



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:31 PM UTC

PDB ID : 5J4B / pdb_00005j4b
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with cisplatin (co-crystallized) and bound to mRNA and A-, P- and E-site tRNAs at 2.6Å resolution
Authors : Melnikov, S.V.; Soll, D.; Steitz, T.A.; Polikanov, Y.S.
Deposited on : 2016-03-31
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

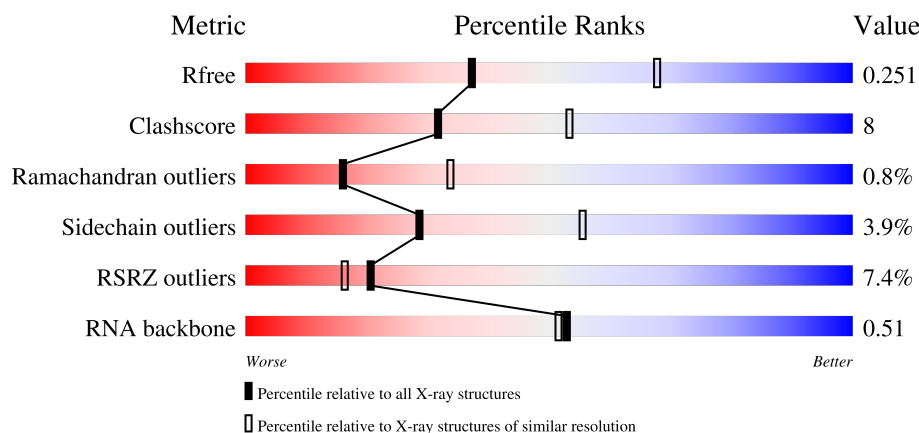
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	6% 67% 25% 7%
1	2A	2915	3% 57% 32% 7%
2	1B	121	76% 21%

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Mol	Chain	Length	Quality of chain
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	
14	2S	112	

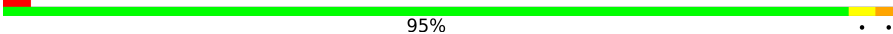
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25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

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Mol	Chain	Length	Quality of chain
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	
39	2h	138	

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Mol	Chain	Length	Quality of chain
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	
52	1u	27	

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Mol	Chain	Length	Quality of chain
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	17	102	-	-	-	X
56	MG	1A	3385	-	-	-	X
56	MG	1a	1691	-	-	-	X
56	MG	1a	1725	-	-	-	X
56	MG	1a	1747	-	-	-	X
56	MG	1a	1755	-	-	-	X
56	MG	2a	1673	-	-	-	X
56	MG	2a	1849	-	-	-	X
56	MG	2x	101	-	-	-	X
56	MG	2x	102	-	-	-	X
58	CPT	1A	4179	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 301328 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	1	0
			61875	27541	11577	19885	2872			
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	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1220	Total	Mg	0	0
			1220	1220		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	11	Total	Mg	0	0
			11	11		
56	1F	7	Total	Mg	0	0
			7	7		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1O	6	Total 6	Mg 6	0	0
56	1P	3	Total 3	Mg 3	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	8	Total 8	Mg 8	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	4	Total 4	Mg 4	0	0
56	1X	5	Total 5	Mg 5	0	0
56	1Y	4	Total 4	Mg 4	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	10	6	Total 6	Mg 6	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	2	Total 2	Mg 2	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	2	Total 2	Mg 2	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	4	Total 4	Mg 4	0	0
56	18	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	19	2	Total 2	Mg 2	0	0
56	1a	284	Total 284	Mg 284	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1n	3	Total 3	Mg 3	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	11	Total 11	Mg 11	0	0
56	1x	18	Total 18	Mg 18	0	0
56	1y	5	Total 5	Mg 5	0	0
56	2A	937	Total 937	Mg 937	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	5	Total 5	Mg 5	0	0
56	2E	9	Total 9	Mg 9	0	0
56	2F	7	Total 7	Mg 7	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2P	3	Total 3	Mg 3	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	3	Total 3	Mg 3	0	0
56	2S	1	Total 1	Mg 1	0	0
56	2T	2	Total 2	Mg 2	0	0
56	2U	3	Total 3	Mg 3	0	0
56	2V	1	Total 1	Mg 1	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	2	Total 2	Mg 2	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2a	256	Total 256	Mg 256	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0

