	0.74	7 (3%) 48 50	62, 72, 78, 83	0
36	1e	148/162 (91%)	0.63	2 (1%) 73 75	58, 68, 77, 81	0
36	2e	148/162 (91%)	1.30	28 (18%) 4 4	68, 79, 85, 87	0
37	1f	100/101 (99%)	0.56	1 (1%) 79 80	60, 70, 77, 80	0
37	2f	100/101 (99%)	0.71	3 (3%) 52 55	65, 74, 80, 84	0
38	1g	155/156 (99%)	0.61	11 (7%) 23 24	64, 73, 83, 85	0
38	2g	155/156 (99%)	1.16	25 (16%) 5 5	71, 80, 86, 90	0
39	1h	137/138 (99%)	0.55	2 (1%) 71 73	56, 70, 76, 82	0
39	2h	137/138 (99%)	1.26	22 (16%) 5 5	72, 79, 84, 87	0
40	1i	127/128 (99%)	1.20	19 (14%) 6 6	62, 79, 83, 86	0
40	2i	127/128 (99%)	1.95	56 (44%) 1 0	72, 84, 89, 90	0
41	1j	97/105 (92%)	1.38	20 (20%) 3 3	65, 80, 87, 89	0
41	2j	96/105 (91%)	2.32	62 (64%) 0 0	78, 86, 91, 92	0
42	1k	114/129 (88%)	0.70	5 (4%) 39 40	51, 69, 78, 80	0
42	2k	114/129 (88%)	1.00	14 (12%) 9 9	60, 76, 82, 84	0
43	1l	121/132 (91%)	0.49	4 (3%) 49 51	52, 63, 71, 77	0
43	2l	121/132 (91%)	1.04	15 (12%) 9 9	63, 73, 80, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.84	8 (6%) 26 26	61, 72, 80, 88	0
44	2m	122/126 (96%)	2.02	48 (39%) 1 0	76, 83, 88, 91	0
45	1n	60/61 (98%)	1.19	4 (6%) 25 26	67, 72, 78, 80	0
45	2n	60/61 (98%)	3.10	49 (81%) 0 0	80, 86, 89, 91	0
46	1o	88/89 (98%)	0.62	4 (4%) 39 39	55, 68, 77, 82	0
46	2o	88/89 (98%)	0.91	5 (5%) 30 31	65, 76, 82, 86	0
47	1p	82/88 (93%)	1.13	11 (13%) 8 7	62, 74, 79, 84	0
47	2p	82/88 (93%)	1.00	5 (6%) 28 28	62, 71, 78, 82	0
48	1q	99/105 (94%)	0.94	6 (6%) 28 28	58, 69, 77, 80	0
48	2q	99/105 (94%)	0.81	7 (7%) 23 24	64, 76, 83, 88	0
49	1r	68/88 (77%)	0.62	5 (7%) 22 23	62, 70, 77, 79	0
49	2r	68/88 (77%)	0.74	2 (2%) 54 56	65, 74, 80, 84	0
50	1s	83/93 (89%)	0.71	4 (4%) 36 37	66, 75, 83, 86	0
50	2s	83/93 (89%)	2.28	53 (63%) 0 0	79, 86, 91, 95	0
51	1t	96/106 (90%)	1.08	12 (12%) 9 9	63, 73, 81, 83	0
51	2t	96/106 (90%)	0.91	11 (11%) 11 10	64, 72, 81, 84	0
52	1u	23/27 (85%)	1.29	3 (13%) 9 8	67, 70, 75, 76	0
52	2u	23/27 (85%)	2.07	11 (47%) 0 0	78, 82, 86, 87	0
53	1v	13/24 (54%)	0.79	2 (15%) 6 6	50, 72, 84, 93	0
53	2v	13/24 (54%)	1.80	4 (30%) 1 1	75, 86, 93, 100	0
54	1w	64/76 (84%)	1.31	10 (15%) 6 6	73, 92, 100, 105	0
54	1y	67/76 (88%)	1.04	10 (14%) 7 6	43, 91, 98, 100	0
54	2w	62/76 (81%)	1.67	18 (29%) 1 1	86, 97, 102, 105	0
54	2y	66/76 (86%)	1.15	7 (10%) 13 13	60, 96, 99, 103	0
55	1x	71/77 (92%)	0.20	1 (1%) 73 75	32, 64, 84, 91	0
55	2x	71/77 (92%)	0.56	2 (2%) 55 57	53, 82, 89, 99	0
All	All	20861/21748 (95%)	0.39	1583 (7%) 21 21	22, 68, 89, 106	0

The worst 5 of 1583 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	10.0
44	2m	124	PRO	9.7

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	7.6
45	2n	2	ALA	7.2
44	2m	102	ARG	7.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
54	PSU	2y	55	20/21	0.51	0.17	93,99,111,111	0
54	G7M	2w	46	24/25	0.53	0.14	79,96,103,111	0
54	G7M	1w	46	24/25	0.53	0.16	77,91,102,115	0
54	G7M	1y	46	24/25	0.57	0.17	88,96,103,115	0
54	G7M	2y	46	24/25	0.62	0.17	92,94,99,121	0
54	5MU	2y	54	21/22	0.64	0.16	90,98,103,120	0
54	4SU	2y	8	20/21	0.68	0.15	93,97,104,110	0
54	PSU	2w	55	20/21	0.69	0.15	86,94,99,102	0
54	PSU	2y	32	20/21	0.70	0.14	82,91,98,105	0
54	5MU	2w	54	21/22	0.72	0.14	78,87,93,95	0
54	PSU	1y	55	20/21	0.72	0.14	89,95,102,107	0
54	MIA	2y	37	22/30	0.72	0.14	81,93,103,114	0
54	4SU	1y	8	20/21	0.73	0.14	90,96,99,108	0
54	5MU	1y	54	21/22	0.73	0.14	85,90,96,110	0
54	4SU	2w	8	20/21	0.75	0.12	90,97,105,113	0
54	4SU	1w	8	20/21	0.77	0.12	86,92,103,105	0
54	PSU	1w	55	20/21	0.81	0.11	82,90,97,97	0
54	PSU	1y	39	20/21	0.82	0.11	84,86,98,98	0
32	2MG	2a	1207	24/25	0.82	0.14	85,90,95,106	0
54	PSU	1y	32	20/21	0.83	0.13	83,88,93,93	0
54	PSU	2y	39	20/21	0.84	0.11	83,87,98,104	0
54	MIA	1y	37	22/30	0.84	0.12	82,86,92,101	0
55	4SU	2x	8	20/21	0.85	0.12	81,86,90,90	0
55	PSU	2x	55	20/21	0.86	0.11	75,81,86,87	0
54	PSU	2w	32	20/21	0.86	0.14	81,90,95,102	0
54	MIA	2w	37	25/30	0.86	0.16	77,88,93,107	0
54	MIA	1w	37	29/30	0.86	0.17	64,73,76,98	0
54	PSU	2w	39	20/21	0.87	0.11	83,90,94,95	0
32	PSU	2a	516	20/21	0.88	0.12	76,82,87,88	0
1	5MU	2A	1915	21/22	0.88	0.11	76,80,84,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	PSU	1w	32	20/21	0.89	0.13	73,78,84,85	0
32	G7M	2a	527	24/25	0.89	0.13	65,73,80,84	0
32	M2G	2a	966	25/26	0.89	0.18	67,74,87,91	0
55	5MC	2x	32	21/22	0.89	0.14	72,78,82,82	0
55	5MU	2x	54	21/22	0.90	0.11	74,83,88,91	0
32	5MC	2a	1404	21/22	0.90	0.13	59,65,70,73	0
1	PSU	2A	1911	20/21	0.90	0.10	67,70,76,79	0
1	PSU	2A	1917	20/21	0.91	0.09	66,74,79,81	0
54	5MU	1w	54	21/22	0.91	0.09	70,81,85,87	0
32	4OC	2a	1402	22/23	0.92	0.13	58,70,74,80	0
55	PSU	1x	55	20/21	0.92	0.10	60,68,74,78	0
43	0TD	2l	92	10/11	0.92	0.11	69,74,79,90	0
1	OMC	2A	1920	21/22	0.92	0.12	61,70,74,76	0
32	5MC	2a	967	21/22	0.92	0.14	72,77,85,88	0
54	PSU	1w	39	20/21	0.92	0.11	73,78,86,88	0
32	5MC	2a	1400	21/22	0.92	0.15	69,75,80,88	0
32	MA6	2a	1518	24/25	0.93	0.13	53,74,78,81	0
43	0TD	1l	92	10/11	0.93	0.10	57,60,65,78	0
32	2MG	1a	1207	24/25	0.93	0.10	71,75,78,81	0
32	UR3	2a	1498	21/22	0.93	0.13	63,65,70,73	0
32	PSU	1a	516	20/21	0.94	0.09	64,70,73,74	0
1	5MU	1A	1915	21/22	0.94	0.10	57,62,68,70	0
32	5MC	2a	1407	21/22	0.94	0.12	59,64,72,77	0
55	5MU	1x	54	21/22	0.94	0.10	66,72,76,80	0
32	5MC	1a	967	21/22	0.95	0.10	58,63,68,69	0
1	5MC	2A	1942	21/22	0.95	0.10	58,64,67,68	0
1	5MC	2A	1962	21/22	0.95	0.10	44,57,65,67	0
32	G7M	1a	527	24/25	0.95	0.09	51,54,59,60	0
32	MA6	2a	1519	24/25	0.95	0.13	58,71,75,77	0
55	5MC	1x	32	21/22	0.95	0.12	54,61,66,75	0
1	5MC	1A	1942	21/22	0.96	0.08	37,43,49,55	0
55	4SU	1x	8	20/21	0.96	0.08	58,66,71,71	0
32	5MC	1a	1400	21/22	0.96	0.11	51,57,60,63	0
32	MA6	1a	1519	24/25	0.96	0.11	45,50,56,62	0
32	M2G	1a	966	25/26	0.96	0.11	56,62,68,69	0
1	PSU	1A	1917	20/21	0.96	0.07	52,57,61,63	0
55	31H	2x	76	32/33	0.96	0.10	44,49,61,62	0
1	OMU	2A	2552	21/22	0.97	0.08	42,50,56,61	0
32	5MC	1a	1407	21/22	0.97	0.09	42,45,50,51	0
32	MA6	1a	1518	24/25	0.97	0.09	39,49,54,54	0
1	OMC	1A	1920	21/22	0.97	0.07	41,49,53,56	0
1	PSU	1A	1911	20/21	0.97	0.08	43,53,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	1A	2605	20/21	0.97	0.06	25,30,34,37	0
1	5MU	2A	1939	21/22	0.97	0.08	38,45,50,52	0
32	4OC	1a	1402	22/23	0.97	0.10	46,50,59,59	0
32	5MC	1a	1404	21/22	0.97	0.09	44,50,53,55	0
1	OMG	2A	2251	24/25	0.97	0.08	45,48,54,61	0
1	2MA	2A	2503	23/24	0.97	0.09	39,42,46,47	0
55	31H	1x	76	32/33	0.98	0.07	25,31,37,44	10
1	5MU	1A	1939	21/22	0.98	0.05	27,33,37,39	0
1	PSU	2A	2605	20/21	0.98	0.06	36,43,48,50	0
1	5MC	1A	1962	21/22	0.98	0.07	35,42,47,53	0
1	OMU	1A	2552	21/22	0.98	0.06	29,34,38,41	0
32	UR3	1a	1498	21/22	0.99	0.07	43,48,51,52	0
1	2MA	1A	2503	23/24	0.99	0.05	21,26,29,31	0
1	OMG	1A	2251	24/25	0.99	0.04	28,31,34,37	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, 95<sup>th</sup> 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	104	1/1	0.43	0.26	95,95,95,95	0
56	MG	2A	3665	1/1	0.52	0.24	87,87,87,87	0
56	MG	2a	3107	1/1	0.55	0.33	80,80,80,80	0
56	MG	2a	3225	1/1	0.57	0.22	84,84,84,84	0
56	MG	1B	3630	1/1	0.57	0.24	81,81,81,81	0
56	MG	2a	3208	1/1	0.60	0.30	80,80,80,80	0
56	MG	2A	3312	1/1	0.60	0.39	80,80,80,80	0
56	MG	2A	3321	1/1	0.60	0.37	89,89,89,89	0
56	MG	2A	3494	1/1	0.62	0.20	77,77,77,77	0
56	MG	2A	3446	1/1	0.63	0.40	91,91,91,91	0
56	MG	2A	3679	1/1	0.63	0.26	81,81,81,81	0
56	MG	2A	3415	1/1	0.64	0.26	84,84,84,84	0
56	MG	1A	3535	1/1	0.64	0.27	67,67,67,67	0
56	MG	2A	3223	1/1	0.64	0.34	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3476	1/1	0.65	0.26	83,83,83,83	0
56	MG	2A	3319	1/1	0.65	0.31	86,86,86,86	0
56	MG	2w	107	1/1	0.66	0.22	84,84,84,84	0
56	MG	2A	3359	1/1	0.66	0.36	83,83,83,83	0
56	MG	20	104	1/1	0.67	0.20	76,76,76,76	0
56	MG	2A	3712	1/1	0.67	0.17	87,87,87,87	0
56	MG	2A	3773	1/1	0.67	0.26	74,74,74,74	0
56	MG	2a	3057	1/1	0.68	0.28	86,86,86,86	0
56	MG	2A	3396	1/1	0.68	0.23	81,81,81,81	0
56	MG	1a	1718	1/1	0.68	0.17	71,71,71,71	0
56	MG	1A	3741	1/1	0.68	0.19	71,71,71,71	0
56	MG	1a	1641	1/1	0.68	0.41	85,85,85,85	0
56	MG	2A	3542	1/1	0.68	0.24	72,72,72,72	0
56	MG	2y	105	1/1	0.68	0.30	99,99,99,99	0
56	MG	2A	3816	1/1	0.69	0.17	70,70,70,70	0
56	MG	2A	3698	1/1	0.69	0.23	65,65,65,65	0
56	MG	1A	4011	1/1	0.69	0.15	76,76,76,76	0
56	MG	1A	3845	1/1	0.69	0.26	74,74,74,74	0
56	MG	2a	3148	1/1	0.69	0.36	84,84,84,84	0
56	MG	2A	3346	1/1	0.70	0.30	90,90,90,90	0
56	MG	2G	201	1/1	0.70	0.27	83,83,83,83	0
56	MG	2A	3708	1/1	0.70	0.26	80,80,80,80	0
56	MG	2j	201	1/1	0.70	0.14	77,77,77,77	0
56	MG	2A	3258	1/1	0.70	0.26	83,83,83,83	0
56	MG	1A	3100	1/1	0.70	0.15	79,79,79,79	0
56	MG	2a	3111	1/1	0.70	0.41	84,84,84,84	0
56	MG	2A	3269	1/1	0.71	0.13	83,83,83,83	0
56	MG	1A	3797	1/1	0.71	0.22	81,81,81,81	0
56	MG	2A	3352	1/1	0.71	0.17	82,82,82,82	0
56	MG	1A	3898	1/1	0.71	0.22	49,49,49,49	0
56	MG	2a	3212	1/1	0.72	0.21	76,76,76,76	0
56	MG	2a	3068	1/1	0.72	0.17	85,85,85,85	0
56	MG	2A	3758	1/1	0.72	0.19	73,73,73,73	0
56	MG	2q	202	1/1	0.72	0.16	86,86,86,86	0
56	MG	2w	105	1/1	0.72	0.15	91,91,91,91	0
56	MG	2A	3091	1/1	0.72	0.29	88,88,88,88	0
56	MG	1a	1743	1/1	0.72	0.27	83,83,83,83	0
56	MG	2a	3063	1/1	0.72	0.36	84,84,84,84	0
56	MG	2A	3343	1/1	0.73	0.16	82,82,82,82	0
56	MG	2A	3300	1/1	0.73	0.27	68,68,68,68	0
56	MG	2A	3694	1/1	0.73	0.22	76,76,76,76	0
56	MG	2a	3007	1/1	0.73	0.22	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3028	1/1	0.73	0.27	85,85,85,85	0
56	MG	2A	3347	1/1	0.73	0.33	88,88,88,88	0
56	MG	2A	3349	1/1	0.73	0.12	92,92,92,92	0
56	MG	2A	3175	1/1	0.73	0.22	77,77,77,77	0
56	MG	2A	3500	1/1	0.73	0.31	86,86,86,86	0
56	MG	2A	3356	1/1	0.73	0.28	78,78,78,78	0
56	MG	2A	3293	1/1	0.74	0.17	79,79,79,79	0
56	MG	1A	3860	1/1	0.74	0.18	77,77,77,77	0
56	MG	2a	3135	1/1	0.74	0.29	91,91,91,91	0
56	MG	1A	3479	1/1	0.74	0.19	78,78,78,78	0
56	MG	1A	3568	1/1	0.74	0.18	71,71,71,71	0
56	MG	1A	4092	1/1	0.74	0.22	86,86,86,86	0
56	MG	2A	3097	1/1	0.74	0.21	80,80,80,80	0
56	MG	1A	4098	1/1	0.74	0.30	78,78,78,78	0
56	MG	2A	3655	1/1	0.74	0.17	75,75,75,75	0
56	MG	2w	102	1/1	0.74	0.17	98,98,98,98	0
56	MG	1A	3707	1/1	0.74	0.21	71,71,71,71	0
56	MG	1U	212	1/1	0.74	0.39	55,55,55,55	0
56	MG	1l	104	1/1	0.74	0.20	84,84,84,84	0
56	MG	2A	3275	1/1	0.74	0.20	78,78,78,78	0
56	MG	2A	3345	1/1	0.75	0.26	84,84,84,84	0
56	MG	1a	1698	1/1	0.75	0.28	79,79,79,79	0
56	MG	2a	3125	1/1	0.75	0.29	85,85,85,85	0
56	MG	2A	3472	1/1	0.75	0.19	85,85,85,85	0
56	MG	2A	3110	1/1	0.75	0.12	81,81,81,81	0
56	MG	2A	3810	1/1	0.75	0.18	71,71,71,71	0
56	MG	1a	1711	1/1	0.75	0.40	78,78,78,78	0
56	MG	2A	3859	1/1	0.75	0.23	81,81,81,81	0
56	MG	1A	4094	1/1	0.75	0.18	65,65,65,65	0
56	MG	2A	3625	1/1	0.75	0.21	64,64,64,64	0
56	MG	2A	3249	1/1	0.75	0.22	82,82,82,82	0
56	MG	1A	3689	1/1	0.75	0.24	69,69,69,69	0
56	MG	2A	3378	1/1	0.75	0.22	79,79,79,79	0
56	MG	2A	3395	1/1	0.75	0.31	78,78,78,78	0
56	MG	1A	3755	1/1	0.75	0.14	64,64,64,64	0
56	MG	2y	107	1/1	0.75	0.25	96,96,96,96	0
56	MG	1A	3529	1/1	0.76	0.14	80,80,80,80	0
56	MG	2A	3325	1/1	0.76	0.17	71,71,71,71	0
56	MG	2a	3106	1/1	0.76	0.26	80,80,80,80	0
56	MG	2A	3408	1/1	0.76	0.15	78,78,78,78	0
56	MG	2A	3331	1/1	0.76	0.29	77,77,77,77	0
56	MG	2a	3112	1/1	0.76	0.17	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1O	206	1/1	0.76	0.32	70,70,70,70	0
56	MG	1a	1739	1/1	0.76	0.20	88,88,88,88	0
56	MG	1A	4041	1/1	0.76	0.10	61,61,61,61	0
56	MG	1a	1791	1/1	0.76	0.11	81,81,81,81	0
56	MG	1a	1812	1/1	0.76	0.21	80,80,80,80	0
56	MG	2B	220	1/1	0.76	0.24	80,80,80,80	0
56	MG	2A	3606	1/1	0.76	0.16	82,82,82,82	0
56	MG	1A	3249	1/1	0.76	0.23	79,79,79,79	0
56	MG	25	104	1/1	0.76	0.24	82,82,82,82	0
56	MG	1A	3815	1/1	0.76	0.25	69,69,69,69	0
56	MG	2a	3008	1/1	0.76	0.47	84,84,84,84	0
56	MG	2A	3101	1/1	0.76	0.31	81,81,81,81	0
56	MG	2a	3042	1/1	0.76	0.23	86,86,86,86	0
56	MG	1A	3999	1/1	0.76	0.15	75,75,75,75	0
56	MG	2a	3197	1/1	0.77	0.26	84,84,84,84	0
56	MG	2A	3115	1/1	0.77	0.25	71,71,71,71	0
56	MG	1w	104	1/1	0.77	0.15	84,84,84,84	0
56	MG	1x	101	1/1	0.77	0.14	69,69,69,69	0
56	MG	2a	3231	1/1	0.77	0.29	79,79,79,79	0
56	MG	2A	3229	1/1	0.77	0.22	65,65,65,65	0
56	MG	1A	4080	1/1	0.77	0.23	66,66,66,66	0
56	MG	1a	1780	1/1	0.77	0.12	77,77,77,77	0
56	MG	2a	3122	1/1	0.77	0.25	82,82,82,82	0
56	MG	1A	4035	1/1	0.77	0.21	60,60,60,60	0
56	MG	2a	3053	1/1	0.77	0.17	87,87,87,87	0
56	MG	2a	3142	1/1	0.77	0.27	74,74,74,74	0
56	MG	1A	4099	1/1	0.77	0.17	62,62,62,62	0
56	MG	2a	3082	1/1	0.78	0.30	78,78,78,78	0
56	MG	1a	1713	1/1	0.78	0.52	82,82,82,82	0
56	MG	2A	3031	1/1	0.78	0.17	61,61,61,61	0
56	MG	1D	311	1/1	0.78	0.29	72,72,72,72	0
56	MG	2A	3815	1/1	0.78	0.13	84,84,84,84	0
56	MG	1A	4024	1/1	0.78	0.12	69,69,69,69	0
56	MG	2A	3280	1/1	0.78	0.22	76,76,76,76	0
56	MG	2A	3885	1/1	0.78	0.34	88,88,88,88	0
56	MG	2B	208	1/1	0.78	0.15	76,76,76,76	0
56	MG	2A	3290	1/1	0.78	0.25	86,86,86,86	0
56	MG	1A	3208	1/1	0.78	0.22	81,81,81,81	0
56	MG	2Z	301	1/1	0.78	0.14	86,86,86,86	0
56	MG	1A	4036	1/1	0.78	0.14	53,53,53,53	0
56	MG	1A	3531	1/1	0.78	0.14	69,69,69,69	0
56	MG	2A	3670	1/1	0.78	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	3622	1/1	0.78	0.23	63,63,63,63	0
56	MG	2A	3689	1/1	0.78	0.15	65,65,65,65	0
56	MG	2A	3196	1/1	0.78	0.15	81,81,81,81	0
56	MG	1n	101	1/1	0.78	0.46	74,74,74,74	0
56	MG	2a	3055	1/1	0.78	0.19	79,79,79,79	0
56	MG	1A	3263	1/1	0.78	0.15	59,59,59,59	0
56	MG	2A	3417	1/1	0.78	0.19	78,78,78,78	0
56	MG	2A	3728	1/1	0.78	0.18	71,71,71,71	0
56	MG	2A	3094	1/1	0.79	0.26	52,52,52,52	0
56	MG	2a	3177	1/1	0.79	0.18	79,79,79,79	0
56	MG	2a	3196	1/1	0.79	0.27	82,82,82,82	0
56	MG	1A	3293	1/1	0.79	0.17	54,54,54,54	0
56	MG	2A	3358	1/1	0.79	0.21	75,75,75,75	0
56	MG	1a	1722	1/1	0.79	0.18	74,74,74,74	0
56	MG	2a	3217	1/1	0.79	0.35	67,67,67,67	0
56	MG	2A	3360	1/1	0.79	0.17	72,72,72,72	0
56	MG	2A	3375	1/1	0.79	0.17	80,80,80,80	0
56	MG	2A	3506	1/1	0.79	0.19	65,65,65,65	0
56	MG	2A	3103	1/1	0.79	0.23	64,64,64,64	0
56	MG	2v	101	1/1	0.79	0.31	85,85,85,85	0
56	MG	2A	3591	1/1	0.79	0.20	79,79,79,79	0
56	MG	1x	107	1/1	0.79	0.28	77,77,77,77	0
56	MG	2A	3610	1/1	0.79	0.22	69,69,69,69	0
56	MG	1A	3693	1/1	0.79	0.15	71,71,71,71	0
56	MG	2a	3041	1/1	0.79	0.38	72,72,72,72	0
56	MG	1A	4044	1/1	0.79	0.17	52,52,52,52	0
56	MG	2a	3084	1/1	0.80	0.30	80,80,80,80	0
56	MG	2A	3116	1/1	0.80	0.38	80,80,80,80	0
56	MG	2A	3322	1/1	0.80	0.25	75,75,75,75	0
56	MG	2a	3109	1/1	0.80	0.20	73,73,73,73	0
56	MG	2A	3126	1/1	0.80	0.11	71,71,71,71	0
56	MG	1A	3753	1/1	0.80	0.28	69,69,69,69	0
56	MG	2A	3338	1/1	0.80	0.35	75,75,75,75	0
56	MG	2a	3124	1/1	0.80	0.41	81,81,81,81	0
56	MG	2A	3873	1/1	0.80	0.20	76,76,76,76	0
56	MG	1A	3344	1/1	0.80	0.28	68,68,68,68	0
56	MG	2A	3203	1/1	0.80	0.29	82,82,82,82	0
56	MG	2B	214	1/1	0.80	0.19	70,70,70,70	0
56	MG	1A	3396	1/1	0.80	0.21	79,79,79,79	0
56	MG	1x	108	1/1	0.80	0.36	82,82,82,82	0
56	MG	2A	3231	1/1	0.80	0.31	68,68,68,68	0
56	MG	2A	3023	1/1	0.80	0.26	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3399	1/1	0.80	0.25	81,81,81,81	0
56	MG	2A	3063	1/1	0.80	0.18	62,62,62,62	0
56	MG	1A	3466	1/1	0.80	0.17	70,70,70,70	0
56	MG	1A	3162	1/1	0.80	0.25	70,70,70,70	0
56	MG	1a	1749	1/1	0.80	0.29	74,74,74,74	0
56	MG	2p	101	1/1	0.80	0.27	81,81,81,81	0
56	MG	1A	3477	1/1	0.80	0.25	72,72,72,72	0
56	MG	2a	3044	1/1	0.80	0.33	76,76,76,76	0
56	MG	2v	102	1/1	0.80	0.32	80,80,80,80	0
56	MG	15	106	1/1	0.80	0.26	47,47,47,47	0
56	MG	1A	3343	1/1	0.80	0.17	64,64,64,64	0
56	MG	2A	3315	1/1	0.80	0.22	54,54,54,54	0
56	MG	2A	3410	1/1	0.80	0.14	71,71,71,71	0
56	MG	1A	3528	1/1	0.80	0.16	80,80,80,80	0
56	MG	2A	3767	1/1	0.80	0.16	58,58,58,58	0
56	MG	2A	3263	1/1	0.81	0.26	77,77,77,77	0
56	MG	2a	3009	1/1	0.81	0.32	78,78,78,78	0
56	MG	2a	3011	1/1	0.81	0.38	77,77,77,77	0
56	MG	2a	3141	1/1	0.81	0.30	81,81,81,81	0
56	MG	2A	3083	1/1	0.81	0.22	68,68,68,68	0
56	MG	2a	3036	1/1	0.81	0.38	83,83,83,83	0
56	MG	1A	3557	1/1	0.81	0.12	75,75,75,75	0
56	MG	1A	3883	1/1	0.81	0.24	58,58,58,58	0
56	MG	1A	3742	1/1	0.81	0.14	59,59,59,59	0
56	MG	2A	3478	1/1	0.81	0.30	73,73,73,73	0
56	MG	2A	3881	1/1	0.81	0.10	64,64,64,64	0
56	MG	1a	1638	1/1	0.81	0.24	71,71,71,71	0
56	MG	2a	3222	1/1	0.81	0.11	78,78,78,78	0
56	MG	1A	3968	1/1	0.81	0.14	69,69,69,69	0
56	MG	2a	3227	1/1	0.81	0.11	79,79,79,79	0
56	MG	2B	211	1/1	0.81	0.25	81,81,81,81	0
56	MG	2g	201	1/1	0.81	0.20	80,80,80,80	0
56	MG	2a	3069	1/1	0.81	0.30	78,78,78,78	0
56	MG	2a	3075	1/1	0.81	0.20	74,74,74,74	0
56	MG	2A	3386	1/1	0.81	0.21	79,79,79,79	0
56	MG	2A	3704	1/1	0.81	0.14	78,78,78,78	0
56	MG	2A	3525	1/1	0.81	0.28	70,70,70,70	0
56	MG	2A	3533	1/1	0.81	0.26	76,76,76,76	0
56	MG	1A	3975	1/1	0.81	0.27	74,74,74,74	0
56	MG	21	101	1/1	0.81	0.26	89,89,89,89	0
56	MG	1A	3823	1/1	0.81	0.23	62,62,62,62	0
56	MG	1A	3791	1/1	0.81	0.10	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3123	1/1	0.81	0.29	77,77,77,77	0
56	MG	2A	3394	1/1	0.82	0.25	77,77,77,77	0
56	MG	1a	1669	1/1	0.82	0.25	72,72,72,72	0
56	MG	1A	3526	1/1	0.82	0.16	66,66,66,66	0
56	MG	2A	3402	1/1	0.82	0.31	66,66,66,66	0
56	MG	1A	3809	1/1	0.82	0.14	55,55,55,55	0
56	MG	2a	3002	1/1	0.82	0.20	73,73,73,73	0
56	MG	1A	3671	1/1	0.82	0.11	46,46,46,46	0
56	MG	1a	1714	1/1	0.82	0.36	78,78,78,78	0
56	MG	2A	3061	1/1	0.82	0.21	63,63,63,63	0
56	MG	2a	3181	1/1	0.82	0.11	84,84,84,84	0
56	MG	2A	3432	1/1	0.82	0.27	74,74,74,74	0
56	MG	1A	3385	1/1	0.82	0.12	77,77,77,77	0
56	MG	2a	3034	1/1	0.82	0.16	87,87,87,87	0
56	MG	2A	3719	1/1	0.82	0.21	72,72,72,72	0
56	MG	1A	4058	1/1	0.82	0.25	69,69,69,69	0
56	MG	2a	3218	1/1	0.82	0.30	75,75,75,75	0
56	MG	2A	3736	1/1	0.82	0.15	62,62,62,62	0