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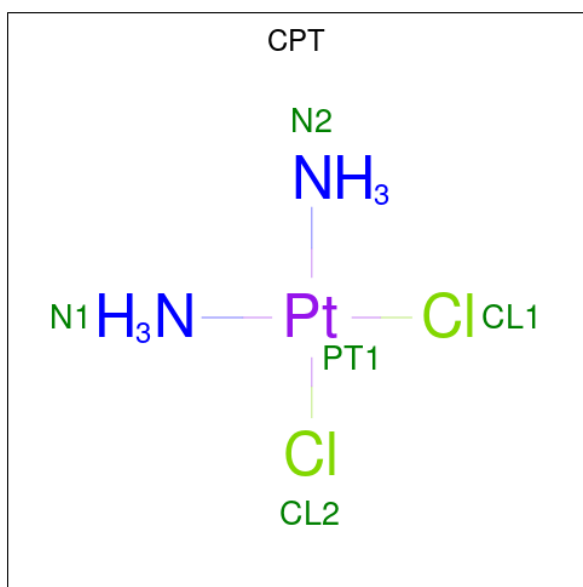
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2l	3	Total 3	Mg 3	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	4	Total 4	Mg 4	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	4	Total 4	Mg 4	0	0
56	2w	8	Total 8	Mg 8	0	0
56	2x	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	2A	1	Total 1	K 1	0	0

- Molecule 58 is Cisplatin (CCD ID: CPT) (formula: Cl₂H₆N₂Pt).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1A	1	Total	N	Pt		0	0
			3	2	1			
58	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2A	1	Total	N	Pt		0	0
			3	2	1			

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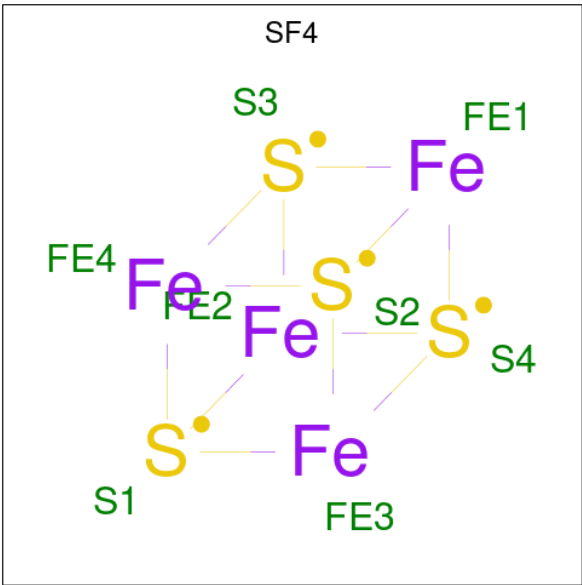
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
58	2I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		

- 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		
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: Fe₄S₄).



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	2299	Total	O	0	0
			2299	2299		
61	1B	68	Total	O	0	0
			68	68		
61	1D	29	Total	O	0	0
			29	29		
61	1E	30	Total	O	0	0
			30	30		
61	1F	17	Total	O	0	0
			17	17		
61	1G	8	Total	O	0	0
			8	8		
61	1H	1	Total	O	0	0
			1	1		
61	1I	2	Total	O	0	0
			2	2		
61	1N	5	Total	O	0	0
			5	5		
61	1O	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1P	21	Total 21	O 21	0	0
61	1Q	13	Total 13	O 13	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	14	Total 14	O 14	0	0
61	1V	12	Total 12	O 12	0	0
61	1W	7	Total 7	O 7	0	0
61	1X	8	Total 8	O 8	0	0
61	1Y	9	Total 9	O 9	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	11	Total 11	O 11	0	0
61	12	4	Total 4	O 4	0	0
61	13	5	Total 5	O 5	0	0
61	14	1	Total 1	O 1	0	0
61	15	6	Total 6	O 6	0	0
61	16	3	Total 3	O 3	0	0
61	17	10	Total 10	O 10	0	0
61	18	11	Total 11	O 11	0	0
61	1a	516	Total 516	O 516	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1b	1	Total 1	O 1	0	0
61	1c	1	Total 1	O 1	0	0
61	1d	3	Total 3	O 3	0	0
61	1e	2	Total 2	O 2	0	0
61	1g	2	Total 2	O 2	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	8	Total 8	O 8	0	0
61	1m	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	21	Total 21	O 21	0	0
61	1x	14	Total 14	O 14	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	1402	Total 1402	O 1402	0	0
61	2B	27	Total 27	O 27	0	0
61	2D	26	Total 26	O 26	0	0
61	2E	17	Total 17	O 17	0	0
61	2F	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2I	4	Total 4	O 4	0	0
61	2N	3	Total 3	O 3	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	15	Total 15	O 15	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	6	Total 6	O 6	0	0
61	21	12	Total 12	O 12	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	3	Total 3	O 3	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0

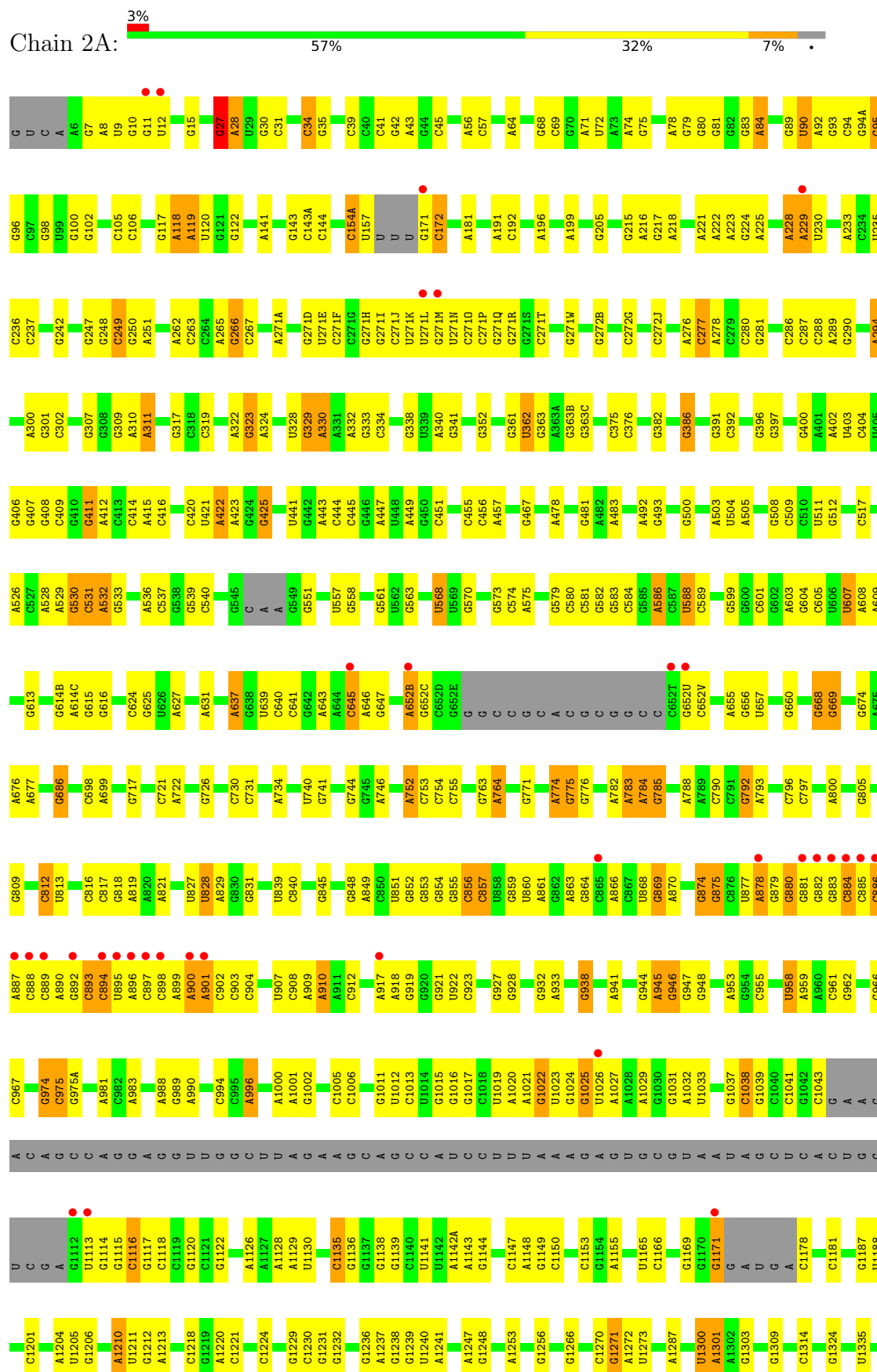
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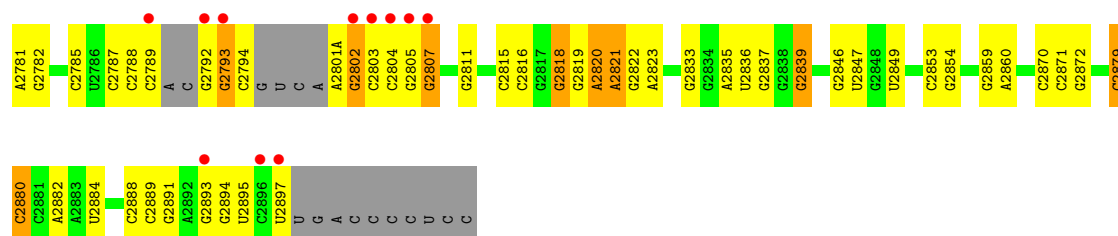
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	380	Total 380	O 380	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2f	1	Total 1	O 1	0	0
61	2g	2	Total 2	O 2	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	7	Total 7	O 7	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2u	2	Total 2	O 2	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	7	Total 7	O 7	0	0
61	2y	20	Total 20	O 20	0	0