56	MG	1A	3546	1/1	0.82	0.28	67,67,67,67	0
56	MG	2a	3226	1/1	0.82	0.13	79,79,79,79	0
56	MG	2A	3485	1/1	0.82	0.18	75,75,75,75	0
56	MG	1A	4086	1/1	0.82	0.25	59,59,59,59	0
56	MG	2A	3271	1/1	0.82	0.32	88,88,88,88	0
56	MG	2A	3502	1/1	0.82	0.12	64,64,64,64	0
56	MG	1Z	301	1/1	0.82	0.12	72,72,72,72	0
56	MG	1A	4090	1/1	0.82	0.21	69,69,69,69	0
56	MG	1A	3854	1/1	0.82	0.21	73,73,73,73	0
56	MG	2A	3879	1/1	0.82	0.22	68,68,68,68	0
56	MG	1a	1615	1/1	0.82	0.14	73,73,73,73	0
56	MG	2A	3590	1/1	0.82	0.20	72,72,72,72	0
56	MG	2A	3294	1/1	0.82	0.29	73,73,73,73	0
56	MG	1e	201	1/1	0.82	0.16	84,84,84,84	0
56	MG	1A	4093	1/1	0.82	0.18	78,78,78,78	0
56	MG	1A	3501	1/1	0.82	0.14	76,76,76,76	0
56	MG	1A	3936	1/1	0.83	0.13	53,53,53,53	0
56	MG	2A	3268	1/1	0.83	0.23	70,70,70,70	0
56	MG	1A	3966	1/1	0.83	0.11	55,55,55,55	0
56	MG	2A	3828	1/1	0.83	0.14	63,63,63,63	0
56	MG	2a	3088	1/1	0.83	0.22	82,82,82,82	0
56	MG	1a	1764	1/1	0.83	0.16	81,81,81,81	0
56	MG	2A	3870	1/1	0.83	0.17	71,71,71,71	0
56	MG	1A	3594	1/1	0.83	0.15	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	3596	1/1	0.83	0.25	71,71,71,71	0
56	MG	2A	3374	1/1	0.83	0.27	65,65,65,65	0
56	MG	1A	3308	1/1	0.83	0.28	60,60,60,60	0
56	MG	2A	3376	1/1	0.83	0.17	78,78,78,78	0
56	MG	1a	1639	1/1	0.83	0.19	64,64,64,64	0
56	MG	1A	3398	1/1	0.83	0.24	69,69,69,69	0
56	MG	2B	217	1/1	0.83	0.12	77,77,77,77	0
56	MG	1s	101	1/1	0.83	0.17	77,77,77,77	0
56	MG	2A	3661	1/1	0.83	0.27	71,71,71,71	0
56	MG	2A	3304	1/1	0.83	0.21	88,88,88,88	0
56	MG	1A	3348	1/1	0.83	0.19	64,64,64,64	0
56	MG	2A	3676	1/1	0.83	0.15	67,67,67,67	0
56	MG	1w	107	1/1	0.83	0.15	85,85,85,85	0
56	MG	2A	3181	1/1	0.83	0.22	74,74,74,74	0
56	MG	2a	3203	1/1	0.83	0.13	80,80,80,80	0
56	MG	1A	3488	1/1	0.83	0.16	77,77,77,77	0
56	MG	1A	3433	1/1	0.83	0.31	80,80,80,80	0
56	MG	2A	3702	1/1	0.83	0.12	80,80,80,80	0
56	MG	2A	3211	1/1	0.83	0.17	76,76,76,76	0
56	MG	2a	3012	1/1	0.83	0.26	75,75,75,75	0
56	MG	2a	3015	1/1	0.83	0.38	80,80,80,80	0
56	MG	2a	3020	1/1	0.83	0.26	77,77,77,77	0
56	MG	2a	3023	1/1	0.83	0.24	87,87,87,87	0
56	MG	2a	3024	1/1	0.83	0.19	74,74,74,74	0
56	MG	1A	3509	1/1	0.83	0.20	78,78,78,78	0
56	MG	2A	3710	1/1	0.83	0.17	75,75,75,75	0
56	MG	1A	3068	1/1	0.83	0.15	52,52,52,52	0
56	MG	2A	3717	1/1	0.83	0.23	67,67,67,67	0
56	MG	2A	3449	1/1	0.83	0.32	70,70,70,70	0
56	MG	2a	3043	1/1	0.83	0.23	77,77,77,77	0
56	MG	1O	201	1/1	0.83	0.14	72,72,72,72	0
56	MG	2A	3475	1/1	0.83	0.26	76,76,76,76	0
56	MG	2A	3742	1/1	0.83	0.20	73,73,73,73	0
56	MG	2y	103	1/1	0.83	0.15	90,90,90,90	0
56	MG	2A	3237	1/1	0.83	0.27	72,72,72,72	0
56	MG	1A	3570	1/1	0.83	0.28	61,61,61,61	0
56	MG	1A	4074	1/1	0.83	0.10	52,52,52,52	0
56	MG	2A	3254	1/1	0.84	0.20	71,71,71,71	0
56	MG	2A	3687	1/1	0.84	0.17	71,71,71,71	0
56	MG	1A	3602	1/1	0.84	0.25	63,63,63,63	0
56	MG	1a	1679	1/1	0.84	0.17	81,81,81,81	0
56	MG	1x	111	1/1	0.84	0.21	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	1y	101	1/1	0.84	0.11	91,91,91,91	0
56	MG	2a	3048	1/1	0.84	0.29	80,80,80,80	0
56	MG	2A	3008	1/1	0.84	0.24	73,73,73,73	0
56	MG	1a	1683	1/1	0.84	0.19	78,78,78,78	0
56	MG	1A	3603	1/1	0.84	0.28	58,58,58,58	0
56	MG	2A	3406	1/1	0.84	0.17	76,76,76,76	0
56	MG	2A	3407	1/1	0.84	0.13	82,82,82,82	0
56	MG	1a	1710	1/1	0.84	0.16	72,72,72,72	0
56	MG	1A	4006	1/1	0.84	0.20	33,33,33,33	0
56	MG	2A	3412	1/1	0.84	0.24	73,73,73,73	0
56	MG	2A	3740	1/1	0.84	0.14	75,75,75,75	0
56	MG	1A	3299	1/1	0.84	0.34	68,68,68,68	0
56	MG	1A	3545	1/1	0.84	0.29	62,62,62,62	0
56	MG	2A	3761	1/1	0.84	0.16	40,40,40,40	0
56	MG	2A	3426	1/1	0.84	0.23	65,65,65,65	0
56	MG	1B	3631	1/1	0.84	0.11	73,73,73,73	0
56	MG	2A	3306	1/1	0.84	0.44	66,66,66,66	0
56	MG	2a	3118	1/1	0.84	0.16	76,76,76,76	0
56	MG	2A	3811	1/1	0.84	0.13	75,75,75,75	0
56	MG	2A	3813	1/1	0.84	0.14	73,73,73,73	0
56	MG	2A	3310	1/1	0.84	0.22	69,69,69,69	0
56	MG	1A	3353	1/1	0.84	0.20	70,70,70,70	0
56	MG	2a	3129	1/1	0.84	0.24	78,78,78,78	0
56	MG	2A	3098	1/1	0.84	0.22	75,75,75,75	0
56	MG	1A	3360	1/1	0.84	0.15	71,71,71,71	0
56	MG	2A	3861	1/1	0.84	0.11	56,56,56,56	0
56	MG	1A	3846	1/1	0.84	0.14	55,55,55,55	0
56	MG	1A	3716	1/1	0.84	0.13	46,46,46,46	0
56	MG	2A	3497	1/1	0.84	0.44	81,81,81,81	0
56	MG	2A	3111	1/1	0.84	0.19	71,71,71,71	0
56	MG	2A	3327	1/1	0.84	0.17	71,71,71,71	0
56	MG	2a	3200	1/1	0.84	0.24	82,82,82,82	0
56	MG	1W	207	1/1	0.84	0.22	38,38,38,38	0
56	MG	1A	3730	1/1	0.84	0.13	67,67,67,67	0
56	MG	2a	3209	1/1	0.84	0.21	80,80,80,80	0
56	MG	1Z	302	1/1	0.84	0.14	77,77,77,77	0
56	MG	1a	1800	1/1	0.84	0.14	73,73,73,73	0
56	MG	1A	3732	1/1	0.84	0.24	71,71,71,71	0
56	MG	1A	3473	1/1	0.84	0.15	60,60,60,60	0
56	MG	2A	3601	1/1	0.84	0.22	92,92,92,92	0
56	MG	1f	202	1/1	0.84	0.28	74,74,74,74	0
56	MG	1a	1601	1/1	0.84	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	3228	1/1	0.84	0.40	78,78,78,78	0
56	MG	2A	3613	1/1	0.84	0.16	69,69,69,69	0
56	MG	2A	3614	1/1	0.84	0.27	63,63,63,63	0
56	MG	2A	3616	1/1	0.84	0.20	71,71,71,71	0
56	MG	2A	3617	1/1	0.84	0.14	66,66,66,66	0
56	MG	1A	3914	1/1	0.84	0.10	47,47,47,47	0
56	MG	2r	101	1/1	0.84	0.12	77,77,77,77	0
56	MG	1A	3254	1/1	0.84	0.14	69,69,69,69	0
56	MG	1w	106	1/1	0.84	0.10	72,72,72,72	0
56	MG	1A	3231	1/1	0.84	0.16	69,69,69,69	0
56	MG	2a	3016	1/1	0.84	0.21	73,73,73,73	0
56	MG	2A	3364	1/1	0.84	0.60	85,85,85,85	0
56	MG	2y	102	1/1	0.84	0.13	94,94,94,94	0
56	MG	2A	3671	1/1	0.84	0.13	77,77,77,77	0
56	MG	2A	3672	1/1	0.84	0.12	76,76,76,76	0
56	MG	1A	3137	1/1	0.84	0.21	57,57,57,57	0
56	MG	2a	3032	1/1	0.84	0.39	79,79,79,79	0
56	MG	1A	3264	1/1	0.85	0.13	64,64,64,64	0
56	MG	1A	3332	1/1	0.85	0.26	61,61,61,61	0
56	MG	2A	3609	1/1	0.85	0.24	69,69,69,69	0
56	MG	2A	3844	1/1	0.85	0.13	46,46,46,46	0
56	MG	2A	3851	1/1	0.85	0.12	67,67,67,67	0
56	MG	2a	3099	1/1	0.85	0.28	73,73,73,73	0
56	MG	1a	1633	1/1	0.85	0.25	81,81,81,81	0
56	MG	2A	3132	1/1	0.85	0.13	60,60,60,60	0
56	MG	2A	3866	1/1	0.85	0.14	68,68,68,68	0
56	MG	1A	3911	1/1	0.85	0.20	46,46,46,46	0
56	MG	2A	3177	1/1	0.85	0.15	66,66,66,66	0
56	MG	2a	3113	1/1	0.85	0.27	77,77,77,77	0
56	MG	2a	3114	1/1	0.85	0.36	83,83,83,83	0
56	MG	1A	3337	1/1	0.85	0.13	63,63,63,63	0
56	MG	2a	3119	1/1	0.85	0.23	72,72,72,72	0
56	MG	2A	3880	1/1	0.85	0.18	60,60,60,60	0
56	MG	2A	3191	1/1	0.85	0.18	72,72,72,72	0
56	MG	2A	3006	1/1	0.85	0.30	65,65,65,65	0
56	MG	1A	3054	1/1	0.85	0.16	51,51,51,51	0
56	MG	2A	3206	1/1	0.85	0.33	74,74,74,74	0
56	MG	2a	3133	1/1	0.85	0.27	75,75,75,75	0
56	MG	2B	213	1/1	0.85	0.23	71,71,71,71	0
56	MG	2a	3136	1/1	0.85	0.29	65,65,65,65	0
56	MG	2A	3207	1/1	0.85	0.14	69,69,69,69	0
56	MG	1S	201	1/1	0.85	0.36	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	2A	3215	1/1	0.85	0.16	69,69,69,69	0
56	MG	2A	3419	1/1	0.85	0.23	69,69,69,69	0
56	MG	2A	3218	1/1	0.85	0.29	75,75,75,75	0
56	MG	2a	3194	1/1	0.85	0.19	79,79,79,79	0
56	MG	1a	1672	1/1	0.85	0.14	63,63,63,63	0
56	MG	2A	3439	1/1	0.85	0.33	60,60,60,60	0
56	MG	2A	3691	1/1	0.85	0.12	73,73,73,73	0
56	MG	28	103	1/1	0.85	0.30	65,65,65,65	0
56	MG	2A	3339	1/1	0.85	0.27	63,63,63,63	0
56	MG	2A	3342	1/1	0.85	0.14	82,82,82,82	0
56	MG	2A	3456	1/1	0.85	0.23	58,58,58,58	0
56	MG	2a	3216	1/1	0.85	0.21	76,76,76,76	0
56	MG	2A	3458	1/1	0.85	0.28	71,71,71,71	0
56	MG	1A	3092	1/1	0.85	0.20	68,68,68,68	0
56	MG	2A	3709	1/1	0.85	0.12	68,68,68,68	0
56	MG	2a	3223	1/1	0.85	0.19	84,84,84,84	0
56	MG	1a	1802	1/1	0.85	0.10	81,81,81,81	0
56	MG	1a	1682	1/1	0.85	0.29	75,75,75,75	0
56	MG	2A	3716	1/1	0.85	0.19	76,76,76,76	0
56	MG	2A	3483	1/1	0.85	0.21	76,76,76,76	0
56	MG	2A	3238	1/1	0.85	0.14	64,64,64,64	0
56	MG	2A	3727	1/1	0.85	0.19	68,68,68,68	0
56	MG	2A	3348	1/1	0.85	0.15	90,90,90,90	0
56	MG	2l	204	1/1	0.85	0.17	84,84,84,84	0
56	MG	2A	3734	1/1	0.85	0.15	79,79,79,79	0
56	MG	1A	3850	1/1	0.85	0.10	67,67,67,67	0
56	MG	1a	1694	1/1	0.85	0.26	63,63,63,63	0
56	MG	1Y	201	1/1	0.85	0.25	63,63,63,63	0
56	MG	1A	3542	1/1	0.85	0.28	57,57,57,57	0
56	MG	2w	101	1/1	0.85	0.26	82,82,82,82	0
56	MG	1w	101	1/1	0.85	0.20	70,70,70,70	0
56	MG	2w	104	1/1	0.85	0.14	76,76,76,76	0
56	MG	1B	3611	1/1	0.85	0.16	63,63,63,63	0
56	MG	1A	3474	1/1	0.85	0.12	61,61,61,61	0
56	MG	2A	3807	1/1	0.85	0.09	61,61,61,61	0
56	MG	2A	3547	1/1	0.85	0.16	59,59,59,59	0
56	MG	2a	3062	1/1	0.85	0.39	74,74,74,74	0
56	MG	1B	3629	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3113	1/1	0.85	0.12	67,67,67,67	0
56	MG	2A	3751	1/1	0.86	0.18	68,68,68,68	0
56	MG	1a	1671	1/1	0.86	0.11	62,62,62,62	0
56	MG	2a	3058	1/1	0.86	0.20	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1w	105	1/1	0.86	0.15	73,73,73,73	0
56	MG	1A	3475	1/1	0.86	0.18	76,76,76,76	0
56	MG	1A	3098	1/1	0.86	0.21	74,74,74,74	0
56	MG	2A	3786	1/1	0.86	0.18	61,61,61,61	0
56	MG	2A	3806	1/1	0.86	0.13	61,61,61,61	0
56	MG	1A	4031	1/1	0.86	0.12	68,68,68,68	0
56	MG	1A	3039	1/1	0.86	0.24	67,67,67,67	0
56	MG	1A	3867	1/1	0.86	0.10	50,50,50,50	0
56	MG	1a	1695	1/1	0.86	0.30	64,64,64,64	0
56	MG	2a	3101	1/1	0.86	0.46	79,79,79,79	0
56	MG	2A	3350	1/1	0.86	0.19	76,76,76,76	0
56	MG	1A	4039	1/1	0.86	0.36	65,65,65,65	0
56	MG	1a	1701	1/1	0.86	0.21	73,73,73,73	0
56	MG	1a	1703	1/1	0.86	0.40	76,76,76,76	0
56	MG	2A	3568	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3874	1/1	0.86	0.20	58,58,58,58	0
56	MG	1A	3413	1/1	0.86	0.19	66,66,66,66	0
56	MG	1A	4057	1/1	0.86	0.14	63,63,63,63	0
56	MG	2A	3367	1/1	0.86	0.15	70,70,70,70	0
56	MG	2A	3371	1/1	0.86	0.13	69,69,69,69	0
56	MG	2A	3875	1/1	0.86	0.16	71,71,71,71	0
56	MG	2A	3876	1/1	0.86	0.22	67,67,67,67	0
56	MG	1A	3424	1/1	0.86	0.25	69,69,69,69	0
56	MG	2A	3064	1/1	0.86	0.18	81,81,81,81	0
56	MG	1A	3907	1/1	0.86	0.10	61,61,61,61	0
56	MG	1A	3807	1/1	0.86	0.09	59,59,59,59	0
56	MG	2B	206	1/1	0.86	0.20	70,70,70,70	0
56	MG	2A	3379	1/1	0.86	0.10	80,80,80,80	0
56	MG	2A	3385	1/1	0.86	0.26	70,70,70,70	0
56	MG	2a	3143	1/1	0.86	0.37	62,62,62,62	0
56	MG	2A	3092	1/1	0.86	0.19	70,70,70,70	0
56	MG	2A	3392	1/1	0.86	0.14	73,73,73,73	0
56	MG	2A	3274	1/1	0.86	0.20	84,84,84,84	0
56	MG	2a	3189	1/1	0.86	0.23	72,72,72,72	0
56	MG	1A	3368	1/1	0.86	0.37	51,51,51,51	0
56	MG	2D	306	1/1	0.86	0.39	59,59,59,59	0
56	MG	2D	307	1/1	0.86	0.16	71,71,71,71	0
56	MG	13	103	1/1	0.86	0.16	59,59,59,59	0
56	MG	2Q	202	1/1	0.86	0.21	65,65,65,65	0
56	MG	1A	3460	1/1	0.86	0.20	64,64,64,64	0
56	MG	2A	3403	1/1	0.86	0.26	73,73,73,73	0
56	MG	2A	3405	1/1	0.86	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3214	1/1	0.86	0.33	63,63,63,63	0
56	MG	1a	1755	1/1	0.86	0.15	81,81,81,81	0
56	MG	26	101	1/1	0.86	0.32	73,73,73,73	0
56	MG	2A	3688	1/1	0.86	0.20	74,74,74,74	0
56	MG	2a	3221	1/1	0.86	0.14	76,76,76,76	0
56	MG	2A	3102	1/1	0.86	0.28	80,80,80,80	0
56	MG	2a	3006	1/1	0.86	0.31	78,78,78,78	0
56	MG	2A	3297	1/1	0.86	0.18	69,69,69,69	0
56	MG	1a	1763	1/1	0.86	0.19	73,73,73,73	0
56	MG	1A	3375	1/1	0.86	0.20	61,61,61,61	0
56	MG	2A	3413	1/1	0.86	0.11	59,59,59,59	0
56	MG	2a	3229	1/1	0.86	0.15	71,71,71,71	0
56	MG	1A	3839	1/1	0.86	0.16	66,66,66,66	0
56	MG	2A	3706	1/1	0.86	0.15	60,60,60,60	0
56	MG	1A	3974	1/1	0.86	0.20	55,55,55,55	0
56	MG	2a	3019	1/1	0.86	0.15	83,83,83,83	0
56	MG	1A	3844	1/1	0.86	0.19	66,66,66,66	0
56	MG	1A	3987	1/1	0.86	0.12	71,71,71,71	0
56	MG	2A	3318	1/1	0.86	0.27	71,71,71,71	0
56	MG	2a	3027	1/1	0.86	0.15	75,75,75,75	0
56	MG	1A	3326	1/1	0.86	0.19	60,60,60,60	0
56	MG	2A	3440	1/1	0.86	0.40	78,78,78,78	0
56	MG	1a	1656	1/1	0.86	0.25	68,68,68,68	0
56	MG	2a	3035	1/1	0.86	0.13	89,89,89,89	0
56	MG	1a	1658	1/1	0.86	0.20	69,69,69,69	0
56	MG	2w	106	1/1	0.86	0.09	82,82,82,82	0
56	MG	1a	1661	1/1	0.86	0.27	82,82,82,82	0
56	MG	2A	3178	1/1	0.86	0.23	76,76,76,76	0
56	MG	1a	1667	1/1	0.86	0.32	70,70,70,70	0
56	MG	1A	3262	1/1	0.86	0.23	76,76,76,76	0
56	MG	2A	3476	1/1	0.86	0.20	74,74,74,74	0
56	MG	2A	3746	1/1	0.86	0.15	61,61,61,61	0
56	MG	2a	3031	1/1	0.87	0.23	71,71,71,71	0
56	MG	1a	1647	1/1	0.87	0.17	69,69,69,69	0
56	MG	2A	3404	1/1	0.87	0.12	72,72,72,72	0
56	MG	2A	3088	1/1	0.87	0.15	57,57,57,57	0
56	MG	1A	3412	1/1	0.87	0.16	59,59,59,59	0
56	MG	2A	3277	1/1	0.87	0.20	75,75,75,75	0
56	MG	2A	3278	1/1	0.87	0.22	68,68,68,68	0
56	MG	1A	3717	1/1	0.87	0.16	67,67,67,67	0
56	MG	2A	3411	1/1	0.87	0.08	79,79,79,79	0
56	MG	1A	3255	1/1	0.87	0.13	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3547	1/1	0.87	0.34	55,55,55,55	0
56	MG	1a	1668	1/1	0.87	0.38	74,74,74,74	0
56	MG	2A	3732	1/1	0.87	0.11	76,76,76,76	0
56	MG	1A	3737	1/1	0.87	0.15	60,60,60,60	0
56	MG	1a	1810	1/1	0.87	0.30	59,59,59,59	0
56	MG	1A	3414	1/1	0.87	0.13	56,56,56,56	0
56	MG	1a	1813	1/1	0.87	0.22	67,67,67,67	0
56	MG	2A	3437	1/1	0.87	0.21	68,68,68,68	0
56	MG	1A	3364	1/1	0.87	0.16	64,64,64,64	0
56	MG	2A	3311	1/1	0.87	0.15	77,77,77,77	0
56	MG	2a	3083	1/1	0.87	0.34	68,68,68,68	0
56	MG	1A	4046	1/1	0.87	0.12	49,49,49,49	0
56	MG	2a	3085	1/1	0.87	0.16	75,75,75,75	0
56	MG	2A	3313	1/1	0.87	0.25	74,74,74,74	0
56	MG	2a	3092	1/1	0.87	0.21	78,78,78,78	0
56	MG	2A	3314	1/1	0.87	0.46	62,62,62,62	0
56	MG	1A	3747	1/1	0.87	0.10	52,52,52,52	0
56	MG	2a	3105	1/1	0.87	0.15	70,70,70,70	0
56	MG	2A	3461	1/1	0.87	0.26	76,76,76,76	0
56	MG	2A	3469	1/1	0.87	0.13	70,70,70,70	0
56	MG	1A	3087	1/1	0.87	0.13	39,39,39,39	0
56	MG	2a	3110	1/1	0.87	0.25	93,93,93,93	0
56	MG	2A	3119	1/1	0.87	0.30	72,72,72,72	0
56	MG	1t	201	1/1	0.87	0.29	66,66,66,66	0
56	MG	1a	1690	1/1	0.87	0.22	57,57,57,57	0
56	MG	2A	3137	1/1	0.87	0.21	66,66,66,66	0
56	MG	2A	3818	1/1	0.87	0.11	82,82,82,82	0
56	MG	2A	3146	1/1	0.87	0.16	76,76,76,76	0
56	MG	2A	3492	1/1	0.87	0.23	62,62,62,62	0
56	MG	2A	3164	1/1	0.87	0.28	80,80,80,80	0
56	MG	2A	3852	1/1	0.87	0.11	71,71,71,71	0
56	MG	2A	3334	1/1	0.87	0.14	67,67,67,67	0
56	MG	2A	3499	1/1	0.87	0.13	73,73,73,73	0
56	MG	1A	3435	1/1	0.87	0.13	54,54,54,54	0
56	MG	1A	3338	1/1	0.87	0.18	58,58,58,58	0
56	MG	2A	3872	1/1	0.87	0.08	69,69,69,69	0
56	MG	2A	3503	1/1	0.87	0.13	64,64,64,64	0
56	MG	1a	1697	1/1	0.87	0.37	73,73,73,73	0
56	MG	2A	3508	1/1	0.87	0.31	70,70,70,70	0
56	MG	2a	3146	1/1	0.87	0.38	72,72,72,72	0
56	MG	2A	3520	1/1	0.87	0.25	60,60,60,60	0
56	MG	2a	3150	1/1	0.87	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3151	1/1	0.87	0.19	65,65,65,65	0
56	MG	1A	3252	1/1	0.87	0.27	48,48,48,48	0
56	MG	1A	3467	1/1	0.87	0.32	71,71,71,71	0
56	MG	1x	106	1/1	0.87	0.23	67,67,67,67	0
56	MG	2B	201	1/1	0.87	0.23	76,76,76,76	0
56	MG	2A	3545	1/1	0.87	0.26	66,66,66,66	0
56	MG	2A	3201	1/1	0.87	0.15	58,58,58,58	0
56	MG	1A	3647	1/1	0.87	0.18	62,62,62,62	0
56	MG	2A	3585	1/1	0.87	0.13	53,53,53,53	0
56	MG	2a	3205	1/1	0.87	0.17	66,66,66,66	0
56	MG	15	107	1/1	0.87	0.15	65,65,65,65	0
56	MG	1x	110	1/1	0.87	0.19	70,70,70,70	0
56	MG	1A	3651	1/1	0.87	0.12	79,79,79,79	0
56	MG	1x	113	1/1	0.87	0.31	66,66,66,66	0
56	MG	2A	3216	1/1	0.87	0.46	80,80,80,80	0
56	MG	2F	305	1/1	0.87	0.10	76,76,76,76	0
56	MG	2A	3217	1/1	0.87	0.22	81,81,81,81	0
56	MG	1A	3324	1/1	0.87	0.28	63,63,63,63	0
56	MG	2R	201	1/1	0.87	0.21	70,70,70,70	0
56	MG	2V	201	1/1	0.87	0.29	51,51,51,51	0
56	MG	2A	3220	1/1	0.87	0.19	56,56,56,56	0
56	MG	1a	1625	1/1	0.87	0.33	71,71,71,71	0
56	MG	1a	1631	1/1	0.87	0.40	73,73,73,73	0
56	MG	1A	3829	1/1	0.87	0.16	42,42,42,42	0
56	MG	2A	3630	1/1	0.87	0.18	75,75,75,75	0
56	MG	2A	3233	1/1	0.87	0.17	60,60,60,60	0
56	MG	2a	3238	1/1	0.87	0.14	83,83,83,83	0
56	MG	1A	3180	1/1	0.87	0.29	63,63,63,63	0
56	MG	2a	3003	1/1	0.87	0.14	85,85,85,85	0
56	MG	2A	3377	1/1	0.87	0.17	55,55,55,55	0
56	MG	2A	3036	1/1	0.87	0.29	58,58,58,58	0
56	MG	2A	3044	1/1	0.87	0.11	53,53,53,53	0
56	MG	2A	3382	1/1	0.87	0.25	73,73,73,73	0
56	MG	2A	3252	1/1	0.87	0.37	74,74,74,74	0
56	MG	2A	3052	1/1	0.87	0.11	62,62,62,62	0
56	MG	2a	3014	1/1	0.87	0.31	70,70,70,70	0
56	MG	2A	3387	1/1	0.87	0.25	55,55,55,55	0
56	MG	2A	3054	1/1	0.87	0.21	69,69,69,69	0
56	MG	1A	3539	1/1	0.87	0.17	66,66,66,66	0
56	MG	2A	3266	1/1	0.87	0.11	60,60,60,60	0
56	MG	1A	3328	1/1	0.87	0.12	50,50,50,50	0
56	MG	2x	105	1/1	0.87	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2y	101	1/1	0.87	0.10	77,77,77,77	0
56	MG	2A	3397	1/1	0.87	0.15	69,69,69,69	0
56	MG	2a	3025	1/1	0.87	0.28	72,72,72,72	0
56	MG	2a	3026	1/1	0.87	0.13	82,82,82,82	0
56	MG	2A	3700	1/1	0.87	0.18	74,74,74,74	0
56	MG	1a	1754	1/1	0.87	0.18	81,81,81,81	0
56	MG	2A	3772	1/1	0.88	0.15	74,74,74,74	0
56	MG	2a	3054	1/1	0.88	0.23	86,86,86,86	0
56	MG	1A	3927	1/1	0.88	0.15	70,70,70,70	0
56	MG	2A	3782	1/1	0.88	0.11	79,79,79,79	0
56	MG	1A	3513	1/1	0.88	0.26	68,68,68,68	0
56	MG	2a	3060	1/1	0.88	0.17	78,78,78,78	0
56	MG	1A	3816	1/1	0.88	0.13	41,41,41,41	0
56	MG	2A	3059	1/1	0.88	0.34	77,77,77,77	0
56	MG	2a	3065	1/1	0.88	0.20	75,75,75,75	0
56	MG	2a	3066	1/1	0.88	0.17	87,87,87,87	0
56	MG	2a	3067	1/1	0.88	0.23	69,69,69,69	0
56	MG	1A	3569	1/1	0.88	0.20	63,63,63,63	0
56	MG	1a	1636	1/1	0.88	0.25	79,79,79,79	0
56	MG	1A	4095	1/1	0.88	0.12	72,72,72,72	0
56	MG	1A	3373	1/1	0.88	0.12	57,57,57,57	0
56	MG	1A	3731	1/1	0.88	0.14	52,52,52,52	0
56	MG	2A	3509	1/1	0.88	0.15	69,69,69,69	0
56	MG	2A	3825	1/1	0.88	0.10	79,79,79,79	0
56	MG	2A	3518	1/1	0.88	0.10	59,59,59,59	0
56	MG	2a	3090	1/1	0.88	0.23	69,69,69,69	0
56	MG	2A	3363	1/1	0.88	0.13	69,69,69,69	0
56	MG	2A	3521	1/1	0.88	0.32	79,79,79,79	0
56	MG	2A	3248	1/1	0.88	0.12	71,71,71,71	0
56	MG	2a	3103	1/1	0.88	0.21	81,81,81,81	0
56	MG	2a	3104	1/1	0.88	0.34	76,76,76,76	0
56	MG	2A	3090	1/1	0.88	0.16	56,56,56,56	0
56	MG	2A	3535	1/1	0.88	0.09	63,63,63,63	0
56	MG	1a	1775	1/1	0.88	0.09	88,88,88,88	0
56	MG	2A	3373	1/1	0.88	0.32	59,59,59,59	0
56	MG	1A	3374	1/1	0.88	0.34	66,66,66,66	0
56	MG	1a	1649	1/1	0.88	0.25	74,74,74,74	0