G2849	A2746	A2602	A2447	C2328	C2226	A2157	G2054	U1939	A1817	U1648	A1540	G1401	A1222
G2856	A2747	C2603	G2448	G2331	G2227	C2158	A2055	C1942	A1822	A1649	A1541	G1402	C1223
U2857	C2756	G2604	A2451	A2332	A2228	C2159	C2061	G1951	U1827	C1650	U1543	A1405	C1224
U2858	G2757	A2614	C2452	A2337	G2229	C2160	G2065	G1952	C1828	G1652	C1544	A1406	G1232
U2859	G2760	G2615	C2453	C2338	G2230	C2162	C2066	U1953	U1829	A1654	C1545	G1410	C1246
A2870	G2764	U2616	G2459	A2339	G2231	G2163	G2071	A1954	G1830	A1655	G1546	A1411	C1247
G2874	G2768	U2617	A2460	G2340	G2232	C2164	G2077	G1955	G1831	C1656	C1547	U1418	G1248
G2877	G2769	G2620	C2476	G2342	G2233	C2166	C2077	A1959	G1832	C1552	C1553	U1250	U1249
A2878	A2770	U2621	G2480	G2343	G2234	C2167	G2078	A1960	A1833	G1680	A1554	A1425	A1255
G2879	A2771	C2622	A2481	G2344	A2237	G2168	A2081	U1961	A1834	A1688	C1555	G1426	A1256
C2880	A2777	U2623	G2482	G2345	C2238	G2170	A2082	G1964	G1842	G1689	A1556	A1430	U1257
C2881	A2778	C2624	A2483	A2347	U2245	G2171	G2083	C1968	G1845	G1694	U1560	G1431	A1258
G2882	G2779	G2625	A2484	A2348	G2246	G2172	A2084	U1977	A1860	C1695	C1561	C1432	U1259
C2889	G2790	A2641	C2496	G2353	G2250	G2173	G2091	G1969	G1847	U1701	U1562	C1433	C1263
C2890	A2791	C2642	C2497	G2354	G2251	G2174	G2092	A1974	G1848	G1721	G1563	U1442	G1282
C2891	G2792	C2658	A2488	C2359	U2255	G2175	U2108	A1975	G1849	U1735	A1575	G1462	G1289
C2892	G2793	U2659	C2489	G2362	U2256	G2176	G2109	G1976	A1877	U1740	C1579	C1463	A1299
U2897	G2798	C2660	A2490	A2363	U2257	G2177	U2121	G1987	A1878	G1743	G	G1464	G1302
C2898	C2799	U2661	U2504	G2364	G2263	G2178	U2122	C1988	U1879	U1747	U	A1465	G1310
C2899	U2799	U2662	U2505	A2367	C2266	G2179	U2123	C1989	U1880	A1767	A	U1466	A1311