56	MG	2A	3571	1/1	0.88	0.18	56,56,56,56	0
56	MG	2A	3581	1/1	0.88	0.26	65,65,65,65	0
56	MG	1a	1654	1/1	0.88	0.18	70,70,70,70	0
56	MG	1B	3618	1/1	0.88	0.08	47,47,47,47	0
56	MG	1A	3417	1/1	0.88	0.23	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	2A	3884	1/1	0.88	0.18	68,68,68,68	0
56	MG	1B	3623	1/1	0.88	0.15	59,59,59,59	0
56	MG	1B	3626	1/1	0.88	0.18	62,62,62,62	0
56	MG	2B	203	1/1	0.88	0.26	81,81,81,81	0
56	MG	2B	204	1/1	0.88	0.20	81,81,81,81	0
56	MG	1A	4004	1/1	0.88	0.11	39,39,39,39	0
56	MG	1A	3187	1/1	0.88	0.12	52,52,52,52	0
56	MG	2B	209	1/1	0.88	0.23	74,74,74,74	0
56	MG	2a	3137	1/1	0.88	0.29	71,71,71,71	0
56	MG	2a	3140	1/1	0.88	0.31	67,67,67,67	0
56	MG	1l	202	1/1	0.88	0.13	73,73,73,73	0
56	MG	2A	3388	1/1	0.88	0.34	68,68,68,68	0
56	MG	1A	3333	1/1	0.88	0.11	52,52,52,52	0
56	MG	1B	3635	1/1	0.88	0.14	72,72,72,72	0
56	MG	2a	3147	1/1	0.88	0.11	63,63,63,63	0
56	MG	2A	3283	1/1	0.88	0.20	75,75,75,75	0
56	MG	2A	3288	1/1	0.88	0.16	66,66,66,66	0
56	MG	2A	3635	1/1	0.88	0.16	67,67,67,67	0
56	MG	2a	3162	1/1	0.88	0.13	83,83,83,83	0
56	MG	2a	3166	1/1	0.88	0.10	78,78,78,78	0
56	MG	2a	3174	1/1	0.88	0.09	86,86,86,86	0
56	MG	2F	301	1/1	0.88	0.10	50,50,50,50	0
56	MG	2a	3180	1/1	0.88	0.10	72,72,72,72	0
56	MG	1a	1674	1/1	0.88	0.23	82,82,82,82	0
56	MG	2A	3399	1/1	0.88	0.31	68,68,68,68	0
56	MG	1A	3334	1/1	0.88	0.24	69,69,69,69	0
56	MG	2A	3128	1/1	0.88	0.17	59,59,59,59	0
56	MG	2A	3296	1/1	0.88	0.43	78,78,78,78	0
56	MG	2V	202	1/1	0.88	0.11	71,71,71,71	0
56	MG	1A	3855	1/1	0.88	0.16	59,59,59,59	0
56	MG	2A	3673	1/1	0.88	0.18	76,76,76,76	0
56	MG	2a	3206	1/1	0.88	0.15	69,69,69,69	0
56	MG	2a	3207	1/1	0.88	0.16	68,68,68,68	0
56	MG	2A	3133	1/1	0.88	0.08	76,76,76,76	0
56	MG	1A	3482	1/1	0.88	0.17	63,63,63,63	0
56	MG	2a	3211	1/1	0.88	0.16	75,75,75,75	0
56	MG	1a	1686	1/1	0.88	0.27	81,81,81,81	0
56	MG	2A	3157	1/1	0.88	0.30	64,64,64,64	0
56	MG	2A	3159	1/1	0.88	0.20	65,65,65,65	0
56	MG	1A	3865	1/1	0.88	0.12	63,63,63,63	0
56	MG	2a	3005	1/1	0.88	0.33	77,77,77,77	0
56	MG	2a	3219	1/1	0.88	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3168	1/1	0.88	0.23	67,67,67,67	0
56	MG	1a	1691	1/1	0.88	0.29	60,60,60,60	0
56	MG	1A	3657	1/1	0.88	0.11	69,69,69,69	0
56	MG	2A	3317	1/1	0.88	0.12	80,80,80,80	0
56	MG	2A	3421	1/1	0.88	0.22	55,55,55,55	0
56	MG	2A	3425	1/1	0.88	0.23	49,49,49,49	0
56	MG	2a	3013	1/1	0.88	0.25	72,72,72,72	0
56	MG	1A	3871	1/1	0.88	0.21	62,62,62,62	0
56	MG	2A	3431	1/1	0.88	0.16	56,56,56,56	0
56	MG	2a	3235	1/1	0.88	0.27	68,68,68,68	0
56	MG	2a	3236	1/1	0.88	0.21	72,72,72,72	0
56	MG	2a	3237	1/1	0.88	0.32	69,69,69,69	0
56	MG	2A	3180	1/1	0.88	0.18	54,54,54,54	0
56	MG	2a	3017	1/1	0.88	0.30	77,77,77,77	0
56	MG	1A	3760	1/1	0.88	0.16	44,44,44,44	0
56	MG	2l	202	1/1	0.88	0.24	79,79,79,79	0
56	MG	2A	3189	1/1	0.88	0.19	68,68,68,68	0
56	MG	1A	3764	1/1	0.88	0.23	58,58,58,58	0
56	MG	2A	3443	1/1	0.88	0.44	67,67,67,67	0
56	MG	2A	3193	1/1	0.88	0.23	73,73,73,73	0
56	MG	2t	201	1/1	0.88	0.21	62,62,62,62	0
56	MG	2A	3329	1/1	0.88	0.15	67,67,67,67	0
56	MG	2A	3731	1/1	0.88	0.13	64,64,64,64	0
56	MG	1A	3133	1/1	0.88	0.17	58,58,58,58	0
56	MG	2a	3030	1/1	0.88	0.15	75,75,75,75	0
56	MG	2A	3333	1/1	0.88	0.12	69,69,69,69	0
56	MG	1A	3495	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3739	1/1	0.88	0.12	62,62,62,62	0
56	MG	2A	3337	1/1	0.88	0.14	79,79,79,79	0
56	MG	1a	1709	1/1	0.88	0.23	65,65,65,65	0
56	MG	1A	3908	1/1	0.88	0.13	70,70,70,70	0
56	MG	1A	3079	1/1	0.88	0.13	60,60,60,60	0
56	MG	1A	3303	1/1	0.88	0.17	48,48,48,48	0
56	MG	1A	4088	1/1	0.88	0.17	61,61,61,61	0
56	MG	1a	1602	1/1	0.88	0.20	65,65,65,65	0
56	MG	2y	106	1/1	0.88	0.36	79,79,79,79	0
56	MG	2a	3049	1/1	0.88	0.24	72,72,72,72	0
56	MG	2A	3279	1/1	0.89	0.42	75,75,75,75	0
56	MG	2A	3744	1/1	0.89	0.12	76,76,76,76	0
56	MG	1A	3315	1/1	0.89	0.08	51,51,51,51	0
56	MG	2A	3055	1/1	0.89	0.29	73,73,73,73	0
56	MG	2A	3752	1/1	0.89	0.16	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	2A	3057	1/1	0.89	0.14	72,72,72,72	0
56	MG	1B	3625	1/1	0.89	0.11	60,60,60,60	0
56	MG	2A	3060	1/1	0.89	0.16	63,63,63,63	0
56	MG	1A	3514	1/1	0.89	0.14	62,62,62,62	0
56	MG	2a	3071	1/1	0.89	0.12	76,76,76,76	0
56	MG	2A	3444	1/1	0.89	0.31	68,68,68,68	0
56	MG	2A	3781	1/1	0.89	0.16	72,72,72,72	0
56	MG	1A	3523	1/1	0.89	0.20	54,54,54,54	0
56	MG	1A	3150	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3789	1/1	0.89	0.08	79,79,79,79	0
56	MG	2a	3087	1/1	0.89	0.21	65,65,65,65	0
56	MG	2A	3065	1/1	0.89	0.11	78,78,78,78	0
56	MG	2A	3302	1/1	0.89	0.34	76,76,76,76	0
56	MG	2a	3091	1/1	0.89	0.16	72,72,72,72	0
56	MG	1A	3024	1/1	0.89	0.16	58,58,58,58	0
56	MG	2A	3468	1/1	0.89	0.21	70,70,70,70	0
56	MG	1A	3440	1/1	0.89	0.27	59,59,59,59	0
56	MG	2A	3307	1/1	0.89	0.22	70,70,70,70	0
56	MG	1A	3454	1/1	0.89	0.11	60,60,60,60	0
56	MG	1a	1705	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3819	1/1	0.89	0.12	62,62,62,62	0
56	MG	1a	1708	1/1	0.89	0.34	74,74,74,74	0
56	MG	1E	317	1/1	0.89	0.07	41,41,41,41	0
56	MG	2A	3831	1/1	0.89	0.10	58,58,58,58	0
56	MG	2A	3838	1/1	0.89	0.09	74,74,74,74	0
56	MG	1G	204	1/1	0.89	0.10	60,60,60,60	0
56	MG	2A	3486	1/1	0.89	0.14	64,64,64,64	0
56	MG	2A	3489	1/1	0.89	0.17	77,77,77,77	0
56	MG	2a	3116	1/1	0.89	0.17	71,71,71,71	0
56	MG	1A	3455	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3457	1/1	0.89	0.15	71,71,71,71	0
56	MG	1A	3458	1/1	0.89	0.17	55,55,55,55	0
56	MG	1U	203	1/1	0.89	0.15	38,38,38,38	0
56	MG	1A	3251	1/1	0.89	0.08	58,58,58,58	0
56	MG	1a	1723	1/1	0.89	0.31	63,63,63,63	0
56	MG	2A	3324	1/1	0.89	0.35	75,75,75,75	0
56	MG	1a	1736	1/1	0.89	0.10	72,72,72,72	0
56	MG	1A	3330	1/1	0.89	0.13	59,59,59,59	0
56	MG	1A	3083	1/1	0.89	0.23	44,44,44,44	0
56	MG	1Y	202	1/1	0.89	0.12	74,74,74,74	0
56	MG	2a	3139	1/1	0.89	0.31	69,69,69,69	0
56	MG	1a	1753	1/1	0.89	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3787	1/1	0.89	0.11	46,46,46,46	0
56	MG	1A	3026	1/1	0.89	0.18	64,64,64,64	0
56	MG	1a	1759	1/1	0.89	0.30	71,71,71,71	0
56	MG	1a	1760	1/1	0.89	0.13	73,73,73,73	0
56	MG	1A	3559	1/1	0.89	0.17	63,63,63,63	0
56	MG	1A	4012	1/1	0.89	0.15	57,57,57,57	0
56	MG	1a	1766	1/1	0.89	0.13	73,73,73,73	0
56	MG	1A	3300	1/1	0.89	0.19	54,54,54,54	0
56	MG	1a	1776	1/1	0.89	0.11	77,77,77,77	0
56	MG	2a	3165	1/1	0.89	0.10	88,88,88,88	0
56	MG	1a	1779	1/1	0.89	0.10	72,72,72,72	0
56	MG	2a	3171	1/1	0.89	0.10	74,74,74,74	0
56	MG	1A	3027	1/1	0.89	0.17	74,74,74,74	0
56	MG	2B	218	1/1	0.89	0.15	71,71,71,71	0
56	MG	2A	3586	1/1	0.89	0.17	56,56,56,56	0
56	MG	1a	1784	1/1	0.89	0.11	66,66,66,66	0
56	MG	2a	3182	1/1	0.89	0.13	83,83,83,83	0
56	MG	17	104	1/1	0.89	0.14	59,59,59,59	0
56	MG	2A	3599	1/1	0.89	0.15	68,68,68,68	0
56	MG	2A	3354	1/1	0.89	0.24	69,69,69,69	0
56	MG	2A	3602	1/1	0.89	0.10	65,65,65,65	0
56	MG	2a	3199	1/1	0.89	0.28	71,71,71,71	0
56	MG	1A	3259	1/1	0.89	0.20	53,53,53,53	0
56	MG	2A	3182	1/1	0.89	0.22	67,67,67,67	0
56	MG	2T	201	1/1	0.89	0.13	65,65,65,65	0
56	MG	2A	3184	1/1	0.89	0.28	75,75,75,75	0
56	MG	1A	3576	1/1	0.89	0.15	55,55,55,55	0
56	MG	1A	3820	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	3587	1/1	0.89	0.12	52,52,52,52	0
56	MG	2A	3195	1/1	0.89	0.29	73,73,73,73	0
56	MG	1A	3408	1/1	0.89	0.22	64,64,64,64	0
56	MG	2A	3198	1/1	0.89	0.11	61,61,61,61	0
56	MG	1b	301	1/1	0.89	0.17	78,78,78,78	0
56	MG	2A	3645	1/1	0.89	0.18	52,52,52,52	0
56	MG	1A	3309	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	4055	1/1	0.89	0.09	55,55,55,55	0
56	MG	1A	3311	1/1	0.89	0.38	71,71,71,71	0
56	MG	1A	3486	1/1	0.89	0.22	54,54,54,54	0
56	MG	1n	102	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3381	1/1	0.89	0.26	65,65,65,65	0
56	MG	1a	1640	1/1	0.89	0.23	74,74,74,74	0
56	MG	1A	4063	1/1	0.89	0.13	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	3313	1/1	0.89	0.25	63,63,63,63	0
56	MG	2A	3682	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3650	1/1	0.89	0.16	61,61,61,61	0
56	MG	2A	3221	1/1	0.89	0.17	63,63,63,63	0
56	MG	1a	1650	1/1	0.89	0.35	76,76,76,76	0
56	MG	1A	3314	1/1	0.89	0.29	63,63,63,63	0
56	MG	1A	3420	1/1	0.89	0.10	49,49,49,49	0
56	MG	1A	3670	1/1	0.89	0.13	64,64,64,64	0
56	MG	1A	3506	1/1	0.89	0.21	50,50,50,50	0
56	MG	2A	3701	1/1	0.89	0.19	62,62,62,62	0
56	MG	1a	1662	1/1	0.89	0.14	67,67,67,67	0
56	MG	2A	3242	1/1	0.89	0.16	53,53,53,53	0
56	MG	1A	3507	1/1	0.89	0.11	67,67,67,67	0
56	MG	1A	3869	1/1	0.89	0.09	58,58,58,58	0
56	MG	1A	3421	1/1	0.89	0.25	72,72,72,72	0
56	MG	1A	3872	1/1	0.89	0.16	74,74,74,74	0
56	MG	2A	3711	1/1	0.89	0.11	85,85,85,85	0
56	MG	1A	3700	1/1	0.89	0.12	73,73,73,73	0
56	MG	2A	3005	1/1	0.89	0.27	67,67,67,67	0
56	MG	2w	103	1/1	0.89	0.24	86,86,86,86	0
56	MG	1B	3602	1/1	0.89	0.25	57,57,57,57	0
56	MG	2A	3267	1/1	0.89	0.37	69,69,69,69	0
56	MG	1A	3875	1/1	0.89	0.10	53,53,53,53	0
56	MG	1a	1681	1/1	0.89	0.18	79,79,79,79	0
56	MG	2x	102	1/1	0.89	0.20	74,74,74,74	0
56	MG	2a	3045	1/1	0.89	0.28	71,71,71,71	0
56	MG	2A	3028	1/1	0.89	0.37	61,61,61,61	0
56	MG	1A	3510	1/1	0.89	0.11	65,65,65,65	0
56	MG	2a	3051	1/1	0.89	0.17	82,82,82,82	0
56	MG	1B	3621	1/1	0.89	0.09	57,57,57,57	0
56	MG	1a	1685	1/1	0.89	0.16	62,62,62,62	0
56	MG	2A	3422	1/1	0.89	0.18	54,54,54,54	0
56	MG	1A	3890	1/1	0.89	0.13	38,38,38,38	0
57	K	2x	101	1/1	0.89	0.19	83,83,83,83	0
56	MG	2A	3270	1/1	0.90	0.26	67,67,67,67	0
56	MG	1A	3358	1/1	0.90	0.16	58,58,58,58	0
56	MG	2a	3046	1/1	0.90	0.26	71,71,71,71	0
56	MG	1A	3608	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	4059	1/1	0.90	0.07	19,19,19,19	0
56	MG	2A	3276	1/1	0.90	0.11	68,68,68,68	0
56	MG	1a	1724	1/1	0.90	0.23	66,66,66,66	0
56	MG	2A	3067	1/1	0.90	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3420	1/1	0.90	0.30	57,57,57,57	0
56	MG	1A	3624	1/1	0.90	0.08	13,13,13,13	0
56	MG	1a	1737	1/1	0.90	0.18	63,63,63,63	0
56	MG	2a	3059	1/1	0.90	0.15	88,88,88,88	0
56	MG	2A	3423	1/1	0.90	0.28	66,66,66,66	0
56	MG	2A	3282	1/1	0.90	0.12	63,63,63,63	0
56	MG	18	107	1/1	0.90	0.11	68,68,68,68	0
56	MG	2a	3064	1/1	0.90	0.08	68,68,68,68	0
56	MG	2A	3429	1/1	0.90	0.35	63,63,63,63	0
56	MG	2A	3430	1/1	0.90	0.20	44,44,44,44	0
56	MG	1A	4066	1/1	0.90	0.06	26,26,26,26	0
56	MG	1A	4069	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3748	1/1	0.90	0.10	65,65,65,65	0
56	MG	1a	1603	1/1	0.90	0.15	70,70,70,70	0
56	MG	2a	3074	1/1	0.90	0.24	76,76,76,76	0
56	MG	2A	3095	1/1	0.90	0.19	49,49,49,49	0
56	MG	1a	1614	1/1	0.90	0.23	72,72,72,72	0
56	MG	1A	3359	1/1	0.90	0.09	61,61,61,61	0
56	MG	2A	3762	1/1	0.90	0.15	69,69,69,69	0
56	MG	2A	3298	1/1	0.90	0.37	71,71,71,71	0
56	MG	1a	1616	1/1	0.90	0.17	68,68,68,68	0
56	MG	1a	1617	1/1	0.90	0.15	63,63,63,63	0
56	MG	2A	3779	1/1	0.90	0.13	42,42,42,42	0
56	MG	1a	1624	1/1	0.90	0.09	60,60,60,60	0
56	MG	2A	3457	1/1	0.90	0.28	63,63,63,63	0
56	MG	2a	3097	1/1	0.90	0.27	66,66,66,66	0
56	MG	2a	3098	1/1	0.90	0.19	83,83,83,83	0
56	MG	1A	3156	1/1	0.90	0.11	52,52,52,52	0
56	MG	1a	1628	1/1	0.90	0.27	62,62,62,62	0
56	MG	2A	3462	1/1	0.90	0.26	56,56,56,56	0
56	MG	2A	3464	1/1	0.90	0.21	61,61,61,61	0
56	MG	2A	3808	1/1	0.90	0.11	52,52,52,52	0
56	MG	2A	3308	1/1	0.90	0.13	68,68,68,68	0
56	MG	1a	1769	1/1	0.90	0.10	69,69,69,69	0
56	MG	1a	1630	1/1	0.90	0.32	73,73,73,73	0
56	MG	1A	3244	1/1	0.90	0.23	70,70,70,70	0
56	MG	1A	3011	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3799	1/1	0.90	0.13	63,63,63,63	0
56	MG	1A	3061	1/1	0.90	0.11	52,52,52,52	0
56	MG	1A	3269	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3916	1/1	0.90	0.12	58,58,58,58	0
56	MG	1A	3923	1/1	0.90	0.11	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	2A	3140	1/1	0.90	0.09	68,68,68,68	0
56	MG	2A	3493	1/1	0.90	0.16	68,68,68,68	0
56	MG	2A	3850	1/1	0.90	0.13	81,81,81,81	0
56	MG	1A	3289	1/1	0.90	0.18	57,57,57,57	0
56	MG	2A	3323	1/1	0.90	0.16	65,65,65,65	0
56	MG	2A	3854	1/1	0.90	0.10	68,68,68,68	0
56	MG	2a	3131	1/1	0.90	0.16	72,72,72,72	0
56	MG	2a	3132	1/1	0.90	0.19	63,63,63,63	0
56	MG	2A	3858	1/1	0.90	0.15	45,45,45,45	0
56	MG	1a	1811	1/1	0.90	0.34	80,80,80,80	0
56	MG	1A	3930	1/1	0.90	0.10	59,59,59,59	0
56	MG	1A	3932	1/1	0.90	0.09	37,37,37,37	0
56	MG	2A	3167	1/1	0.90	0.31	70,70,70,70	0
56	MG	2A	3330	1/1	0.90	0.10	66,66,66,66	0
56	MG	1a	1815	1/1	0.90	0.09	58,58,58,58	0
56	MG	2A	3172	1/1	0.90	0.18	73,73,73,73	0
56	MG	2A	3511	1/1	0.90	0.13	57,57,57,57	0
56	MG	2a	3144	1/1	0.90	0.14	66,66,66,66	0
56	MG	2A	3878	1/1	0.90	0.10	77,77,77,77	0
56	MG	2A	3513	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3516	1/1	0.90	0.10	73,73,73,73	0
56	MG	1A	3493	1/1	0.90	0.17	55,55,55,55	0
56	MG	2A	3335	1/1	0.90	0.19	64,64,64,64	0
56	MG	2a	3159	1/1	0.90	0.11	81,81,81,81	0
56	MG	1B	3615	1/1	0.90	0.10	56,56,56,56	0
56	MG	1a	1657	1/1	0.90	0.27	77,77,77,77	0
56	MG	2B	202	1/1	0.90	0.11	66,66,66,66	0
56	MG	2a	3167	1/1	0.90	0.18	70,70,70,70	0
56	MG	1A	3951	1/1	0.90	0.11	61,61,61,61	0
56	MG	1A	3376	1/1	0.90	0.23	63,63,63,63	0
56	MG	1A	3497	1/1	0.90	0.19	63,63,63,63	0
56	MG	1a	1666	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	3381	1/1	0.90	0.29	66,66,66,66	0
56	MG	1v	101	1/1	0.90	0.26	78,78,78,78	0
56	MG	2a	3188	1/1	0.90	0.15	65,65,65,65	0
56	MG	2B	212	1/1	0.90	0.23	75,75,75,75	0
56	MG	2a	3192	1/1	0.90	0.26	76,76,76,76	0
56	MG	1A	3838	1/1	0.90	0.20	61,61,61,61	0
56	MG	2A	3575	1/1	0.90	0.12	70,70,70,70	0
56	MG	2A	3194	1/1	0.90	0.22	79,79,79,79	0
56	MG	2A	3582	1/1	0.90	0.19	81,81,81,81	0
56	MG	1A	3978	1/1	0.90	0.13	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	1A	3984	1/1	0.90	0.15	73,73,73,73	0
56	MG	1A	3340	1/1	0.90	0.12	61,61,61,61	0
56	MG	2E	305	1/1	0.90	0.18	69,69,69,69	0
56	MG	1A	3992	1/1	0.90	0.09	40,40,40,40	0
56	MG	2A	3594	1/1	0.90	0.26	68,68,68,68	0
56	MG	1A	3843	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3204	1/1	0.90	0.24	63,63,63,63	0
56	MG	1B	3636	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3603	1/1	0.90	0.22	62,62,62,62	0
56	MG	2T	202	1/1	0.90	0.19	66,66,66,66	0
56	MG	1A	4000	1/1	0.90	0.11	59,59,59,59	0
56	MG	1E	303	1/1	0.90	0.27	56,56,56,56	0
56	MG	2A	3365	1/1	0.90	0.16	70,70,70,70	0
56	MG	2A	3612	1/1	0.90	0.18	74,74,74,74	0
56	MG	2A	3214	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3369	1/1	0.90	0.17	65,65,65,65	0
56	MG	1A	3718	1/1	0.90	0.11	53,53,53,53	0
56	MG	1A	3721	1/1	0.90	0.20	64,64,64,64	0
56	MG	29	101	1/1	0.90	0.23	73,73,73,73	0
56	MG	2A	3624	1/1	0.90	0.11	40,40,40,40	0
56	MG	1A	3393	1/1	0.90	0.11	58,58,58,58	0
56	MG	1A	3149	1/1	0.90	0.12	43,43,43,43	0
56	MG	1A	3852	1/1	0.90	0.18	61,61,61,61	0
56	MG	2A	3636	1/1	0.90	0.20	60,60,60,60	0
56	MG	1S	203	1/1	0.90	0.12	76,76,76,76	0
56	MG	1T	201	1/1	0.90	0.20	70,70,70,70	0
56	MG	2a	3239	1/1	0.90	0.23	65,65,65,65	0
56	MG	2d	302	1/1	0.90	0.16	70,70,70,70	0
56	MG	2a	3010	1/1	0.90	0.17	68,68,68,68	0
56	MG	2A	3657	1/1	0.90	0.08	64,64,64,64	0
56	MG	2A	3018	1/1	0.90	0.11	57,57,57,57	0
56	MG	2A	3230	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3294	1/1	0.90	0.14	58,58,58,58	0
56	MG	1A	3733	1/1	0.90	0.17	70,70,70,70	0
56	MG	2A	3029	1/1	0.90	0.14	71,71,71,71	0
56	MG	1V	202	1/1	0.90	0.25	53,53,53,53	0
56	MG	2a	3018	1/1	0.90	0.21	74,74,74,74	0
56	MG	2A	3674	1/1	0.90	0.11	63,63,63,63	0
56	MG	2A	3241	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3856	1/1	0.90	0.10	59,59,59,59	0
56	MG	2A	3393	1/1	0.90	0.24	78,78,78,78	0
56	MG	2A	3039	1/1	0.90	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3195	1/1	0.90	0.28	64,64,64,64	0
56	MG	2A	3045	1/1	0.90	0.21	75,75,75,75	0
56	MG	2A	3051	1/1	0.90	0.18	74,74,74,74	0
56	MG	2A	3257	1/1	0.90	0.14	79,79,79,79	0
56	MG	2x	104	1/1	0.90	0.25	77,77,77,77	0
56	MG	2A	3401	1/1	0.90	0.12	77,77,77,77	0
56	MG	1A	3020	1/1	0.90	0.15	51,51,51,51	0
56	MG	2A	3262	1/1	0.90	0.12	68,68,68,68	0
56	MG	1A	3356	1/1	0.90	0.17	66,66,66,66	0
56	MG	1A	3745	1/1	0.90	0.08	60,60,60,60	0
56	MG	2a	3039	1/1	0.90	0.30	68,68,68,68	0
56	MG	10	107	1/1	0.90	0.15	68,68,68,68	0
56	MG	1A	3525	1/1	0.90	0.19	61,61,61,61	0
56	MG	1a	1715	1/1	0.90	0.10	59,59,59,59	0
56	MG	2a	3033	1/1	0.91	0.11	85,85,85,85	0
56	MG	1a	1696	1/1	0.91	0.38	69,69,69,69	0
56	MG	2A	3695	1/1	0.91	0.22	62,62,62,62	0
56	MG	2A	3696	1/1	0.91	0.20	74,74,74,74	0
56	MG	2a	3037	1/1	0.91	0.23	65,65,65,65	0
56	MG	2A	3697	1/1	0.91	0.20	74,74,74,74	0
56	MG	1O	204	1/1	0.91	0.16	65,65,65,65	0
56	MG	2A	3259	1/1	0.91	0.13	77,77,77,77	0
56	MG	2A	3261	1/1	0.91	0.17	51,51,51,51	0
56	MG	1O	205	1/1	0.91	0.13	71,71,71,71	0
56	MG	1A	3431	1/1	0.91	0.21	58,58,58,58	0
56	MG	1a	1702	1/1	0.91	0.21	69,69,69,69	0
56	MG	2A	3707	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3841	1/1	0.91	0.14	43,43,43,43	0
56	MG	1a	1704	1/1	0.91	0.23	63,63,63,63	0
56	MG	1S	202	1/1	0.91	0.17	60,60,60,60	0
56	MG	1a	1706	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	4009	1/1	0.91	0.09	74,74,74,74	0
56	MG	1A	3295	1/1	0.91	0.13	70,70,70,70	0
56	MG	1T	202	1/1	0.91	0.14	57,57,57,57	0
56	MG	2A	3718	1/1	0.91	0.38	80,80,80,80	0
56	MG	1A	3366	1/1	0.91	0.10	51,51,51,51	0
56	MG	2a	3061	1/1	0.91	0.13	70,70,70,70	0
56	MG	1A	4018	1/1	0.91	0.07	50,50,50,50	0
56	MG	1A	3518	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3730	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3089	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	4027	1/1	0.91	0.14	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	3686	1/1	0.91	0.15	49,49,49,49	0
56	MG	1A	3296	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3284	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3433	1/1	0.91	0.41	71,71,71,71	0
56	MG	2A	3286	1/1	0.91	0.12	72,72,72,72	0