G2900	C2800	A2666	C2510	C2367	C2286	G2180	U2124	G1990	U1882	G1770	C	G1467	G1312
G2901	C2801	A2691	C2511	A2373	A2280	G2181	U2125	C1991	C1883	A1748	G1584	A1473	U1319
G2902	G2802	C2695	G2514	C2376	A2281	G2182	U2126	C1992	U1887	G1749	U	C1474	A1314
G2903	U2803	U2697	A2515	G2377	G2282	G2183	U2127	A1993	C1889	U1768	A1589	C1475	U1338
U2904	C2804	C2698	U2516	G2378	G2283	G2184	C2127	A1994	U1891	G1769	C1590	C1476	G1317
C2905	G2805	U2699	U2517	A2380	A2286	G2185	U2128	U2013	U1892	A1491	A1491	A1318	A1318
U2906	G2806	U2700	U2518	G2389	G2287	G2186	U2129	G2014	C1893	G1776	C1593	U1319	A1320
U	C	A	A2530	C2395	A2290	G2187	U2130	U2015	U1894	G1776	A1605	U1338	U1339
G	U	C	G2541	C2396	G2291	G2188	U2131	G2018	A1899	G1781	A1613	A1500	C1343
A	U	C	A2545	C2397	G2292	G2189	U2132	C2019	U1899	G1787	U1601	U1502	U1346
C	U	C	G2546	G2408	C2295	U2190	U2133	G2018	A1900	A1793	A1617	A1507	A1347
C	U	C	G2547	U2418	C2296	G2191	U2134	C2019	G1896	G1794	A1618	A1516	A1348
C	U	C	G2561	G2419	C2297	G2192	U2135	A2023	U1897	G1795	U1625	G1513	G1349
C	U	C	G2562	G2421	A2298	G2193	U2136	G2024	C1898	A1804	A1626	C1514	G1378
C	U	C	C2563	A2429	A2299	G2194	U2137	G2034	G1905	A1793	A1627	C1515	G1378
C	U	C	U2564	C2430	G2303	G2195	U2138	A2035	A1911	G1794	A1618	A1516	A1388
C	U	C	U2566	A2434	C2304	G2196	U2139	A2036	C1915	G1795	U1625	G1513	A1348
C	U	C	A2576	A2437	G2315	G2197	U2140	A2041	G1921	A1804	A1626	C1514	G1349
C	U	C	A2577	A2438	G2316	G2198	U2141	A2042	A1922	A1809	A1627	C1515	G1378
C	U	C	A2578	A2439	G2317	G2199	U2142	C2043	A1922	U1809	A1627	C1515	G1378
C	U	C	G2579	A2440	A2318	G2200	U2143	G2044	A1911	U1810	A1618	A1516	A1388
C	U	C	G2580	A2441	G2319	G2201	U2144	G2045	C1928	A1811	C1631	G1529	C1391
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• Molecule 1: 23S ribosomal RNA