56	MG	2A	3438	1/1	0.91	0.24	75,75,75,75	0
56	MG	2a	3080	1/1	0.91	0.33	70,70,70,70	0
56	MG	1A	3045	1/1	0.91	0.07	34,34,34,34	0
56	MG	1A	3194	1/1	0.91	0.25	34,34,34,34	0
56	MG	1A	3302	1/1	0.91	0.17	41,41,41,41	0
56	MG	1A	3711	1/1	0.91	0.15	52,52,52,52	0
56	MG	2a	3086	1/1	0.91	0.12	68,68,68,68	0
56	MG	2A	3754	1/1	0.91	0.10	68,68,68,68	0
56	MG	2A	3295	1/1	0.91	0.10	69,69,69,69	0
56	MG	2A	3447	1/1	0.91	0.17	55,55,55,55	0
56	MG	2A	3448	1/1	0.91	0.26	57,57,57,57	0
56	MG	2A	3765	1/1	0.91	0.11	51,51,51,51	0
56	MG	2a	3096	1/1	0.91	0.19	67,67,67,67	0
56	MG	1A	3859	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3770	1/1	0.91	0.13	67,67,67,67	0
56	MG	2A	3451	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3455	1/1	0.91	0.17	68,68,68,68	0
56	MG	1a	1740	1/1	0.91	0.14	57,57,57,57	0
56	MG	1A	4048	1/1	0.91	0.10	51,51,51,51	0
56	MG	2A	3299	1/1	0.91	0.24	77,77,77,77	0
56	MG	2A	3783	1/1	0.91	0.14	79,79,79,79	0
56	MG	2A	3108	1/1	0.91	0.32	56,56,56,56	0
56	MG	2A	3301	1/1	0.91	0.35	73,73,73,73	0
56	MG	2A	3800	1/1	0.91	0.11	80,80,80,80	0
56	MG	1A	3335	1/1	0.91	0.39	68,68,68,68	0
56	MG	16	101	1/1	0.91	0.15	49,49,49,49	0
56	MG	1A	3258	1/1	0.91	0.09	41,41,41,41	0
56	MG	1A	3465	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3141	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3812	1/1	0.91	0.13	77,77,77,77	0
56	MG	1A	3725	1/1	0.91	0.09	48,48,48,48	0
56	MG	2a	3121	1/1	0.91	0.18	79,79,79,79	0
56	MG	2A	3477	1/1	0.91	0.10	69,69,69,69	0
56	MG	1A	3388	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3127	1/1	0.91	0.08	77,77,77,77	0
56	MG	1a	1604	1/1	0.91	0.14	67,67,67,67	0
56	MG	1A	3543	1/1	0.91	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	2a	3130	1/1	0.91	0.16	65,65,65,65	0
56	MG	2A	3487	1/1	0.91	0.27	65,65,65,65	0
56	MG	1A	3469	1/1	0.91	0.15	73,73,73,73	0
56	MG	2A	3834	1/1	0.91	0.14	62,62,62,62	0
56	MG	2A	3134	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3843	1/1	0.91	0.15	59,59,59,59	0
56	MG	1a	1772	1/1	0.91	0.11	79,79,79,79	0
56	MG	1A	3876	1/1	0.91	0.16	43,43,43,43	0
56	MG	2A	3142	1/1	0.91	0.28	68,68,68,68	0
56	MG	1A	4081	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3148	1/1	0.91	0.30	67,67,67,67	0
56	MG	2A	3149	1/1	0.91	0.20	45,45,45,45	0
56	MG	2A	3154	1/1	0.91	0.14	69,69,69,69	0
56	MG	2a	3145	1/1	0.91	0.19	71,71,71,71	0
56	MG	2A	3860	1/1	0.91	0.07	43,43,43,43	0
56	MG	1a	1622	1/1	0.91	0.35	73,73,73,73	0
56	MG	1A	3339	1/1	0.91	0.12	56,56,56,56	0
56	MG	2a	3149	1/1	0.91	0.12	83,83,83,83	0
56	MG	1A	3395	1/1	0.91	0.33	43,43,43,43	0
56	MG	2A	3871	1/1	0.91	0.15	73,73,73,73	0
56	MG	2a	3156	1/1	0.91	0.07	82,82,82,82	0
56	MG	2a	3158	1/1	0.91	0.09	83,83,83,83	0
56	MG	1a	1785	1/1	0.91	0.13	56,56,56,56	0
56	MG	1a	1627	1/1	0.91	0.20	65,65,65,65	0
56	MG	1A	3146	1/1	0.91	0.26	46,46,46,46	0
56	MG	1a	1629	1/1	0.91	0.09	61,61,61,61	0
56	MG	1A	3558	1/1	0.91	0.13	71,71,71,71	0
56	MG	1A	3214	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3099	1/1	0.91	0.11	44,44,44,44	0
56	MG	2A	3530	1/1	0.91	0.13	61,61,61,61	0
56	MG	2A	3340	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3400	1/1	0.91	0.25	39,39,39,39	0
56	MG	1A	3073	1/1	0.91	0.33	65,65,65,65	0
56	MG	2A	3183	1/1	0.91	0.10	56,56,56,56	0
56	MG	2A	3546	1/1	0.91	0.21	60,60,60,60	0
56	MG	1A	3483	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3565	1/1	0.91	0.11	75,75,75,75	0
56	MG	2A	3187	1/1	0.91	0.25	67,67,67,67	0
56	MG	1d	301	1/1	0.91	0.36	66,66,66,66	0
56	MG	1B	3601	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3410	1/1	0.91	0.15	57,57,57,57	0
56	MG	2a	3202	1/1	0.91	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1644	1/1	0.91	0.15	73,73,73,73	0
56	MG	2a	3204	1/1	0.91	0.18	72,72,72,72	0
56	MG	2A	3584	1/1	0.91	0.17	70,70,70,70	0
56	MG	2B	215	1/1	0.91	0.17	73,73,73,73	0
56	MG	1A	3593	1/1	0.91	0.28	50,50,50,50	0
56	MG	1B	3612	1/1	0.91	0.32	66,66,66,66	0
56	MG	2A	3357	1/1	0.91	0.11	68,68,68,68	0
56	MG	1B	3614	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3199	1/1	0.91	0.22	67,67,67,67	0
56	MG	2a	3213	1/1	0.91	0.12	72,72,72,72	0
56	MG	2A	3597	1/1	0.91	0.16	71,71,71,71	0
56	MG	2a	3215	1/1	0.91	0.08	71,71,71,71	0
56	MG	2E	307	1/1	0.91	0.16	74,74,74,74	0
56	MG	2E	308	1/1	0.91	0.13	68,68,68,68	0
56	MG	1A	3411	1/1	0.91	0.18	53,53,53,53	0
56	MG	1A	3106	1/1	0.91	0.39	42,42,42,42	0
56	MG	2a	3220	1/1	0.91	0.20	75,75,75,75	0
56	MG	1A	3601	1/1	0.91	0.20	70,70,70,70	0
56	MG	1A	3954	1/1	0.91	0.07	57,57,57,57	0
56	MG	2A	3366	1/1	0.91	0.18	67,67,67,67	0
56	MG	2a	3224	1/1	0.91	0.11	74,74,74,74	0
56	MG	1A	3956	1/1	0.91	0.09	61,61,61,61	0
56	MG	2A	3210	1/1	0.91	0.14	53,53,53,53	0
56	MG	1A	3963	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3213	1/1	0.91	0.13	69,69,69,69	0
56	MG	1a	1665	1/1	0.91	0.07	74,74,74,74	0
56	MG	1A	3354	1/1	0.91	0.11	61,61,61,61	0
56	MG	1A	3317	1/1	0.91	0.25	59,59,59,59	0
56	MG	1A	3121	1/1	0.91	0.18	53,53,53,53	0
56	MG	1A	3618	1/1	0.91	0.15	46,46,46,46	0
56	MG	27	101	1/1	0.91	0.19	60,60,60,60	0
56	MG	27	102	1/1	0.91	0.12	57,57,57,57	0
56	MG	2a	3240	1/1	0.91	0.14	75,75,75,75	0
56	MG	2A	3626	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3062	1/1	0.91	0.25	59,59,59,59	0
56	MG	2A	3631	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3632	1/1	0.91	0.20	77,77,77,77	0
56	MG	1A	3980	1/1	0.91	0.13	74,74,74,74	0
56	MG	1A	3821	1/1	0.91	0.18	60,60,60,60	0
56	MG	2A	3642	1/1	0.91	0.10	61,61,61,61	0
56	MG	2A	3384	1/1	0.91	0.39	75,75,75,75	0
56	MG	2r	102	1/1	0.91	0.08	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3225	1/1	0.91	0.15	65,65,65,65	0
56	MG	1a	1678	1/1	0.91	0.14	55,55,55,55	0
56	MG	1D	312	1/1	0.91	0.15	38,38,38,38	0
56	MG	2A	3662	1/1	0.91	0.23	71,71,71,71	0
56	MG	2A	3664	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	3626	1/1	0.91	0.14	40,40,40,40	0
56	MG	2A	3667	1/1	0.91	0.14	64,64,64,64	0
56	MG	2A	3389	1/1	0.91	0.12	71,71,71,71	0
56	MG	2A	3390	1/1	0.91	0.16	65,65,65,65	0
56	MG	1E	311	1/1	0.91	0.11	61,61,61,61	0
56	MG	1E	314	1/1	0.91	0.09	69,69,69,69	0
56	MG	1a	1684	1/1	0.91	0.24	80,80,80,80	0
56	MG	2A	3239	1/1	0.91	0.26	65,65,65,65	0
56	MG	1A	3327	1/1	0.91	0.30	62,62,62,62	0
56	MG	1F	311	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3683	1/1	0.91	0.14	63,63,63,63	0
56	MG	1F	313	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3834	1/1	0.91	0.13	47,47,47,47	0
56	MG	1N	201	1/1	0.91	0.24	57,57,57,57	0
56	MG	1A	3361	1/1	0.91	0.12	55,55,55,55	0
56	MG	2A	3693	1/1	0.91	0.14	70,70,70,70	0
56	MG	1A	3511	1/1	0.92	0.09	54,54,54,54	0
56	MG	2A	3656	1/1	0.92	0.12	57,57,57,57	0
56	MG	10	108	1/1	0.92	0.08	53,53,53,53	0
56	MG	1A	4028	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3370	1/1	0.92	0.16	74,74,74,74	0
56	MG	1A	4029	1/1	0.92	0.07	55,55,55,55	0
56	MG	1A	3443	1/1	0.92	0.08	74,74,74,74	0
56	MG	1A	3260	1/1	0.92	0.10	72,72,72,72	0
56	MG	2a	3021	1/1	0.92	0.16	89,89,89,89	0
56	MG	2a	3022	1/1	0.92	0.19	68,68,68,68	0
56	MG	2A	3668	1/1	0.92	0.10	63,63,63,63	0
56	MG	1A	3665	1/1	0.92	0.11	38,38,38,38	0
56	MG	2A	3186	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3049	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3519	1/1	0.92	0.12	63,63,63,63	0
56	MG	19	101	1/1	0.92	0.19	59,59,59,59	0
56	MG	2a	3029	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3192	1/1	0.92	0.19	67,67,67,67	0
56	MG	2A	3677	1/1	0.92	0.09	64,64,64,64	0
56	MG	1A	3521	1/1	0.92	0.27	46,46,46,46	0
56	MG	1A	4045	1/1	0.92	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	1a	1799	1/1	0.92	0.08	77,77,77,77	0
56	MG	2A	3684	1/1	0.92	0.14	71,71,71,71	0
56	MG	2A	3686	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3391	1/1	0.92	0.26	32,32,32,32	0
56	MG	1A	3342	1/1	0.92	0.23	53,53,53,53	0
56	MG	1a	1607	1/1	0.92	0.32	77,77,77,77	0
56	MG	2A	3690	1/1	0.92	0.16	84,84,84,84	0
56	MG	2A	3200	1/1	0.92	0.18	70,70,70,70	0
56	MG	1A	3101	1/1	0.92	0.09	39,39,39,39	0
56	MG	2A	3202	1/1	0.92	0.39	73,73,73,73	0
56	MG	1A	3703	1/1	0.92	0.09	46,46,46,46	0
56	MG	2a	3047	1/1	0.92	0.14	67,67,67,67	0
56	MG	1A	3461	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3163	1/1	0.92	0.19	45,45,45,45	0
56	MG	1A	3713	1/1	0.92	0.11	42,42,42,42	0
56	MG	2A	3699	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3208	1/1	0.92	0.15	67,67,67,67	0
56	MG	2A	3209	1/1	0.92	0.09	58,58,58,58	0
56	MG	1a	1623	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	4064	1/1	0.92	0.15	41,41,41,41	0
56	MG	1A	3868	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3715	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3267	1/1	0.92	0.19	66,66,66,66	0
56	MG	1A	3268	1/1	0.92	0.32	56,56,56,56	0
56	MG	1A	3232	1/1	0.92	0.07	53,53,53,53	0
56	MG	1A	4082	1/1	0.92	0.07	29,29,29,29	0
56	MG	1a	1632	1/1	0.92	0.21	65,65,65,65	0
56	MG	1A	3719	1/1	0.92	0.19	63,63,63,63	0
56	MG	1w	103	1/1	0.92	0.10	80,80,80,80	0
56	MG	2A	3224	1/1	0.92	0.32	70,70,70,70	0
56	MG	1A	3541	1/1	0.92	0.19	50,50,50,50	0
56	MG	2A	3725	1/1	0.92	0.11	60,60,60,60	0
56	MG	2A	3726	1/1	0.92	0.12	51,51,51,51	0
56	MG	2A	3228	1/1	0.92	0.29	51,51,51,51	0
56	MG	1A	3404	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3884	1/1	0.92	0.16	34,34,34,34	0
56	MG	1A	3886	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3728	1/1	0.92	0.10	40,40,40,40	0
56	MG	2A	3234	1/1	0.92	0.19	54,54,54,54	0
56	MG	1x	102	1/1	0.92	0.31	70,70,70,70	0
56	MG	1x	103	1/1	0.92	0.17	57,57,57,57	0
56	MG	1x	104	1/1	0.92	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3240	1/1	0.92	0.07	85,85,85,85	0
56	MG	2A	3743	1/1	0.92	0.11	57,57,57,57	0
56	MG	1a	1643	1/1	0.92	0.16	69,69,69,69	0
56	MG	2a	3093	1/1	0.92	0.19	68,68,68,68	0
56	MG	2a	3095	1/1	0.92	0.16	76,76,76,76	0
56	MG	1A	3891	1/1	0.92	0.07	26,26,26,26	0
56	MG	1A	3892	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3750	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3434	1/1	0.92	0.35	70,70,70,70	0
56	MG	2a	3100	1/1	0.92	0.27	55,55,55,55	0
56	MG	1A	3893	1/1	0.92	0.09	33,33,33,33	0
56	MG	1A	4103	1/1	0.92	0.31	62,62,62,62	0
56	MG	2A	3757	1/1	0.92	0.10	75,75,75,75	0
56	MG	2A	3253	1/1	0.92	0.29	62,62,62,62	0
56	MG	2A	3759	1/1	0.92	0.12	77,77,77,77	0
56	MG	1A	3894	1/1	0.92	0.09	54,54,54,54	0
56	MG	1A	3323	1/1	0.92	0.12	55,55,55,55	0
56	MG	1B	3609	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3766	1/1	0.92	0.20	52,52,52,52	0
56	MG	1A	3901	1/1	0.92	0.12	27,27,27,27	0
56	MG	1A	3544	1/1	0.92	0.23	50,50,50,50	0
56	MG	2A	3014	1/1	0.92	0.08	50,50,50,50	0
56	MG	2A	3016	1/1	0.92	0.10	75,75,75,75	0
56	MG	2A	3265	1/1	0.92	0.17	68,68,68,68	0
56	MG	2A	3017	1/1	0.92	0.25	59,59,59,59	0
56	MG	1B	3613	1/1	0.92	0.29	75,75,75,75	0
56	MG	1A	3409	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3024	1/1	0.92	0.19	65,65,65,65	0
56	MG	2A	3460	1/1	0.92	0.26	70,70,70,70	0
56	MG	2A	3795	1/1	0.92	0.09	80,80,80,80	0
56	MG	2a	3126	1/1	0.92	0.19	70,70,70,70	0
56	MG	1A	3287	1/1	0.92	0.11	49,49,49,49	0
56	MG	1A	3912	1/1	0.92	0.18	31,31,31,31	0
56	MG	2A	3463	1/1	0.92	0.27	61,61,61,61	0
56	MG	1A	3325	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3809	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	3556	1/1	0.92	0.10	63,63,63,63	0
56	MG	2A	3038	1/1	0.92	0.09	34,34,34,34	0
56	MG	1A	3478	1/1	0.92	0.12	62,62,62,62	0
56	MG	2a	3138	1/1	0.92	0.37	75,75,75,75	0
56	MG	2A	3043	1/1	0.92	0.17	80,80,80,80	0
56	MG	1A	3925	1/1	0.92	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1673	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	3288	1/1	0.92	0.17	56,56,56,56	0
56	MG	1a	1677	1/1	0.92	0.32	61,61,61,61	0
56	MG	2A	3820	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3480	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3565	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3481	1/1	0.92	0.16	65,65,65,65	0
56	MG	2A	3488	1/1	0.92	0.15	64,64,64,64	0
56	MG	1B	3633	1/1	0.92	0.08	46,46,46,46	0
56	MG	2A	3841	1/1	0.92	0.11	52,52,52,52	0
56	MG	1B	3634	1/1	0.92	0.09	68,68,68,68	0
56	MG	2a	3152	1/1	0.92	0.09	84,84,84,84	0
56	MG	1A	3942	1/1	0.92	0.07	35,35,35,35	0
56	MG	2a	3157	1/1	0.92	0.08	72,72,72,72	0
56	MG	1A	3758	1/1	0.92	0.10	53,53,53,53	0
56	MG	1D	305	1/1	0.92	0.10	48,48,48,48	0
56	MG	2a	3160	1/1	0.92	0.13	69,69,69,69	0
56	MG	1a	1688	1/1	0.92	0.09	66,66,66,66	0
56	MG	2a	3163	1/1	0.92	0.06	93,93,93,93	0
56	MG	1A	3167	1/1	0.92	0.20	61,61,61,61	0
56	MG	2A	3068	1/1	0.92	0.19	67,67,67,67	0
56	MG	2A	3069	1/1	0.92	0.11	53,53,53,53	0
56	MG	2A	3074	1/1	0.92	0.11	61,61,61,61	0
56	MG	2A	3075	1/1	0.92	0.22	78,78,78,78	0
56	MG	1A	3363	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3962	1/1	0.92	0.09	57,57,57,57	0
56	MG	1E	308	1/1	0.92	0.26	66,66,66,66	0
56	MG	2A	3514	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	3765	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3775	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3519	1/1	0.92	0.14	44,44,44,44	0
56	MG	2a	3193	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3485	1/1	0.92	0.21	53,53,53,53	0
56	MG	1a	1699	1/1	0.92	0.26	68,68,68,68	0
56	MG	2A	3523	1/1	0.92	0.14	56,56,56,56	0
56	MG	2a	3198	1/1	0.92	0.13	71,71,71,71	0
56	MG	1A	3970	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3883	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3096	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	3973	1/1	0.92	0.09	53,53,53,53	0
56	MG	2A	3316	1/1	0.92	0.21	73,73,73,73	0
56	MG	1A	3247	1/1	0.92	0.29	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	1A	3170	1/1	0.92	0.10	56,56,56,56	0
56	MG	1N	202	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3976	1/1	0.92	0.10	60,60,60,60	0
56	MG	2A	3564	1/1	0.92	0.13	52,52,52,52	0
56	MG	1O	203	1/1	0.92	0.23	64,64,64,64	0
56	MG	2B	210	1/1	0.92	0.15	75,75,75,75	0
56	MG	1A	3490	1/1	0.92	0.12	57,57,57,57	0
56	MG	1A	3006	1/1	0.92	0.16	62,62,62,62	0
56	MG	2A	3573	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3598	1/1	0.92	0.22	56,56,56,56	0
56	MG	2A	3326	1/1	0.92	0.12	57,57,57,57	0
56	MG	2B	216	1/1	0.92	0.15	76,76,76,76	0
56	MG	1P	206	1/1	0.92	0.22	46,46,46,46	0
56	MG	1A	3181	1/1	0.92	0.21	61,61,61,61	0
56	MG	2B	219	1/1	0.92	0.23	83,83,83,83	0
56	MG	2A	3118	1/1	0.92	0.15	56,56,56,56	0
56	MG	2D	305	1/1	0.92	0.34	48,48,48,48	0
56	MG	1A	3182	1/1	0.92	0.12	56,56,56,56	0
56	MG	2A	3332	1/1	0.92	0.16	60,60,60,60	0
56	MG	2E	303	1/1	0.92	0.34	69,69,69,69	0
56	MG	2A	3125	1/1	0.92	0.23	67,67,67,67	0
56	MG	1A	3996	1/1	0.92	0.07	37,37,37,37	0
56	MG	2A	3595	1/1	0.92	0.12	58,58,58,58	0
56	MG	2a	3230	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3119	1/1	0.92	0.37	48,48,48,48	0
56	MG	1A	3502	1/1	0.92	0.35	52,52,52,52	0
56	MG	2A	3129	1/1	0.92	0.15	71,71,71,71	0
56	MG	2P	202	1/1	0.92	0.16	63,63,63,63	0
56	MG	2A	3130	1/1	0.92	0.13	57,57,57,57	0
56	MG	2Q	204	1/1	0.92	0.13	58,58,58,58	0
56	MG	1A	3434	1/1	0.92	0.10	69,69,69,69	0
56	MG	2d	301	1/1	0.92	0.34	66,66,66,66	0
56	MG	2R	202	1/1	0.92	0.10	56,56,56,56	0
56	MG	1a	1730	1/1	0.92	0.09	73,73,73,73	0
56	MG	2A	3608	1/1	0.92	0.13	60,60,60,60	0
56	MG	2U	201	1/1	0.92	0.17	62,62,62,62	0
56	MG	1U	204	1/1	0.92	0.11	47,47,47,47	0
56	MG	1A	3825	1/1	0.92	0.07	54,54,54,54	0
56	MG	2X	101	1/1	0.92	0.10	65,65,65,65	0
56	MG	2Y	201	1/1	0.92	0.18	61,61,61,61	0
56	MG	1A	3046	1/1	0.92	0.08	42,42,42,42	0
56	MG	1W	206	1/1	0.92	0.15	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	4010	1/1	0.92	0.08	81,81,81,81	0
56	MG	2I	102	1/1	0.92	0.36	57,57,57,57	0
56	MG	1a	1745	1/1	0.92	0.12	72,72,72,72	0
56	MG	1a	1748	1/1	0.92	0.09	66,66,66,66	0
56	MG	2A	3619	1/1	0.92	0.12	55,55,55,55	0
56	MG	2A	3620	1/1	0.92	0.12	71,71,71,71	0
56	MG	2A	3152	1/1	0.92	0.11	57,57,57,57	0
56	MG	2A	3153	1/1	0.92	0.27	63,63,63,63	0
56	MG	2a	3001	1/1	0.92	0.10	69,69,69,69	0
56	MG	1X	107	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3833	1/1	0.92	0.08	47,47,47,47	0
56	MG	2a	3004	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3439	1/1	0.92	0.09	50,50,50,50	0
56	MG	1A	3646	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3128	1/1	0.92	0.07	76,76,76,76	0
56	MG	10	103	1/1	0.92	0.15	55,55,55,55	0
56	MG	1a	1761	1/1	0.92	0.17	63,63,63,63	0
56	MG	1a	1762	1/1	0.92	0.08	65,65,65,65	0
56	MG	2A	3651	1/1	0.92	0.17	49,49,49,49	0
57	K	1A	3571	1/1	0.92	0.28	75,75,75,75	0
56	MG	2A	3652	1/1	0.92	0.11	53,53,53,53	0
56	MG	2A	3491	1/1	0.93	0.22	63,63,63,63	0
56	MG	1A	4102	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3619	1/1	0.93	0.09	41,41,41,41	0
56	MG	2A	3774	1/1	0.93	0.15	60,60,60,60	0
56	MG	1a	1782	1/1	0.93	0.10	68,68,68,68	0
56	MG	1A	3620	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3122	1/1	0.93	0.18	41,41,41,41	0
56	MG	1a	1626	1/1	0.93	0.15	70,70,70,70	0
56	MG	2A	3501	1/1	0.93	0.27	63,63,63,63	0
56	MG	1B	3607	1/1	0.93	0.14	69,69,69,69	0
56	MG	2A	3794	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3144	1/1	0.93	0.16	51,51,51,51	0
56	MG	2A	3796	1/1	0.93	0.11	71,71,71,71	0
56	MG	2A	3504	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3803	1/1	0.93	0.15	72,72,72,72	0
56	MG	2A	3145	1/1	0.93	0.20	59,59,59,59	0
56	MG	1B	3608	1/1	0.93	0.26	72,72,72,72	0
56	MG	1A	3808	1/1	0.93	0.08	49,49,49,49	0
56	MG	1a	1806	1/1	0.93	0.09	75,75,75,75	0
56	MG	1A	3298	1/1	0.93	0.24	54,54,54,54	0
56	MG	1A	3627	1/1	0.93	0.12	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	1A	3960	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3517	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3155	1/1	0.93	0.10	56,56,56,56	0
56	MG	1A	3633	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3817	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3029	1/1	0.93	0.15	37,37,37,37	0
56	MG	1A	3129	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	3025	1/1	0.93	0.15	36,36,36,36	0
56	MG	2A	3169	1/1	0.93	0.13	46,46,46,46	0
56	MG	2A	3336	1/1	0.93	0.08	54,54,54,54	0
56	MG	2A	3832	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	3972	1/1	0.93	0.10	46,46,46,46	0
56	MG	1B	3624	1/1	0.93	0.15	60,60,60,60	0
56	MG	1A	3824	1/1	0.93	0.35	43,43,43,43	0
56	MG	2A	3842	1/1	0.93	0.10	78,78,78,78	0
56	MG	1A	3135	1/1	0.93	0.25	36,36,36,36	0
56	MG	1B	3627	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3548	1/1	0.93	0.25	56,56,56,56	0
56	MG	1A	3826	1/1	0.93	0.07	42,42,42,42	0
56	MG	2A	3344	1/1	0.93	0.29	73,73,73,73	0
56	MG	1A	3257	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3832	1/1	0.93	0.07	40,40,40,40	0
56	MG	1A	3202	1/1	0.93	0.07	48,48,48,48	0
56	MG	1A	3345	1/1	0.93	0.16	53,53,53,53	0
56	MG	2A	3578	1/1	0.93	0.10	40,40,40,40	0
56	MG	2A	3865	1/1	0.93	0.09	40,40,40,40	0
56	MG	2a	3120	1/1	0.93	0.16	72,72,72,72	0
56	MG	1A	3346	1/1	0.93	0.27	37,37,37,37	0
56	MG	1A	3673	1/1	0.93	0.10	34,34,34,34	0
56	MG	1D	302	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3840	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3355	1/1	0.93	0.10	74,74,74,74	0
56	MG	1A	3998	1/1	0.93	0.08	47,47,47,47	0
56	MG	2a	3128	1/1	0.93	0.16	67,67,67,67	0
56	MG	1A	3205	1/1	0.93	0.23	64,64,64,64	0
56	MG	2A	3593	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3351	1/1	0.93	0.24	39,39,39,39	0
56	MG	1x	105	1/1	0.93	0.18	57,57,57,57	0
56	MG	1E	305	1/1	0.93	0.21	38,38,38,38	0
56	MG	2A	3361	1/1	0.93	0.14	72,72,72,72	0
56	MG	1A	4003	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3352	1/1	0.93	0.28	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3696	1/1	0.93	0.06	37,37,37,37	0
56	MG	1A	3207	1/1	0.93	0.11	61,61,61,61	0
56	MG	1x	112	1/1	0.93	0.11	72,72,72,72	0
56	MG	1F	304	1/1	0.93	0.13	45,45,45,45	0
56	MG	2B	205	1/1	0.93	0.11	58,58,58,58	0
56	MG	2A	3205	1/1	0.93	0.36	72,72,72,72	0
56	MG	1A	3166	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3372	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3001	1/1	0.93	0.46	69,69,69,69	0
56	MG	2A	3003	1/1	0.93	0.24	66,66,66,66	0
56	MG	2A	3004	1/1	0.93	0.33	63,63,63,63	0
56	MG	2A	3618	1/1	0.93	0.08	65,65,65,65	0
56	MG	1A	3058	1/1	0.93	0.08	44,44,44,44	0
56	MG	1A	3217	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3622	1/1	0.93	0.10	74,74,74,74	0
56	MG	2A	3007	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3549	1/1	0.93	0.26	58,58,58,58	0
56	MG	2A	3380	1/1	0.93	0.26	71,71,71,71	0
56	MG	1A	3550	1/1	0.93	0.32	52,52,52,52	0
56	MG	1A	4025	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	3552	1/1	0.93	0.22	65,65,65,65	0
56	MG	1a	1687	1/1	0.93	0.25	69,69,69,69	0
56	MG	2A	3020	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3554	1/1	0.93	0.37	73,73,73,73	0
56	MG	2A	3222	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3864	1/1	0.93	0.07	34,34,34,34	0
56	MG	2a	3172	1/1	0.93	0.07	80,80,80,80	0
56	MG	1A	3415	1/1	0.93	0.10	52,52,52,52	0
56	MG	2a	3175	1/1	0.93	0.16	58,58,58,58	0
56	MG	2a	3176	1/1	0.93	0.07	90,90,90,90	0
56	MG	2F	304	1/1	0.93	0.20	59,59,59,59	0
56	MG	1A	3416	1/1	0.93	0.19	45,45,45,45	0
56	MG	2A	3227	1/1	0.93	0.17	74,74,74,74	0
56	MG	1Q	206	1/1	0.93	0.08	42,42,42,42	0
56	MG	2a	3186	1/1	0.93	0.22	61,61,61,61	0
56	MG	1R	201	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3720	1/1	0.93	0.08	67,67,67,67	0
56	MG	1A	3319	1/1	0.93	0.24	35,35,35,35	0
56	MG	1A	3218	1/1	0.93	0.13	40,40,40,40	0
56	MG	2A	3400	1/1	0.93	0.11	74,74,74,74	0
56	MG	2a	3195	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3224	1/1	0.93	0.12	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	2A	3235	1/1	0.93	0.23	49,49,49,49	0
56	MG	1A	3422	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3046	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3048	1/1	0.93	0.17	55,55,55,55	0
56	MG	1A	3168	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3426	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	4053	1/1	0.93	0.08	51,51,51,51	0
56	MG	2A	3409	1/1	0.93	0.17	76,76,76,76	0
56	MG	2A	3245	1/1	0.93	0.20	72,72,72,72	0
56	MG	25	101	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	3276	1/1	0.93	0.26	42,42,42,42	0
56	MG	1a	1707	1/1	0.93	0.10	65,65,65,65	0
56	MG	1V	206	1/1	0.93	0.13	67,67,67,67	0
56	MG	1V	207	1/1	0.93	0.11	56,56,56,56	0
56	MG	1W	201	1/1	0.93	0.31	62,62,62,62	0
56	MG	2A	3256	1/1	0.93	0.07	66,66,66,66	0
56	MG	1W	202	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3734	1/1	0.93	0.13	50,50,50,50	0
56	MG	1A	3579	1/1	0.93	0.23	47,47,47,47	0
56	MG	2A	3260	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3424	1/1	0.93	0.33	58,58,58,58	0
56	MG	2A	3066	1/1	0.93	0.23	66,66,66,66	0
56	MG	1A	3582	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3427	1/1	0.93	0.37	59,59,59,59	0
56	MG	1a	1716	1/1	0.93	0.35	58,58,58,58	0
56	MG	1a	1717	1/1	0.93	0.26	54,54,54,54	0
56	MG	1A	3585	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3743	1/1	0.93	0.08	63,63,63,63	0
56	MG	2A	3080	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3082	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3169	1/1	0.93	0.17	44,44,44,44	0
56	MG	2A	3085	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3086	1/1	0.93	0.11	52,52,52,52	0
56	MG	2a	3233	1/1	0.93	0.20	74,74,74,74	0
56	MG	1A	4068	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3441	1/1	0.93	0.29	68,68,68,68	0
56	MG	1A	3233	1/1	0.93	0.32	55,55,55,55	0
56	MG	1A	4071	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3371	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	4075	1/1	0.93	0.09	27,27,27,27	0
56	MG	11	105	1/1	0.93	0.11	63,63,63,63	0
56	MG	12	101	1/1	0.93	0.09	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	3450	1/1	0.93	0.14	84,84,84,84	0
56	MG	1A	3048	1/1	0.93	0.06	25,25,25,25	0
56	MG	1A	3331	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3245	1/1	0.93	0.11	63,63,63,63	0
56	MG	1A	4083	1/1	0.93	0.11	46,46,46,46	0
56	MG	2q	201	1/1	0.93	0.14	85,85,85,85	0
56	MG	1A	4085	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3291	1/1	0.93	0.09	67,67,67,67	0
56	MG	18	105	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3763	1/1	0.93	0.17	67,67,67,67	0
56	MG	1A	3448	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3453	1/1	0.93	0.15	40,40,40,40	0
56	MG	2A	3465	1/1	0.93	0.12	44,44,44,44	0
56	MG	2A	3466	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	4091	1/1	0.93	0.13	45,45,45,45	0
56	MG	2A	3114	1/1	0.93	0.19	72,72,72,72	0
56	MG	1A	3246	1/1	0.93	0.19	67,67,67,67	0
56	MG	2A	3474	1/1	0.93	0.25	66,66,66,66	0
56	MG	1A	3778	1/1	0.93	0.07	20,20,20,20	0
56	MG	1A	3616	1/1	0.93	0.09	54,54,54,54	0
56	MG	2x	103	1/1	0.93	0.11	63,63,63,63	0
56	MG	1a	1767	1/1	0.93	0.19	62,62,62,62	0
56	MG	2A	3123	1/1	0.93	0.26	69,69,69,69	0
56	MG	1A	3082	1/1	0.93	0.19	50,50,50,50	0
56	MG	1a	1770	1/1	0.93	0.09	76,76,76,76	0
56	MG	2a	3052	1/1	0.93	0.18	74,74,74,74	0
56	MG	1A	4096	1/1	0.93	0.08	54,54,54,54	0
56	MG	2A	3309	1/1	0.93	0.19	68,68,68,68	0
56	MG	1A	3929	1/1	0.93	0.11	42,42,42,42	0
56	MG	2a	3056	1/1	0.93	0.26	68,68,68,68	0
56	MG	1A	3795	1/1	0.93	0.06	44,44,44,44	0
56	MG	2A	3769	1/1	0.93	0.21	73,73,73,73	0
56	MG	1A	3588	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3241	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	3931	1/1	0.94	0.09	60,60,60,60	0
56	MG	2A	3669	1/1	0.94	0.17	69,69,69,69	0
56	MG	1A	3050	1/1	0.94	0.14	31,31,31,31	0
56	MG	1A	3935	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3595	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	3767	1/1	0.94	0.09	54,54,54,54	0
56	MG	1a	1659	1/1	0.94	0.11	57,57,57,57	0
56	MG	1a	1660	1/1	0.94	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3492	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3398	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3052	1/1	0.94	0.09	45,45,45,45	0
56	MG	1a	1663	1/1	0.94	0.21	70,70,70,70	0
56	MG	1A	3783	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3685	1/1	0.94	0.21	45,45,45,45	0
56	MG	1A	3957	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3600	1/1	0.94	0.32	63,63,63,63	0
56	MG	1A	3961	1/1	0.94	0.13	62,62,62,62	0
56	MG	1A	3126	1/1	0.94	0.13	49,49,49,49	0
56	MG	1a	1670	1/1	0.94	0.21	70,70,70,70	0
56	MG	2A	3226	1/1	0.94	0.12	65,65,65,65	0
56	MG	1A	3419	1/1	0.94	0.09	63,63,63,63	0
56	MG	1A	3053	1/1	0.94	0.06	56,56,56,56	0
56	MG	1A	3605	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3803	1/1	0.94	0.11	30,30,30,30	0
56	MG	1A	3035	1/1	0.94	0.06	51,51,51,51	0
56	MG	2A	3232	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3609	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3033	1/1	0.94	0.17	58,58,58,58	0
56	MG	2A	3035	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	3312	1/1	0.94	0.32	64,64,64,64	0
56	MG	1A	3810	1/1	0.94	0.06	26,26,26,26	0
56	MG	2A	3705	1/1	0.94	0.07	68,68,68,68	0
56	MG	1A	3132	1/1	0.94	0.10	40,40,40,40	0
56	MG	2A	3041	1/1	0.94	0.21	61,61,61,61	0
56	MG	2A	3042	1/1	0.94	0.26	62,62,62,62	0
56	MG	1A	3977	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3243	1/1	0.94	0.15	69,69,69,69	0
56	MG	1A	3093	1/1	0.94	0.12	58,58,58,58	0
56	MG	2A	3428	1/1	0.94	0.40	65,65,65,65	0
56	MG	2A	3246	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	3427	1/1	0.94	0.12	61,61,61,61	0
56	MG	1A	3430	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3250	1/1	0.94	0.26	64,64,64,64	0
56	MG	2A	3722	1/1	0.94	0.10	38,38,38,38	0
56	MG	2A	3047	1/1	0.94	0.21	61,61,61,61	0
56	MG	1A	3985	1/1	0.94	0.09	70,70,70,70	0
56	MG	2A	3435	1/1	0.94	0.33	68,68,68,68	0
56	MG	1A	3183	1/1	0.94	0.15	73,73,73,73	0
56	MG	2A	3255	1/1	0.94	0.28	73,73,73,73	0
56	MG	1E	316	1/1	0.94	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3989	1/1	0.94	0.11	67,67,67,67	0
56	MG	1a	1693	1/1	0.94	0.35	60,60,60,60	0
56	MG	1F	301	1/1	0.94	0.12	43,43,43,43	0
56	MG	1A	3990	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3362	1/1	0.94	0.14	62,62,62,62	0
56	MG	2A	3741	1/1	0.94	0.19	61,61,61,61	0
56	MG	1F	312	1/1	0.94	0.12	61,61,61,61	0
56	MG	2a	3078	1/1	0.94	0.21	65,65,65,65	0
56	MG	2A	3062	1/1	0.94	0.07	54,54,54,54	0
56	MG	2a	3081	1/1	0.94	0.28	75,75,75,75	0
56	MG	2A	3264	1/1	0.94	0.15	65,65,65,65	0
56	MG	2A	3745	1/1	0.94	0.15	65,65,65,65	0
56	MG	1A	3515	1/1	0.94	0.13	35,35,35,35	0
56	MG	1G	201	1/1	0.94	0.09	42,42,42,42	0
56	MG	2A	3749	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3453	1/1	0.94	0.23	56,56,56,56	0
56	MG	1G	202	1/1	0.94	0.23	67,67,67,67	0
56	MG	2a	3089	1/1	0.94	0.18	75,75,75,75	0
56	MG	1G	203	1/1	0.94	0.05	75,75,75,75	0
56	MG	1A	3997	1/1	0.94	0.12	65,65,65,65	0
56	MG	2A	3755	1/1	0.94	0.10	63,63,63,63	0
56	MG	1I	201	1/1	0.94	0.10	65,65,65,65	0
56	MG	1A	3637	1/1	0.94	0.07	38,38,38,38	0
56	MG	2A	3273	1/1	0.94	0.22	75,75,75,75	0
56	MG	2A	3760	1/1	0.94	0.19	70,70,70,70	0
56	MG	1A	3516	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3316	1/1	0.94	0.21	62,62,62,62	0
56	MG	2A	3763	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3830	1/1	0.94	0.06	32,32,32,32	0
56	MG	2a	3102	1/1	0.94	0.10	69,69,69,69	0
56	MG	1A	3185	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	4005	1/1	0.94	0.07	20,20,20,20	0
56	MG	1A	3134	1/1	0.94	0.26	34,34,34,34	0
56	MG	1A	3655	1/1	0.94	0.07	35,35,35,35	0
56	MG	1Q	205	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3367	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3663	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3441	1/1	0.94	0.22	55,55,55,55	0
56	MG	2A	3287	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	4014	1/1	0.94	0.06	30,30,30,30	0
56	MG	1A	3668	1/1	0.94	0.06	28,28,28,28	0
56	MG	1A	4019	1/1	0.94	0.07	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	3189	1/1	0.94	0.13	35,35,35,35	0
56	MG	1a	1726	1/1	0.94	0.19	71,71,71,71	0
56	MG	1A	3527	1/1	0.94	0.19	44,44,44,44	0
56	MG	1a	1731	1/1	0.94	0.06	48,48,48,48	0
56	MG	2A	3797	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3799	1/1	0.94	0.12	75,75,75,75	0
56	MG	1A	3094	1/1	0.94	0.18	43,43,43,43	0
56	MG	1U	205	1/1	0.94	0.29	49,49,49,49	0
56	MG	2A	3105	1/1	0.94	0.14	71,71,71,71	0
56	MG	2a	3127	1/1	0.94	0.26	67,67,67,67	0
56	MG	2A	3106	1/1	0.94	0.22	78,78,78,78	0
56	MG	2A	3495	1/1	0.94	0.10	40,40,40,40	0
56	MG	2A	3496	1/1	0.94	0.06	62,62,62,62	0
56	MG	1A	3004	1/1	0.94	0.06	28,28,28,28	0
56	MG	1A	3848	1/1	0.94	0.19	55,55,55,55	0
56	MG	2A	3303	1/1	0.94	0.13	79,79,79,79	0
56	MG	2a	3134	1/1	0.94	0.22	62,62,62,62	0
56	MG	1A	3196	1/1	0.94	0.07	46,46,46,46	0
56	MG	2A	3814	1/1	0.94	0.10	63,63,63,63	0
56	MG	1a	1744	1/1	0.94	0.15	71,71,71,71	0
56	MG	1A	4032	1/1	0.94	0.08	53,53,53,53	0
56	MG	1a	1747	1/1	0.94	0.09	59,59,59,59	0
56	MG	2A	3505	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3691	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3821	1/1	0.94	0.11	65,65,65,65	0
56	MG	2A	3117	1/1	0.94	0.28	62,62,62,62	0
56	MG	2A	3826	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3198	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3537	1/1	0.94	0.27	41,41,41,41	0
56	MG	1A	4040	1/1	0.94	0.09	53,53,53,53	0
56	MG	2A	3124	1/1	0.94	0.20	67,67,67,67	0
56	MG	2A	3515	1/1	0.94	0.07	57,57,57,57	0
56	MG	1A	3040	1/1	0.94	0.09	38,38,38,38	0
56	MG	1a	1757	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3378	1/1	0.94	0.08	50,50,50,50	0
56	MG	2a	3153	1/1	0.94	0.06	64,64,64,64	0
56	MG	2a	3154	1/1	0.94	0.08	96,96,96,96	0
56	MG	1A	3379	1/1	0.94	0.10	38,38,38,38	0
56	MG	2A	3848	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3861	1/1	0.94	0.09	69,69,69,69	0
56	MG	2A	3320	1/1	0.94	0.17	76,76,76,76	0
56	MG	2A	3522	1/1	0.94	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3329	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3855	1/1	0.94	0.06	27,27,27,27	0
56	MG	2A	3856	1/1	0.94	0.10	73,73,73,73	0
56	MG	2A	3524	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	4050	1/1	0.94	0.12	34,34,34,34	0
56	MG	2A	3529	1/1	0.94	0.14	53,53,53,53	0
56	MG	10	104	1/1	0.94	0.15	50,50,50,50	0
56	MG	2a	3173	1/1	0.94	0.07	67,67,67,67	0
56	MG	2A	3863	1/1	0.94	0.16	56,56,56,56	0
56	MG	2A	3531	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3532	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3868	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3463	1/1	0.94	0.17	68,68,68,68	0
56	MG	1A	3142	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3541	1/1	0.94	0.16	68,68,68,68	0
56	MG	1A	3017	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3874	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3141	1/1	0.94	0.17	45,45,45,45	0
56	MG	2a	3190	1/1	0.94	0.22	78,78,78,78	0
56	MG	2a	3191	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3018	1/1	0.94	0.10	36,36,36,36	0
56	MG	1a	1771	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3870	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3553	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3557	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3558	1/1	0.94	0.13	55,55,55,55	0
56	MG	2A	3561	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4060	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3147	1/1	0.94	0.17	63,63,63,63	0
56	MG	2a	3201	1/1	0.94	0.11	69,69,69,69	0
56	MG	1A	4061	1/1	0.94	0.16	59,59,59,59	0
56	MG	1A	4062	1/1	0.94	0.12	39,39,39,39	0
56	MG	1A	3468	1/1	0.94	0.14	43,43,43,43	0
56	MG	1A	3272	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3873	1/1	0.94	0.06	26,26,26,26	0
56	MG	2A	3580	1/1	0.94	0.08	48,48,48,48	0
56	MG	18	106	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3156	1/1	0.94	0.12	71,71,71,71	0
56	MG	2A	3341	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	4067	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3158	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3472	1/1	0.94	0.10	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	2A	3160	1/1	0.94	0.14	66,66,66,66	0
56	MG	2A	3161	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3213	1/1	0.94	0.13	56,56,56,56	0
56	MG	2A	3165	1/1	0.94	0.13	63,63,63,63	0
56	MG	2A	3596	1/1	0.94	0.19	64,64,64,64	0
56	MG	1A	3723	1/1	0.94	0.14	63,63,63,63	0
56	MG	2D	303	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3877	1/1	0.94	0.10	33,33,33,33	0
56	MG	2A	3600	1/1	0.94	0.10	74,74,74,74	0
56	MG	1A	3001	1/1	0.94	0.13	48,48,48,48	0
56	MG	2E	301	1/1	0.94	0.25	64,64,64,64	0
56	MG	2E	302	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3353	1/1	0.94	0.15	63,63,63,63	0
56	MG	1a	1606	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3173	1/1	0.94	0.20	75,75,75,75	0
56	MG	2A	3174	1/1	0.94	0.22	68,68,68,68	0
56	MG	1A	3336	1/1	0.94	0.21	58,58,58,58	0
56	MG	2a	3232	1/1	0.94	0.17	73,73,73,73	0
56	MG	2F	302	1/1	0.94	0.12	65,65,65,65	0
56	MG	2A	3176	1/1	0.94	0.21	59,59,59,59	0
56	MG	2A	3611	1/1	0.94	0.07	45,45,45,45	0
56	MG	1a	1613	1/1	0.94	0.07	73,73,73,73	0
56	MG	2N	201	1/1	0.94	0.09	70,70,70,70	0
56	MG	2P	201	1/1	0.94	0.08	67,67,67,67	0
56	MG	1A	3152	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3889	1/1	0.94	0.07	44,44,44,44	0
56	MG	2A	3615	1/1	0.94	0.12	62,62,62,62	0
56	MG	2A	3362	1/1	0.94	0.20	74,74,74,74	0