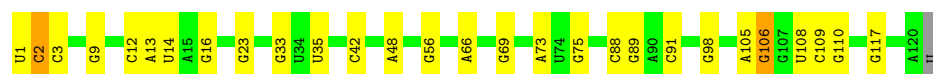


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628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642



- Molecule 2: 5S ribosomal RNA

Chain 1B: 76% 21% ..



- Molecule 2: 5S ribosomal RNA

Chain 2B: 2% 45% 46% 7% .



- Molecule 3: 50S ribosomal protein L2

Chain 1D: 2% 80% 18% .



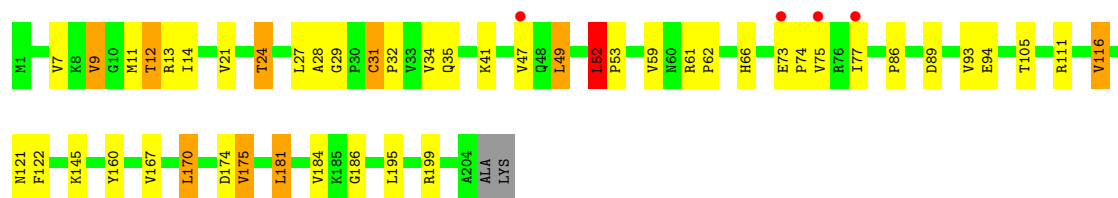
- Molecule 3: 50S ribosomal protein L2

Chain 2D: 81% 18%

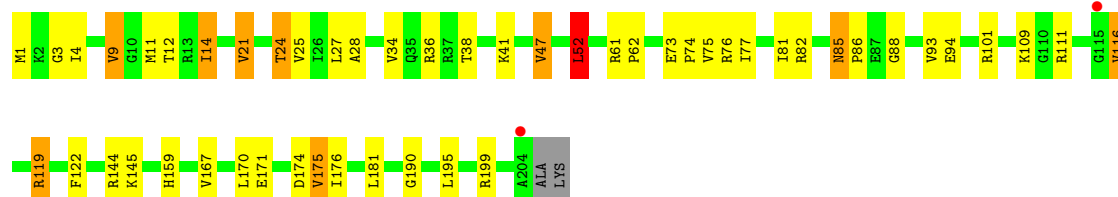
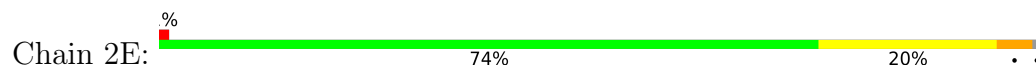


- Molecule 4: 50S ribosomal protein L3

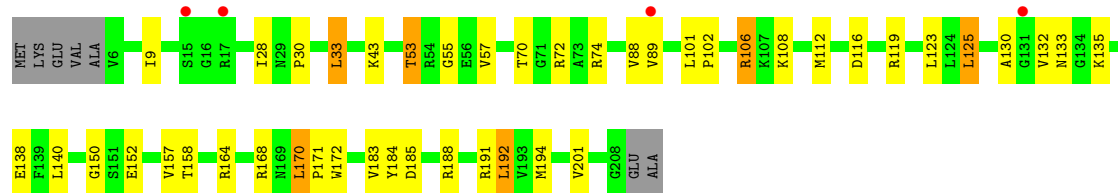
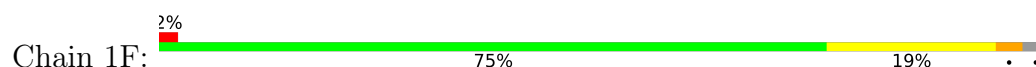
Chain 1E: 2% 76% 18% ..



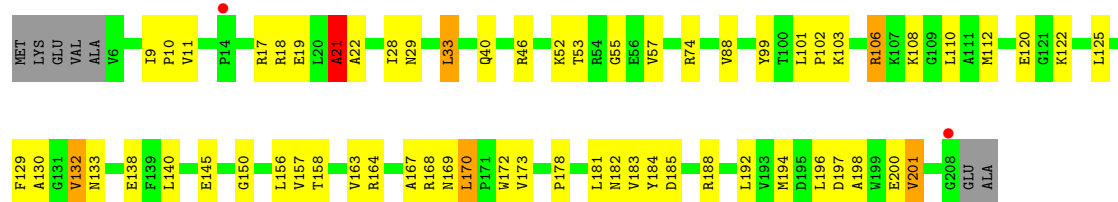
• Molecule 4: 50S ribosomal protein L3



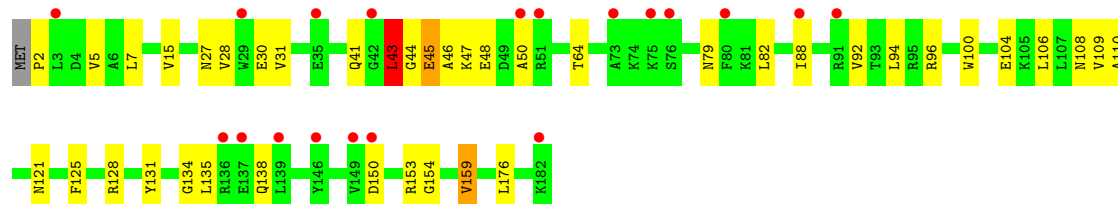
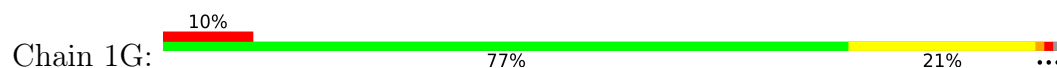
• Molecule 5: 50S ribosomal protein L4