56	MG	1A	3153	1/1	0.94	0.11	44,44,44,44	0
56	MG	1A	3562	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	3403	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3292	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	3219	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3368	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3896	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3188	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3629	1/1	0.94	0.07	48,48,48,48	0
56	MG	20	102	1/1	0.94	0.08	67,67,67,67	0
56	MG	20	103	1/1	0.94	0.14	69,69,69,69	0
56	MG	1A	3110	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3572	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	3906	1/1	0.94	0.07	30,30,30,30	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	0.94	0.11	40,40,40,40	0
56	MG	1A	3744	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3638	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3640	1/1	0.94	0.12	69,69,69,69	0
56	MG	1A	3118	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3022	1/1	0.94	0.11	45,45,45,45	0
56	MG	1A	4101	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3748	1/1	0.94	0.08	59,59,59,59	0
56	MG	2A	3654	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3750	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3919	1/1	0.94	0.26	40,40,40,40	0
56	MG	1A	3584	1/1	0.94	0.25	38,38,38,38	0
56	MG	2A	3659	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3924	1/1	0.94	0.18	42,42,42,42	0
56	MG	1A	3234	1/1	0.94	0.07	64,64,64,64	0
56	MG	2A	3663	1/1	0.94	0.21	58,58,58,58	0
56	MG	1A	3487	1/1	0.94	0.21	47,47,47,47	0
56	MG	1A	3081	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3250	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3025	1/1	0.95	0.10	66,66,66,66	0
56	MG	2A	3026	1/1	0.95	0.12	53,53,53,53	0
56	MG	1B	3616	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3958	1/1	0.95	0.06	63,63,63,63	0
56	MG	2A	3030	1/1	0.95	0.17	51,51,51,51	0
56	MG	1A	3109	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3805	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3436	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3305	1/1	0.95	0.25	63,63,63,63	0
56	MG	1A	3617	1/1	0.95	0.07	31,31,31,31	0
56	MG	1A	3355	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3967	1/1	0.95	0.05	28,28,28,28	0
56	MG	2A	3040	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3508	1/1	0.95	0.16	66,66,66,66	0
56	MG	1A	3814	1/1	0.95	0.28	34,34,34,34	0
56	MG	2a	3038	1/1	0.95	0.29	62,62,62,62	0
56	MG	1A	3425	1/1	0.95	0.09	48,48,48,48	0
56	MG	2a	3040	1/1	0.95	0.16	80,80,80,80	0
56	MG	1A	3307	1/1	0.95	0.07	51,51,51,51	0
56	MG	1B	3632	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3211	1/1	0.95	0.37	44,44,44,44	0
56	MG	1A	3818	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3819	1/1	0.95	0.08	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	2A	3452	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3253	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3310	1/1	0.95	0.06	56,56,56,56	0
56	MG	2A	3053	1/1	0.95	0.16	71,71,71,71	0
56	MG	1A	3822	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3981	1/1	0.95	0.13	51,51,51,51	0
56	MG	2A	3459	1/1	0.95	0.29	61,61,61,61	0
56	MG	1A	3982	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3058	1/1	0.95	0.28	68,68,68,68	0
56	MG	1A	3983	1/1	0.95	0.06	70,70,70,70	0
56	MG	1A	3059	1/1	0.95	0.24	60,60,60,60	0
56	MG	1A	3097	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3986	1/1	0.95	0.07	71,71,71,71	0
56	MG	1E	312	1/1	0.95	0.05	24,24,24,24	0
56	MG	2A	3272	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3256	1/1	0.95	0.18	41,41,41,41	0
56	MG	2A	3470	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3436	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3215	1/1	0.95	0.25	43,43,43,43	0
56	MG	2A	3753	1/1	0.95	0.06	80,80,80,80	0
56	MG	1a	1692	1/1	0.95	0.39	72,72,72,72	0
56	MG	1A	3991	1/1	0.95	0.09	29,29,29,29	0
56	MG	1A	3654	1/1	0.95	0.07	30,30,30,30	0
56	MG	2A	3073	1/1	0.95	0.07	62,62,62,62	0
56	MG	2a	3073	1/1	0.95	0.52	83,83,83,83	0
56	MG	2A	3480	1/1	0.95	0.09	62,62,62,62	0
56	MG	1F	309	1/1	0.95	0.06	45,45,45,45	0
56	MG	2a	3077	1/1	0.95	0.22	66,66,66,66	0
56	MG	2A	3281	1/1	0.95	0.06	62,62,62,62	0
56	MG	1A	3831	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3077	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3764	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3079	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3365	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3216	1/1	0.95	0.22	48,48,48,48	0
56	MG	1A	3662	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3289	1/1	0.95	0.24	62,62,62,62	0
56	MG	2A	3771	1/1	0.95	0.06	62,62,62,62	0
56	MG	2A	3084	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3837	1/1	0.95	0.17	66,66,66,66	0
56	MG	2A	3292	1/1	0.95	0.18	73,73,73,73	0
56	MG	2A	3776	1/1	0.95	0.10	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	3442	1/1	0.95	0.09	57,57,57,57	0
56	MG	2a	3094	1/1	0.95	0.26	72,72,72,72	0
56	MG	1A	3154	1/1	0.95	0.21	42,42,42,42	0
56	MG	1A	3446	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3447	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3784	1/1	0.95	0.08	57,57,57,57	0
56	MG	2A	3785	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3530	1/1	0.95	0.10	74,74,74,74	0
56	MG	2A	3787	1/1	0.95	0.14	68,68,68,68	0
56	MG	1N	204	1/1	0.95	0.34	48,48,48,48	0
56	MG	1N	205	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3114	1/1	0.95	0.16	41,41,41,41	0
56	MG	1A	3449	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3450	1/1	0.95	0.30	48,48,48,48	0
56	MG	1A	3451	1/1	0.95	0.17	36,36,36,36	0
56	MG	2A	3510	1/1	0.95	0.06	77,77,77,77	0
56	MG	2A	3100	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3804	1/1	0.95	0.14	56,56,56,56	0
56	MG	2A	3305	1/1	0.95	0.14	64,64,64,64	0
56	MG	1A	3540	1/1	0.95	0.24	44,44,44,44	0
56	MG	1A	3370	1/1	0.95	0.10	56,56,56,56	0
56	MG	1Q	202	1/1	0.95	0.07	54,54,54,54	0
56	MG	1Q	204	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	4020	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1721	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	4022	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	4023	1/1	0.95	0.10	57,57,57,57	0
56	MG	1R	203	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3261	1/1	0.95	0.13	71,71,71,71	0
56	MG	2A	3817	1/1	0.95	0.06	67,67,67,67	0
56	MG	1a	1727	1/1	0.95	0.13	66,66,66,66	0
56	MG	1A	3702	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3526	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3372	1/1	0.95	0.11	56,56,56,56	0
56	MG	2A	3823	1/1	0.95	0.12	56,56,56,56	0
56	MG	1a	1733	1/1	0.95	0.12	50,50,50,50	0
56	MG	1a	1735	1/1	0.95	0.12	61,61,61,61	0
56	MG	2A	3121	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3704	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3320	1/1	0.95	0.09	60,60,60,60	0
56	MG	2A	3537	1/1	0.95	0.09	56,56,56,56	0
56	MG	2A	3540	1/1	0.95	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3321	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3862	1/1	0.95	0.04	24,24,24,24	0
56	MG	1A	3322	1/1	0.95	0.12	53,53,53,53	0
56	MG	1U	210	1/1	0.95	0.18	43,43,43,43	0
56	MG	2A	3845	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3328	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3157	1/1	0.95	0.14	36,36,36,36	0
56	MG	1A	3462	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3555	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3556	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3220	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3221	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3160	1/1	0.95	0.48	38,38,38,38	0
56	MG	1A	3225	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3138	1/1	0.95	0.19	53,53,53,53	0
56	MG	1A	3386	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3226	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3572	1/1	0.95	0.12	74,74,74,74	0
56	MG	1X	103	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3574	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3869	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3143	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3470	1/1	0.95	0.17	41,41,41,41	0
56	MG	2A	3579	1/1	0.95	0.12	62,62,62,62	0
56	MG	1A	3727	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	4054	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3561	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3228	1/1	0.95	0.13	33,33,33,33	0
56	MG	10	101	1/1	0.95	0.26	46,46,46,46	0
56	MG	2A	3151	1/1	0.95	0.13	62,62,62,62	0
56	MG	2A	3589	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3879	1/1	0.95	0.14	36,36,36,36	0
56	MG	1A	3273	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	3188	1/1	0.95	0.22	39,39,39,39	0
56	MG	1A	3885	1/1	0.95	0.11	39,39,39,39	0
56	MG	2A	3351	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3278	1/1	0.95	0.18	35,35,35,35	0
56	MG	2a	3184	1/1	0.95	0.07	78,78,78,78	0
56	MG	2a	3185	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3888	1/1	0.95	0.08	40,40,40,40	0
56	MG	2a	3187	1/1	0.95	0.11	70,70,70,70	0
56	MG	1A	3279	1/1	0.95	0.36	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	12	102	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3280	1/1	0.95	0.10	36,36,36,36	0
56	MG	1a	1781	1/1	0.95	0.10	50,50,50,50	0
56	MG	13	104	1/1	0.95	0.13	59,59,59,59	0
56	MG	15	101	1/1	0.95	0.27	33,33,33,33	0
56	MG	1A	3740	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3573	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3284	1/1	0.95	0.06	45,45,45,45	0
56	MG	2A	3170	1/1	0.95	0.10	63,63,63,63	0
56	MG	16	102	1/1	0.95	0.07	60,60,60,60	0
56	MG	17	101	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3577	1/1	0.95	0.19	43,43,43,43	0
56	MG	1a	1807	1/1	0.95	0.06	62,62,62,62	0
56	MG	1a	1809	1/1	0.95	0.18	66,66,66,66	0
56	MG	18	101	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3578	1/1	0.95	0.19	53,53,53,53	0
56	MG	2A	3179	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3286	1/1	0.95	0.07	57,57,57,57	0
56	MG	1A	4076	1/1	0.95	0.08	67,67,67,67	0
56	MG	2A	3623	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	4077	1/1	0.95	0.08	53,53,53,53	0
56	MG	2a	3210	1/1	0.95	0.19	72,72,72,72	0
56	MG	1A	3899	1/1	0.95	0.06	31,31,31,31	0
56	MG	1A	3746	1/1	0.95	0.09	56,56,56,56	0
56	MG	2A	3627	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3185	1/1	0.95	0.13	51,51,51,51	0
56	MG	2E	310	1/1	0.95	0.14	73,73,73,73	0
56	MG	1A	3902	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3161	1/1	0.95	0.15	54,54,54,54	0
56	MG	2F	303	1/1	0.95	0.09	51,51,51,51	0
56	MG	1a	1605	1/1	0.95	0.06	63,63,63,63	0
56	MG	1A	3583	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3407	1/1	0.95	0.07	44,44,44,44	0
56	MG	1a	1610	1/1	0.95	0.17	59,59,59,59	0
56	MG	2O	201	1/1	0.95	0.16	67,67,67,67	0
56	MG	2A	3639	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	4087	1/1	0.95	0.19	61,61,61,61	0
56	MG	1A	3909	1/1	0.95	0.09	50,50,50,50	0
56	MG	2Q	203	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	4089	1/1	0.95	0.11	44,44,44,44	0
56	MG	1w	102	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3028	1/1	0.95	0.18	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	1A	3086	1/1	0.95	0.20	33,33,33,33	0
56	MG	2A	3391	1/1	0.95	0.19	66,66,66,66	0
56	MG	1a	1620	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3164	1/1	0.95	0.21	37,37,37,37	0
56	MG	1A	3590	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3762	1/1	0.95	0.06	45,45,45,45	0
56	MG	1A	3591	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	3242	1/1	0.95	0.17	52,52,52,52	0
56	MG	20	101	1/1	0.95	0.20	68,68,68,68	0
56	MG	2a	3241	1/1	0.95	0.13	73,73,73,73	0
56	MG	1A	4097	1/1	0.95	0.23	57,57,57,57	0
56	MG	1A	3076	1/1	0.95	0.19	52,52,52,52	0
56	MG	2A	3666	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3766	1/1	0.95	0.09	22,22,22,22	0
56	MG	1A	3201	1/1	0.95	0.09	34,34,34,34	0
56	MG	2l	203	1/1	0.95	0.08	78,78,78,78	0
56	MG	1A	3489	1/1	0.95	0.14	64,64,64,64	0
56	MG	25	102	1/1	0.95	0.15	55,55,55,55	0
56	MG	25	103	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3776	1/1	0.95	0.08	33,33,33,33	0
56	MG	1A	3016	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3102	1/1	0.95	0.17	43,43,43,43	0
56	MG	1B	3603	1/1	0.95	0.17	57,57,57,57	0
56	MG	1B	3605	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3675	1/1	0.95	0.07	43,43,43,43	0
56	MG	1B	3606	1/1	0.95	0.17	50,50,50,50	0
56	MG	2A	3002	1/1	0.95	0.37	68,68,68,68	0
56	MG	2A	3678	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3248	1/1	0.95	0.12	42,42,42,42	0
56	MG	2A	3681	1/1	0.95	0.25	75,75,75,75	0
56	MG	1a	1642	1/1	0.95	0.21	71,71,71,71	0
56	MG	1A	3941	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3494	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3414	1/1	0.95	0.12	67,67,67,67	0
56	MG	1a	1645	1/1	0.95	0.08	55,55,55,55	0
56	MG	1B	3610	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3010	1/1	0.95	0.12	58,58,58,58	0
56	MG	2A	3011	1/1	0.95	0.09	61,61,61,61	0
56	MG	1a	1648	1/1	0.95	0.21	64,64,64,64	0
56	MG	1A	3949	1/1	0.95	0.10	31,31,31,31	0
56	MG	2A	3692	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3793	1/1	0.95	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3350	1/1	0.95	0.10	43,43,43,43	0
56	MG	1a	1655	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3022	1/1	0.95	0.22	48,48,48,48	0
59	ZN	24	501	1/1	0.95	0.09	108,108,108,108	0
56	MG	1D	308	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3063	1/1	0.96	0.26	57,57,57,57	0
56	MG	1A	3706	1/1	0.96	0.10	26,26,26,26	0
56	MG	1E	301	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3713	1/1	0.96	0.06	68,68,68,68	0
56	MG	2A	3244	1/1	0.96	0.20	59,59,59,59	0
56	MG	1A	3171	1/1	0.96	0.12	42,42,42,42	0
56	MG	1E	304	1/1	0.96	0.26	51,51,51,51	0
56	MG	2A	3247	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3454	1/1	0.96	0.24	57,57,57,57	0
56	MG	2A	3723	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3724	1/1	0.96	0.06	48,48,48,48	0
56	MG	1a	1664	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3037	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3709	1/1	0.96	0.05	30,30,30,30	0
56	MG	1E	307	1/1	0.96	0.18	35,35,35,35	0
56	MG	1A	3847	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3175	1/1	0.96	0.17	30,30,30,30	0
56	MG	1A	3178	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3270	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3853	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3423	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3564	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3271	1/1	0.96	0.13	53,53,53,53	0
56	MG	2A	3467	1/1	0.96	0.20	42,42,42,42	0
56	MG	1a	1675	1/1	0.96	0.10	67,67,67,67	0
56	MG	2A	3050	1/1	0.96	0.11	43,43,43,43	0
56	MG	1F	305	1/1	0.96	0.04	42,42,42,42	0
56	MG	2a	3050	1/1	0.96	0.11	65,65,65,65	0
56	MG	1F	308	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3179	1/1	0.96	0.21	42,42,42,42	0
56	MG	1a	1680	1/1	0.96	0.11	78,78,78,78	0
56	MG	1F	310	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3227	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3065	1/1	0.96	0.29	65,65,65,65	0
56	MG	1A	3002	1/1	0.96	0.20	58,58,58,58	0
56	MG	1A	4015	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	4016	1/1	0.96	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3756	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3863	1/1	0.96	0.07	27,27,27,27	0
56	MG	1A	3724	1/1	0.96	0.13	35,35,35,35	0
56	MG	1a	1689	1/1	0.96	0.19	55,55,55,55	0
56	MG	1A	3009	1/1	0.96	0.05	30,30,30,30	0
56	MG	1A	3866	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3726	1/1	0.96	0.17	57,57,57,57	0
56	MG	1N	203	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3491	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3071	1/1	0.96	0.10	66,66,66,66	0
56	MG	2a	3070	1/1	0.96	0.23	54,54,54,54	0
56	MG	1A	3432	1/1	0.96	0.20	56,56,56,56	0
56	MG	2a	3072	1/1	0.96	0.07	64,64,64,64	0
56	MG	1A	3074	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3184	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3285	1/1	0.96	0.28	53,53,53,53	0
56	MG	2a	3076	1/1	0.96	0.17	55,55,55,55	0
56	MG	1A	3237	1/1	0.96	0.20	56,56,56,56	0
56	MG	2A	3078	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3496	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3238	1/1	0.96	0.12	32,32,32,32	0
56	MG	1P	201	1/1	0.96	0.21	35,35,35,35	0
56	MG	2A	3778	1/1	0.96	0.10	46,46,46,46	0
56	MG	1P	204	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3507	1/1	0.96	0.10	68,68,68,68	0
56	MG	1A	4033	1/1	0.96	0.10	40,40,40,40	0
56	MG	1Q	201	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3498	1/1	0.96	0.06	54,54,54,54	0
56	MG	2A	3087	1/1	0.96	0.09	57,57,57,57	0
56	MG	1Q	203	1/1	0.96	0.07	65,65,65,65	0
56	MG	1A	3586	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3788	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3499	1/1	0.96	0.14	58,58,58,58	0
56	MG	2A	3792	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3793	1/1	0.96	0.08	59,59,59,59	0
56	MG	1A	3500	1/1	0.96	0.16	61,61,61,61	0
56	MG	1A	3882	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	4042	1/1	0.96	0.08	57,57,57,57	0
56	MG	1R	204	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	4043	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3437	1/1	0.96	0.15	53,53,53,53	0
56	MG	1A	3239	1/1	0.96	0.13	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	2A	3099	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3592	1/1	0.96	0.09	46,46,46,46	0
56	MG	1a	1720	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3505	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3528	1/1	0.96	0.11	58,58,58,58	0
56	MG	2a	3108	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3139	1/1	0.96	0.06	20,20,20,20	0
56	MG	1A	4052	1/1	0.96	0.04	38,38,38,38	0
56	MG	1A	3380	1/1	0.96	0.08	51,51,51,51	0
56	MG	2A	3107	1/1	0.96	0.08	61,61,61,61	0
56	MG	1a	1725	1/1	0.96	0.13	60,60,60,60	0
56	MG	1U	208	1/1	0.96	0.21	38,38,38,38	0
56	MG	2a	3115	1/1	0.96	0.09	77,77,77,77	0
56	MG	1A	3291	1/1	0.96	0.22	42,42,42,42	0
56	MG	2A	3112	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3382	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3444	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3543	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3544	1/1	0.96	0.08	66,66,66,66	0
56	MG	1A	3757	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3445	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3759	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3827	1/1	0.96	0.05	45,45,45,45	0
56	MG	1A	3897	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3512	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3051	1/1	0.96	0.11	32,32,32,32	0
56	MG	2A	3122	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3836	1/1	0.96	0.07	45,45,45,45	0
56	MG	1X	102	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3105	1/1	0.96	0.17	48,48,48,48	0
56	MG	2A	3559	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3387	1/1	0.96	0.09	49,49,49,49	0
56	MG	1a	1746	1/1	0.96	0.08	63,63,63,63	0
56	MG	1A	3144	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3612	1/1	0.96	0.11	55,55,55,55	0
56	MG	1Y	203	1/1	0.96	0.19	52,52,52,52	0
56	MG	1a	1751	1/1	0.96	0.08	59,59,59,59	0
56	MG	2A	3131	1/1	0.96	0.15	55,55,55,55	0
56	MG	1a	1752	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3389	1/1	0.96	0.11	54,54,54,54	0
56	MG	2A	3577	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3857	1/1	0.96	0.08	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	3769	1/1	0.96	0.09	25,25,25,25	0
56	MG	2A	3135	1/1	0.96	0.13	59,59,59,59	0
56	MG	2A	3136	1/1	0.96	0.06	54,54,54,54	0
56	MG	1Z	303	1/1	0.96	0.14	56,56,56,56	0
56	MG	2A	3862	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	4072	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3864	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3770	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3771	1/1	0.96	0.05	31,31,31,31	0
56	MG	10	105	1/1	0.96	0.29	68,68,68,68	0
56	MG	1A	3774	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3078	1/1	0.96	0.08	32,32,32,32	0
56	MG	11	102	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	4079	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	3917	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3918	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3452	1/1	0.96	0.09	65,65,65,65	0
56	MG	2A	3150	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3522	1/1	0.96	0.30	45,45,45,45	0
56	MG	2a	3168	1/1	0.96	0.06	58,58,58,58	0
56	MG	2a	3169	1/1	0.96	0.19	64,64,64,64	0
56	MG	1A	3779	1/1	0.96	0.05	64,64,64,64	0
56	MG	1A	3041	1/1	0.96	0.23	35,35,35,35	0
56	MG	15	102	1/1	0.96	0.10	42,42,42,42	0
56	MG	15	103	1/1	0.96	0.23	30,30,30,30	0
56	MG	15	104	1/1	0.96	0.07	32,32,32,32	0
56	MG	2A	3607	1/1	0.96	0.15	57,57,57,57	0
56	MG	15	105	1/1	0.96	0.08	50,50,50,50	0
56	MG	2a	3178	1/1	0.96	0.06	74,74,74,74	0
56	MG	2a	3179	1/1	0.96	0.09	75,75,75,75	0
56	MG	1A	3621	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3790	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3623	1/1	0.96	0.04	42,42,42,42	0
56	MG	1A	3394	1/1	0.96	0.62	48,48,48,48	0
56	MG	2A	3162	1/1	0.96	0.09	64,64,64,64	0
56	MG	2A	3163	1/1	0.96	0.18	54,54,54,54	0
56	MG	1a	1794	1/1	0.96	0.05	82,82,82,82	0
56	MG	1A	3341	1/1	0.96	0.21	41,41,41,41	0
56	MG	2A	3166	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3934	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3456	1/1	0.96	0.09	45,45,45,45	0
56	MG	1a	1805	1/1	0.96	0.06	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3621	1/1	0.96	0.08	72,72,72,72	0
56	MG	18	102	1/1	0.96	0.20	45,45,45,45	0
56	MG	2A	3171	1/1	0.96	0.13	72,72,72,72	0
56	MG	18	104	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3798	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3629	1/1	0.96	0.07	37,37,37,37	0
56	MG	2D	302	1/1	0.96	0.33	70,70,70,70	0
56	MG	1A	3042	1/1	0.96	0.27	38,38,38,38	0
56	MG	2D	304	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3943	1/1	0.96	0.08	66,66,66,66	0
56	MG	1A	3944	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3946	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3804	1/1	0.96	0.07	23,23,23,23	0
56	MG	1A	3043	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3952	1/1	0.96	0.05	63,63,63,63	0
56	MG	2E	304	1/1	0.96	0.21	51,51,51,51	0
56	MG	1e	202	1/1	0.96	0.16	61,61,61,61	0
56	MG	1A	3641	1/1	0.96	0.10	57,57,57,57	0
56	MG	1l	201	1/1	0.96	0.08	76,76,76,76	0
56	MG	2E	309	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3112	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3643	1/1	0.96	0.16	68,68,68,68	0
56	MG	1m	3001	1/1	0.96	0.07	67,67,67,67	0
56	MG	2A	3647	1/1	0.96	0.06	50,50,50,50	0
56	MG	2A	3650	1/1	0.96	0.08	52,52,52,52	0
56	MG	1a	1608	1/1	0.96	0.07	58,58,58,58	0
56	MG	1a	1609	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3653	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3113	1/1	0.96	0.07	46,46,46,46	0
56	MG	1a	1611	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3532	1/1	0.96	0.09	64,64,64,64	0
56	MG	2Q	201	1/1	0.96	0.10	61,61,61,61	0
56	MG	1A	3533	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3534	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3204	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3536	1/1	0.96	0.11	44,44,44,44	0
56	MG	1a	1618	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3965	1/1	0.96	0.05	38,38,38,38	0
56	MG	1A	3659	1/1	0.96	0.07	44,44,44,44	0
56	MG	2T	203	1/1	0.96	0.20	61,61,61,61	0
56	MG	1w	108	1/1	0.96	0.07	88,88,88,88	0
56	MG	2a	3234	1/1	0.96	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	3056	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	3405	1/1	0.96	0.09	51,51,51,51	0
56	MG	2W	201	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3969	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3664	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3971	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	3406	1/1	0.96	0.07	48,48,48,48	0
56	MG	1B	3619	1/1	0.96	0.21	58,58,58,58	0
56	MG	1B	3620	1/1	0.96	0.06	37,37,37,37	0
56	MG	2e	201	1/1	0.96	0.06	75,75,75,75	0
56	MG	2f	201	1/1	0.96	0.11	57,57,57,57	0
56	MG	1A	3117	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3030	1/1	0.96	0.31	32,32,32,32	0
56	MG	2l	201	1/1	0.96	0.09	70,70,70,70	0
56	MG	2A	3212	1/1	0.96	0.09	63,63,63,63	0
56	MG	23	101	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3034	1/1	0.96	0.23	35,35,35,35	0
56	MG	2A	3416	1/1	0.96	0.17	60,60,60,60	0
56	MG	1a	1635	1/1	0.96	0.15	69,69,69,69	0
56	MG	1A	3089	1/1	0.96	0.16	54,54,54,54	0
56	MG	1a	1637	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3677	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3681	1/1	0.96	0.05	22,22,22,22	0
56	MG	2A	3219	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3979	1/1	0.96	0.08	70,70,70,70	0
56	MG	1B	3628	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3471	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3090	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3060	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3009	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3127	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3836	1/1	0.96	0.15	41,41,41,41	0
56	MG	2A	3012	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3047	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3698	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3551	1/1	0.96	0.21	53,53,53,53	0
56	MG	2x	106	1/1	0.96	0.09	58,58,58,58	0
56	MG	1a	1651	1/1	0.96	0.08	58,58,58,58	0
56	MG	1a	1652	1/1	0.96	0.13	54,54,54,54	0
56	MG	1a	1653	1/1	0.96	0.07	57,57,57,57	0
56	MG	1B	3637	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3703	1/1	0.96	0.10	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	3236	1/1	0.96	0.21	44,44,44,44	0
56	MG	1D	301	1/1	0.96	0.25	41,41,41,41	0
56	MG	2A	3442	1/1	0.96	0.25	60,60,60,60	0
56	MG	1A	3005	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3131	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3130	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3581	1/1	0.97	0.39	41,41,41,41	0
56	MG	1A	3155	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3222	1/1	0.97	0.18	42,42,42,42	0
56	MG	1A	3705	1/1	0.97	0.10	30,30,30,30	0
56	MG	1a	1788	1/1	0.97	0.05	65,65,65,65	0
56	MG	1a	1790	1/1	0.97	0.10	72,72,72,72	0
56	MG	2A	3768	1/1	0.97	0.06	59,59,59,59	0
56	MG	2A	3139	1/1	0.97	0.19	46,46,46,46	0
56	MG	1A	3459	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3223	1/1	0.97	0.24	54,54,54,54	0
56	MG	1a	1796	1/1	0.97	0.06	71,71,71,71	0
56	MG	1A	3091	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3517	1/1	0.97	0.19	50,50,50,50	0
56	MG	2A	3775	1/1	0.97	0.20	68,68,68,68	0
56	MG	1a	1801	1/1	0.97	0.06	68,68,68,68	0
56	MG	2A	3777	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3115	1/1	0.97	0.18	35,35,35,35	0
56	MG	2A	3536	1/1	0.97	0.11	42,42,42,42	0
56	MG	2A	3780	1/1	0.97	0.10	63,63,63,63	0
56	MG	1a	1612	1/1	0.97	0.05	64,64,64,64	0
56	MG	2A	3538	1/1	0.97	0.06	41,41,41,41	0
56	MG	2A	3539	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3589	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3158	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3988	1/1	0.97	0.16	62,62,62,62	0
56	MG	1A	3464	1/1	0.97	0.21	41,41,41,41	0
56	MG	1A	3851	1/1	0.97	0.04	59,59,59,59	0
56	MG	1A	3357	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3790	1/1	0.97	0.05	54,54,54,54	0
56	MG	2A	3791	1/1	0.97	0.04	59,59,59,59	0
56	MG	1a	1619	1/1	0.97	0.06	65,65,65,65	0
56	MG	1a	1814	1/1	0.97	0.16	58,58,58,58	0
56	MG	1A	3116	1/1	0.97	0.07	40,40,40,40	0
56	MG	2A	3551	1/1	0.97	0.08	65,65,65,65	0
56	MG	1A	3995	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	3265	1/1	0.97	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3798	1/1	0.97	0.06	73,73,73,73	0
56	MG	1A	3191	1/1	0.97	0.12	52,52,52,52	0
56	MG	1D	304	1/1	0.97	0.07	24,24,24,24	0
56	MG	1f	201	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3722	1/1	0.97	0.04	14,14,14,14	0
56	MG	2A	3805	1/1	0.97	0.10	79,79,79,79	0
56	MG	1A	3857	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3562	1/1	0.97	0.11	42,42,42,42	0
56	MG	1D	309	1/1	0.97	0.10	46,46,46,46	0
56	MG	1D	310	1/1	0.97	0.11	29,29,29,29	0
56	MG	2A	3567	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3858	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	4001	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	4002	1/1	0.97	0.06	62,62,62,62	0
56	MG	1A	3230	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	1634	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3193	1/1	0.97	0.18	38,38,38,38	0
56	MG	1A	3318	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3064	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3103	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3007	1/1	0.97	0.05	39,39,39,39	0
56	MG	1A	3235	1/1	0.97	0.27	39,39,39,39	0
56	MG	1A	3606	1/1	0.97	0.36	62,62,62,62	0
56	MG	2A	3824	1/1	0.97	0.12	61,61,61,61	0
56	MG	1E	315	1/1	0.97	0.17	46,46,46,46	0
56	MG	1A	3607	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	3275	1/1	0.97	0.12	53,53,53,53	0
56	MG	2A	3588	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3197	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3735	1/1	0.97	0.11	58,58,58,58	0
56	MG	2A	3833	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3611	1/1	0.97	0.08	39,39,39,39	0
56	MG	2A	3835	1/1	0.97	0.07	58,58,58,58	0
56	MG	1F	306	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3120	1/1	0.97	0.22	43,43,43,43	0
56	MG	1A	3614	1/1	0.97	0.06	43,43,43,43	0
56	MG	1x	109	1/1	0.97	0.08	32,32,32,32	0
56	MG	1A	3140	1/1	0.97	0.10	50,50,50,50	0
56	MG	2a	3117	1/1	0.97	0.17	66,66,66,66	0
56	MG	1A	3538	1/1	0.97	0.13	43,43,43,43	0
56	MG	2A	3190	1/1	0.97	0.06	59,59,59,59	0
56	MG	2A	3846	1/1	0.97	0.06	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	3847	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3240	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	3281	1/1	0.97	0.29	40,40,40,40	0
56	MG	1A	3878	1/1	0.97	0.04	40,40,40,40	0
56	MG	1A	3429	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3283	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3484	1/1	0.97	0.07	43,43,43,43	0
56	MG	1G	205	1/1	0.97	0.08	64,64,64,64	0
56	MG	1A	3023	1/1	0.97	0.05	20,20,20,20	0
56	MG	1A	4034	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3751	1/1	0.97	0.04	51,51,51,51	0
56	MG	1A	3377	1/1	0.97	0.23	42,42,42,42	0
56	MG	1A	3285	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3095	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3631	1/1	0.97	0.10	44,44,44,44	0
56	MG	1O	202	1/1	0.97	0.15	59,59,59,59	0
56	MG	1A	3632	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3548	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3867	1/1	0.97	0.07	63,63,63,63	0
56	MG	1A	3635	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3636	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3019	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3895	1/1	0.97	0.08	55,55,55,55	0
56	MG	1P	203	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	4047	1/1	0.97	0.04	53,53,53,53	0
56	MG	1a	1676	1/1	0.97	0.11	58,58,58,58	0
56	MG	1P	205	1/1	0.97	0.20	31,31,31,31	0
56	MG	1A	3243	1/1	0.97	0.05	42,42,42,42	0
56	MG	2A	3877	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	4049	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3638	1/1	0.97	0.05	23,23,23,23	0
56	MG	1A	4051	1/1	0.97	0.05	25,25,25,25	0
56	MG	2A	3633	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3124	1/1	0.97	0.20	42,42,42,42	0
56	MG	2a	3155	1/1	0.97	0.06	67,67,67,67	0
56	MG	2A	3032	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3637	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3642	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3034	1/1	0.97	0.13	58,58,58,58	0
56	MG	1A	3900	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3641	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3643	1/1	0.97	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3164	1/1	0.97	0.06	70,70,70,70	0
56	MG	1A	3644	1/1	0.97	0.05	43,43,43,43	0
56	MG	2B	207	1/1	0.97	0.05	67,67,67,67	0
56	MG	1A	3903	1/1	0.97	0.05	39,39,39,39	0
56	MG	2A	3646	1/1	0.97	0.13	60,60,60,60	0
56	MG	1A	3904	1/1	0.97	0.13	36,36,36,36	0
56	MG	2A	3648	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3649	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3418	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3905	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3645	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3773	1/1	0.97	0.06	30,30,30,30	0
56	MG	1A	3206	1/1	0.97	0.14	34,34,34,34	0
56	MG	1U	202	1/1	0.97	0.28	43,43,43,43	0
56	MG	1A	3384	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3553	1/1	0.97	0.07	53,53,53,53	0
56	MG	2D	301	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3658	1/1	0.97	0.20	69,69,69,69	0
56	MG	1A	3145	1/1	0.97	0.05	36,36,36,36	0
56	MG	2A	3660	1/1	0.97	0.09	57,57,57,57	0
56	MG	1U	206	1/1	0.97	0.20	37,37,37,37	0
56	MG	2A	3049	1/1	0.97	0.08	32,32,32,32	0
56	MG	1U	207	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	3913	1/1	0.97	0.07	61,61,61,61	0
56	MG	1a	1700	1/1	0.97	0.32	69,69,69,69	0
56	MG	1U	209	1/1	0.97	0.20	38,38,38,38	0
56	MG	1A	3652	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	4070	1/1	0.97	0.07	54,54,54,54	0
56	MG	2E	306	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3056	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3653	1/1	0.97	0.07	35,35,35,35	0
56	MG	1V	205	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3555	1/1	0.97	0.12	52,52,52,52	0
56	MG	1A	3788	1/1	0.97	0.08	56,56,56,56	0
56	MG	2A	3251	1/1	0.97	0.14	69,69,69,69	0
56	MG	1A	3789	1/1	0.97	0.09	66,66,66,66	0
56	MG	1A	3922	1/1	0.97	0.07	25,25,25,25	0
56	MG	1W	204	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3125	1/1	0.97	0.23	41,41,41,41	0
56	MG	1A	3656	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3792	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	3174	1/1	0.97	0.15	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	1X	104	1/1	0.97	0.19	43,43,43,43	0
56	MG	1X	105	1/1	0.97	0.05	50,50,50,50	0
56	MG	1A	3928	1/1	0.97	0.17	45,45,45,45	0
56	MG	2A	3072	1/1	0.97	0.12	53,53,53,53	0