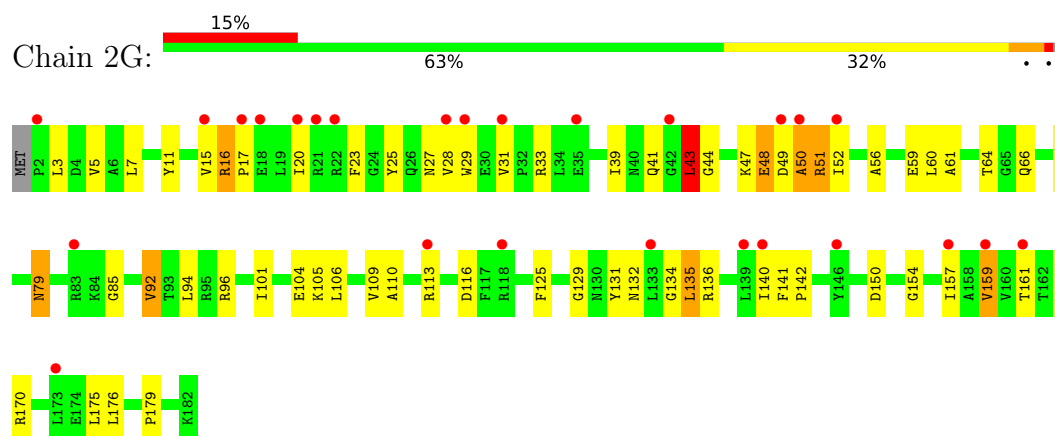
• Molecule 5: 50S ribosomal protein L4



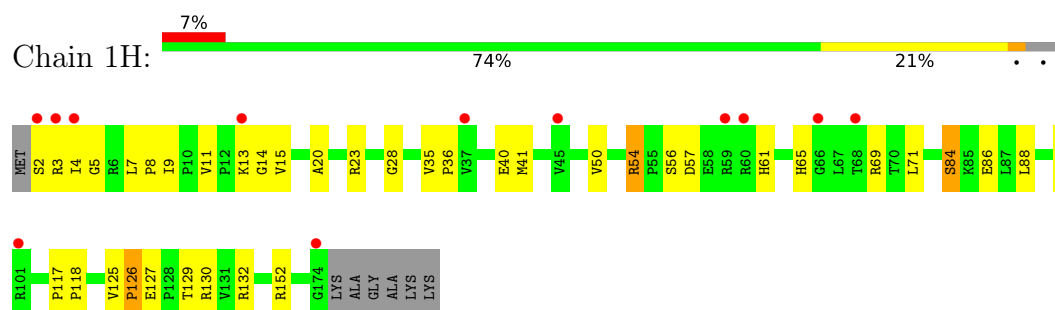
• Molecule 6: 50S ribosomal protein L5



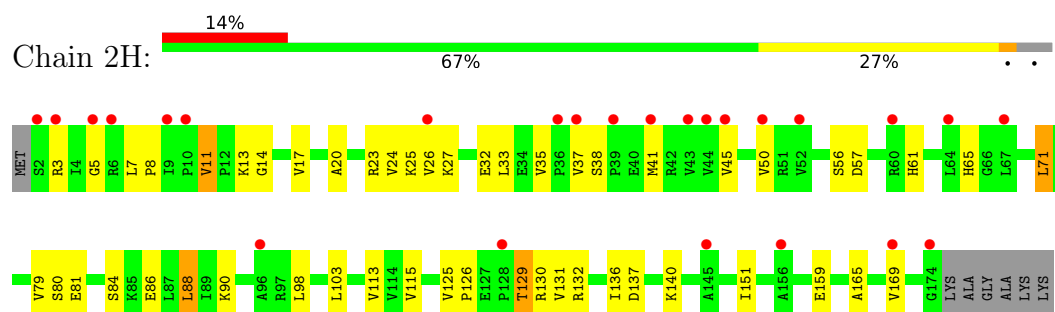
- Molecule 6: 50S ribosomal protein L5



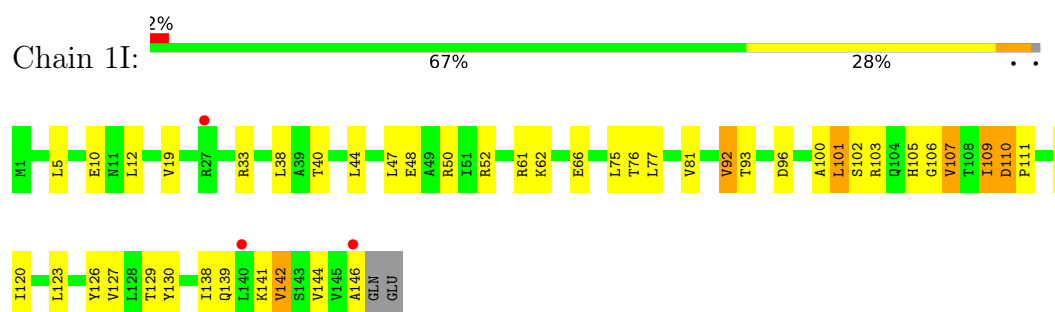
- Molecule 7: 50S ribosomal protein L6



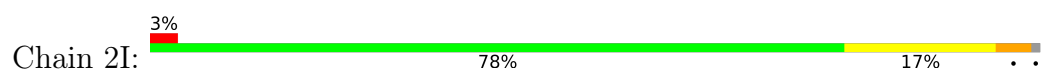
- Molecule 7: 50S ribosomal protein L6

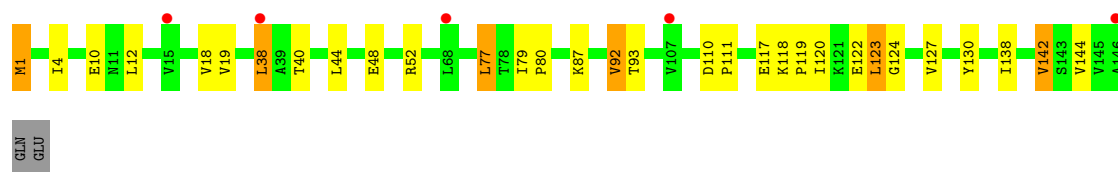


- Molecule 8: 50S ribosomal protein L9

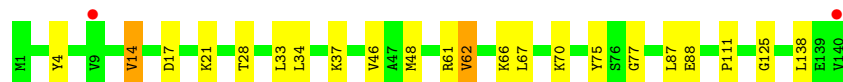
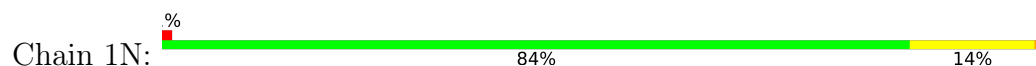