56	MG	1a	1719	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3658	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	4084	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3076	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3212	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3661	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3147	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3800	1/1	0.97	0.08	53,53,53,53	0
56	MG	2A	3081	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3177	1/1	0.97	0.08	25,25,25,25	0
56	MG	10	102	1/1	0.97	0.08	49,49,49,49	0
56	MG	1a	1729	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3392	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3071	1/1	0.97	0.24	37,37,37,37	0
56	MG	1A	3806	1/1	0.97	0.10	46,46,46,46	0
56	MG	10	106	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3666	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3667	1/1	0.97	0.04	27,27,27,27	0
56	MG	2A	3471	1/1	0.97	0.30	52,52,52,52	0
56	MG	1a	1738	1/1	0.97	0.07	63,63,63,63	0
56	MG	11	101	1/1	0.97	0.32	43,43,43,43	0
56	MG	2A	3093	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3088	1/1	0.97	0.18	46,46,46,46	0
56	MG	1a	1741	1/1	0.97	0.05	50,50,50,50	0
56	MG	1A	3669	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3479	1/1	0.97	0.19	48,48,48,48	0
56	MG	1A	3566	1/1	0.97	0.10	41,41,41,41	0
56	MG	28	102	1/1	0.97	0.12	59,59,59,59	0
56	MG	2A	3714	1/1	0.97	0.10	70,70,70,70	0
56	MG	2A	3715	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3481	1/1	0.97	0.12	63,63,63,63	0
56	MG	2A	3482	1/1	0.97	0.09	74,74,74,74	0
56	MG	1A	3567	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3484	1/1	0.97	0.18	48,48,48,48	0
56	MG	2A	3720	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3151	1/1	0.97	0.08	39,39,39,39	0
56	MG	13	102	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3955	1/1	0.97	0.06	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3675	1/1	0.97	0.06	23,23,23,23	0
56	MG	1a	1750	1/1	0.97	0.15	48,48,48,48	0
56	MG	2A	3490	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3504	1/1	0.97	0.16	33,33,33,33	0
56	MG	1A	3679	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3080	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3682	1/1	0.97	0.10	24,24,24,24	0
56	MG	2A	3733	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3109	1/1	0.97	0.12	49,49,49,49	0
56	MG	1B	3604	1/1	0.97	0.20	59,59,59,59	0
56	MG	2A	3737	1/1	0.97	0.05	59,59,59,59	0
56	MG	1A	3684	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3685	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3964	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3397	1/1	0.97	0.08	58,58,58,58	0
56	MG	1A	3687	1/1	0.97	0.11	53,53,53,53	0
56	MG	17	102	1/1	0.97	0.08	30,30,30,30	0
56	MG	1A	3688	1/1	0.97	0.06	36,36,36,36	0
56	MG	1a	1765	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3828	1/1	0.97	0.04	38,38,38,38	0
56	MG	1A	3015	1/1	0.97	0.07	36,36,36,36	0
56	MG	1a	1768	1/1	0.97	0.07	60,60,60,60	0
56	MG	18	103	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3574	1/1	0.97	0.05	27,27,27,27	0
56	MG	1A	3347	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3512	1/1	0.97	0.07	70,70,70,70	0
56	MG	1A	3304	1/1	0.97	0.37	62,62,62,62	0
56	MG	1a	1773	1/1	0.97	0.08	68,68,68,68	0
56	MG	1A	3697	1/1	0.97	0.13	31,31,31,31	0
56	MG	1A	3402	1/1	0.97	0.13	33,33,33,33	0
56	MG	1a	1777	1/1	0.97	0.06	70,70,70,70	0
59	ZN	2Y	202	1/1	0.97	0.05	95,95,95,95	0
56	MG	1A	3835	1/1	0.97	0.09	41,41,41,41	0
59	ZN	2n	501	1/1	0.97	0.07	98,98,98,98	0
56	MG	13	101	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3209	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3780	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3210	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3887	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	4008	1/1	0.98	0.03	32,32,32,32	0
56	MG	1A	3784	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3786	1/1	0.98	0.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3390	1/1	0.98	0.34	35,35,35,35	0
56	MG	1a	1728	1/1	0.98	0.13	58,58,58,58	0
56	MG	1A	3173	1/1	0.98	0.34	37,37,37,37	0
56	MG	1A	4013	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3008	1/1	0.98	0.11	29,29,29,29	0
56	MG	1a	1732	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	3692	1/1	0.98	0.04	35,35,35,35	0
56	MG	1a	1734	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3613	1/1	0.98	0.08	29,29,29,29	0
56	MG	1D	303	1/1	0.98	0.10	44,44,44,44	0
56	MG	17	103	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3694	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3096	1/1	0.98	0.13	25,25,25,25	0
56	MG	1D	306	1/1	0.98	0.17	36,36,36,36	0
56	MG	2A	3534	1/1	0.98	0.05	52,52,52,52	0
56	MG	1D	307	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3794	1/1	0.98	0.03	41,41,41,41	0
56	MG	1A	4021	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3615	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3796	1/1	0.98	0.07	24,24,24,24	0
56	MG	1A	3176	1/1	0.98	0.09	33,33,33,33	0
56	MG	1A	3699	1/1	0.98	0.07	32,32,32,32	0
56	MG	1E	302	1/1	0.98	0.23	36,36,36,36	0
56	MG	1A	4026	1/1	0.98	0.06	57,57,57,57	0
56	MG	1A	3301	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3077	1/1	0.98	0.11	36,36,36,36	0
56	MG	2A	3383	1/1	0.98	0.09	38,38,38,38	0
56	MG	1E	306	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3801	1/1	0.98	0.06	29,29,29,29	0
56	MG	2A	3549	1/1	0.98	0.08	45,45,45,45	0
56	MG	2A	3550	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	4030	1/1	0.98	0.04	47,47,47,47	0
56	MG	1E	309	1/1	0.98	0.05	45,45,45,45	0
56	MG	2A	3554	1/1	0.98	0.03	49,49,49,49	0
56	MG	2A	3738	1/1	0.98	0.05	43,43,43,43	0
56	MG	1a	1758	1/1	0.98	0.07	56,56,56,56	0
56	MG	1E	310	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3802	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3012	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3349	1/1	0.98	0.17	35,35,35,35	0
56	MG	1A	3148	1/1	0.98	0.19	38,38,38,38	0
56	MG	1A	3503	1/1	0.98	0.16	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	3563	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3910	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3019	1/1	0.98	0.17	48,48,48,48	0
56	MG	2A	3566	1/1	0.98	0.09	50,50,50,50	0
56	MG	1F	302	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3708	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3569	1/1	0.98	0.07	55,55,55,55	0
56	MG	2A	3570	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3625	1/1	0.98	0.07	33,33,33,33	0
56	MG	1a	1621	1/1	0.98	0.05	49,49,49,49	0
56	MG	1A	3710	1/1	0.98	0.04	14,14,14,14	0
56	MG	1F	307	1/1	0.98	0.12	35,35,35,35	0
56	MG	2a	3161	1/1	0.98	0.04	69,69,69,69	0
56	MG	1A	3811	1/1	0.98	0.05	24,24,24,24	0
56	MG	1a	1774	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3812	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3401	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3712	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3560	1/1	0.98	0.21	41,41,41,41	0
56	MG	1A	3714	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3583	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3628	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3306	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3630	1/1	0.98	0.09	27,27,27,27	0
56	MG	2A	3587	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3123	1/1	0.98	0.24	42,42,42,42	0
56	MG	1a	1786	1/1	0.98	0.07	49,49,49,49	0
56	MG	1a	1787	1/1	0.98	0.08	77,77,77,77	0
56	MG	1A	3013	1/1	0.98	0.19	28,28,28,28	0
56	MG	2A	3592	1/1	0.98	0.03	33,33,33,33	0
56	MG	1A	3021	1/1	0.98	0.10	24,24,24,24	0
56	MG	28	101	1/1	0.98	0.18	49,49,49,49	0
56	MG	1A	3003	1/1	0.98	0.06	31,31,31,31	0
56	MG	2a	3183	1/1	0.98	0.10	59,59,59,59	0
56	MG	1a	1793	1/1	0.98	0.08	74,74,74,74	0
56	MG	2A	3104	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	4056	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	3010	1/1	0.98	0.06	37,37,37,37	0
56	MG	1a	1798	1/1	0.98	0.04	76,76,76,76	0
56	MG	1A	3933	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3186	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3827	1/1	0.98	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3104	1/1	0.98	0.04	25,25,25,25	0
56	MG	1a	1804	1/1	0.98	0.05	70,70,70,70	0
56	MG	1A	3938	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3939	1/1	0.98	0.04	63,63,63,63	0
56	MG	1A	3084	1/1	0.98	0.07	31,31,31,31	0
56	MG	1a	1646	1/1	0.98	0.09	61,61,61,61	0
56	MG	1A	4065	1/1	0.98	0.03	40,40,40,40	0
56	MG	1A	3085	1/1	0.98	0.15	35,35,35,35	0
56	MG	1P	202	1/1	0.98	0.15	32,32,32,32	0
56	MG	2A	3120	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3190	1/1	0.98	0.20	40,40,40,40	0
56	MG	1A	3229	1/1	0.98	0.22	35,35,35,35	0
56	MG	1A	3945	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3575	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	3947	1/1	0.98	0.04	48,48,48,48	0
56	MG	2A	3801	1/1	0.98	0.04	42,42,42,42	0
56	MG	2A	3802	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	3948	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3108	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	3950	1/1	0.98	0.08	63,63,63,63	0
56	MG	2A	3445	1/1	0.98	0.23	62,62,62,62	0
56	MG	1A	3192	1/1	0.98	0.13	34,34,34,34	0
56	MG	1A	3648	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	3953	1/1	0.98	0.09	49,49,49,49	0
56	MG	2A	3628	1/1	0.98	0.06	44,44,44,44	0
56	MG	1R	202	1/1	0.98	0.22	41,41,41,41	0
56	MG	1A	3649	1/1	0.98	0.04	20,20,20,20	0
56	MG	1A	3520	1/1	0.98	0.10	30,30,30,30	0
56	MG	1A	3736	1/1	0.98	0.06	46,46,46,46	0
56	MG	1A	3159	1/1	0.98	0.07	35,35,35,35	0
56	MG	2A	3634	1/1	0.98	0.06	46,46,46,46	0
56	MG	1A	3739	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3959	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3580	1/1	0.98	0.14	46,46,46,46	0
56	MG	1U	201	1/1	0.98	0.06	29,29,29,29	0
56	MG	1A	3274	1/1	0.98	0.16	41,41,41,41	0
56	MG	2A	3822	1/1	0.98	0.04	50,50,50,50	0
56	MG	1A	3418	1/1	0.98	0.09	43,43,43,43	0
56	MG	1A	3524	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3066	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3369	1/1	0.98	0.18	34,34,34,34	0
56	MG	1A	3849	1/1	0.98	0.06	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	3067	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3277	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3660	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3749	1/1	0.98	0.09	23,23,23,23	0
56	MG	1V	201	1/1	0.98	0.18	35,35,35,35	0
56	MG	1A	3044	1/1	0.98	0.08	35,35,35,35	0
56	MG	1V	204	1/1	0.98	0.19	56,56,56,56	0
56	MG	1A	3236	1/1	0.98	0.15	33,33,33,33	0
56	MG	2A	3840	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3752	1/1	0.98	0.03	23,23,23,23	0
56	MG	1A	4100	1/1	0.98	0.03	35,35,35,35	0
56	MG	1A	3069	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3754	1/1	0.98	0.05	57,57,57,57	0
56	MG	1x	114	1/1	0.98	0.05	72,72,72,72	0
56	MG	1W	203	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3136	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	4104	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3756	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3199	1/1	0.98	0.17	28,28,28,28	0
56	MG	1A	3200	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	3165	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3055	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3761	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3203	1/1	0.98	0.08	22,22,22,22	0
56	MG	1A	3597	1/1	0.98	0.33	38,38,38,38	0
56	MG	1A	3072	1/1	0.98	0.09	19,19,19,19	0
56	MG	1A	3672	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3599	1/1	0.98	0.14	45,45,45,45	0
56	MG	2A	3015	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3674	1/1	0.98	0.06	33,33,33,33	0
56	MG	2a	3079	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3032	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3290	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3033	1/1	0.98	0.29	34,34,34,34	0
56	MG	1A	3772	1/1	0.98	0.04	37,37,37,37	0
56	MG	2A	3498	1/1	0.98	0.06	51,51,51,51	0
56	MG	2A	3680	1/1	0.98	0.05	40,40,40,40	0
56	MG	1B	3617	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3993	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3680	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3075	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	3604	1/1	0.98	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3027	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	3438	1/1	0.98	0.14	48,48,48,48	0
56	MG	1I	103	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3880	1/1	0.98	0.13	41,41,41,41	0
56	MG	1A	3881	1/1	0.98	0.20	36,36,36,36	0
58	A1A1K	1A	4105	34/34	0.98	0.07	24,30,36,53	0
58	A1A1K	2A	3886	34/34	0.98	0.08	39,46,54,56	0
56	MG	1A	3777	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3143	1/1	0.98	0.16	33,33,33,33	0
59	ZN	29	102	1/1	0.98	0.04	79,79,79,79	0
56	MG	2A	3882	1/1	0.98	0.04	52,52,52,52	0
60	SF4	1d	302	8/8	0.98	0.06	67,74,78,79	0
56	MG	2A	3527	1/1	0.99	0.07	46,46,46,46	0
56	MG	1A	4078	1/1	0.99	0.07	41,41,41,41	0
56	MG	2A	3197	1/1	0.99	0.03	54,54,54,54	0
56	MG	1a	1792	1/1	0.99	0.07	49,49,49,49	0
56	MG	1A	3640	1/1	0.99	0.06	27,27,27,27	0
56	MG	2A	3837	1/1	0.99	0.07	46,46,46,46	0
56	MG	2A	3605	1/1	0.99	0.04	44,44,44,44	0
56	MG	2A	3839	1/1	0.99	0.03	56,56,56,56	0
56	MG	1F	303	1/1	0.99	0.11	34,34,34,34	0
56	MG	2A	3070	1/1	0.99	0.07	33,33,33,33	0
56	MG	1A	3057	1/1	0.99	0.09	21,21,21,21	0
56	MG	1a	1797	1/1	0.99	0.04	60,60,60,60	0
56	MG	1A	3070	1/1	0.99	0.09	20,20,20,20	0
56	MG	1A	3622	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3842	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	4038	1/1	0.99	0.02	42,42,42,42	0
56	MG	1A	3994	1/1	0.99	0.06	26,26,26,26	0
56	MG	2A	3849	1/1	0.99	0.05	35,35,35,35	0
56	MG	2A	3473	1/1	0.99	0.13	31,31,31,31	0
56	MG	2A	3013	1/1	0.99	0.05	51,51,51,51	0
56	MG	1a	1803	1/1	0.99	0.03	62,62,62,62	0
56	MG	2A	3853	1/1	0.99	0.07	66,66,66,66	0
56	MG	1A	3138	1/1	0.99	0.09	37,37,37,37	0
56	MG	1a	1742	1/1	0.99	0.07	40,40,40,40	0
56	MG	1A	3690	1/1	0.99	0.08	26,26,26,26	0
56	MG	1A	3915	1/1	0.99	0.09	38,38,38,38	0
56	MG	1a	1808	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3266	1/1	0.99	0.08	41,41,41,41	0
56	MG	2A	3021	1/1	0.99	0.07	30,30,30,30	0
56	MG	1U	211	1/1	0.99	0.21	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	2A	3552	1/1	0.99	0.07	59,59,59,59	0
56	MG	1A	3037	1/1	0.99	0.08	35,35,35,35	0
56	MG	1A	3107	1/1	0.99	0.31	34,34,34,34	0
56	MG	1A	3813	1/1	0.99	0.05	32,32,32,32	0
56	MG	1V	203	1/1	0.99	0.10	33,33,33,33	0
56	MG	1A	3920	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3921	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3383	1/1	0.99	0.17	28,28,28,28	0
56	MG	2A	3560	1/1	0.99	0.12	44,44,44,44	0
56	MG	1A	3781	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3782	1/1	0.99	0.04	46,46,46,46	0
56	MG	1a	1756	1/1	0.99	0.08	61,61,61,61	0
56	MG	1A	4007	1/1	0.99	0.10	24,24,24,24	0
56	MG	1A	3695	1/1	0.99	0.07	30,30,30,30	0
56	MG	1A	3926	1/1	0.99	0.03	37,37,37,37	0
56	MG	1W	205	1/1	0.99	0.06	39,39,39,39	0
56	MG	1A	3610	1/1	0.99	0.06	27,27,27,27	0
56	MG	1A	3785	1/1	0.99	0.04	28,28,28,28	0
56	MG	2A	3644	1/1	0.99	0.09	43,43,43,43	0
56	MG	1X	101	1/1	0.99	0.26	44,44,44,44	0
56	MG	1A	3038	1/1	0.99	0.21	33,33,33,33	0
56	MG	2A	3721	1/1	0.99	0.04	38,38,38,38	0
56	MG	2a	3170	1/1	0.99	0.04	59,59,59,59	0
56	MG	1A	3014	1/1	0.99	0.15	30,30,30,30	0
56	MG	1A	3563	1/1	0.99	0.13	37,37,37,37	0
56	MG	1A	3428	1/1	0.99	0.19	36,36,36,36	0
56	MG	1a	1712	1/1	0.99	0.11	54,54,54,54	0
56	MG	2A	3576	1/1	0.99	0.06	40,40,40,40	0
56	MG	1X	106	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	3701	1/1	0.99	0.07	29,29,29,29	0
56	MG	2A	3729	1/1	0.99	0.03	61,61,61,61	0
56	MG	1A	4017	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3729	1/1	0.99	0.06	27,27,27,27	0
56	MG	1A	3282	1/1	0.99	0.22	36,36,36,36	0
56	MG	1A	3676	1/1	0.99	0.09	34,34,34,34	0
56	MG	1A	3937	1/1	0.99	0.03	13,13,13,13	0
56	MG	2A	3735	1/1	0.99	0.05	45,45,45,45	0
56	MG	1A	3634	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3678	1/1	0.99	0.03	45,45,45,45	0
56	MG	1a	1778	1/1	0.99	0.05	59,59,59,59	0
56	MG	1A	3031	1/1	0.99	0.14	32,32,32,32	0
56	MG	1A	3036	1/1	0.99	0.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3297	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3172	1/1	0.99	0.06	34,34,34,34	0
56	MG	1A	4073	1/1	0.99	0.10	35,35,35,35	0
56	MG	1E	313	1/1	0.99	0.09	30,30,30,30	0
56	MG	1A	3738	1/1	0.99	0.08	33,33,33,33	0
56	MG	1A	3768	1/1	0.99	0.07	39,39,39,39	0
56	MG	2A	3747	1/1	0.99	0.07	53,53,53,53	0
56	MG	1A	3683	1/1	0.99	0.04	33,33,33,33	0
59	ZN	1Y	204	1/1	0.99	0.03	65,65,65,65	0
59	ZN	14	501	1/1	0.99	0.04	87,87,87,87	0
59	ZN	15	108	1/1	0.99	0.05	45,45,45,45	0
59	ZN	16	103	1/1	0.99	0.04	44,44,44,44	0
59	ZN	1n	103	1/1	0.99	0.03	69,69,69,69	0
56	MG	1a	1789	1/1	0.99	0.06	59,59,59,59	0
56	MG	1A	3639	1/1	0.99	0.05	34,34,34,34	0
59	ZN	25	105	1/1	0.99	0.03	53,53,53,53	0
59	ZN	26	102	1/1	0.99	0.04	62,62,62,62	0
56	MG	2A	3829	1/1	0.99	0.15	55,55,55,55	0
56	MG	2A	3830	1/1	0.99	0.06	39,39,39,39	0
56	MG	2A	3598	1/1	0.99	0.08	53,53,53,53	0
60	SF4	2d	303	8/8	0.99	0.04	67,73,82,85	0
56	MG	1A	4037	1/1	1.00	0.03	28,28,28,28	0
56	MG	1A	3940	1/1	1.00	0.05	30,30,30,30	0
59	ZN	19	102	1/1	1.00	0.04	44,44,44,44	0
56	MG	1a	1795	1/1	1.00	0.05	55,55,55,55	0
56	MG	2A	3604	1/1	1.00	0.03	43,43,43,43	0
56	MG	1a	1783	1/1	1.00	0.02	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.