- Molecule 8: 50S ribosomal protein L9

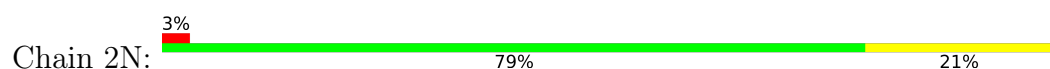




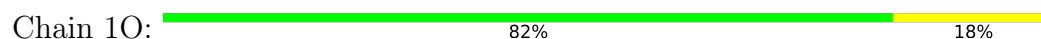
- Molecule 9: 50S ribosomal protein L13



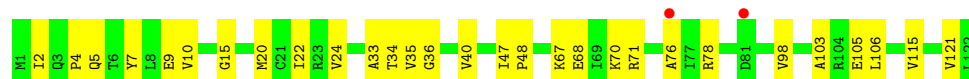
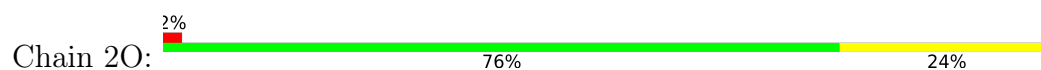
- Molecule 9: 50S ribosomal protein L13



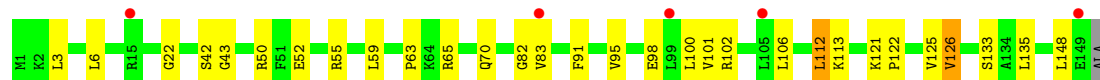
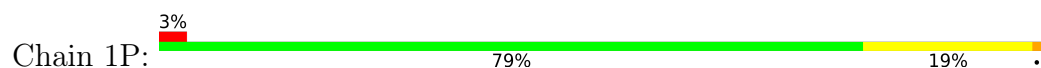
- Molecule 10: 50S ribosomal protein L14



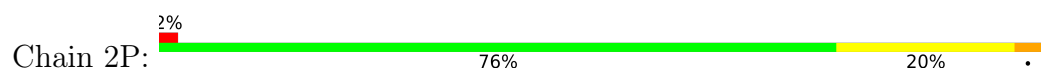
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

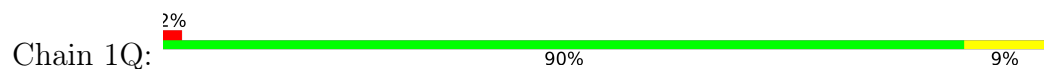


- Molecule 11: 50S ribosomal protein L15

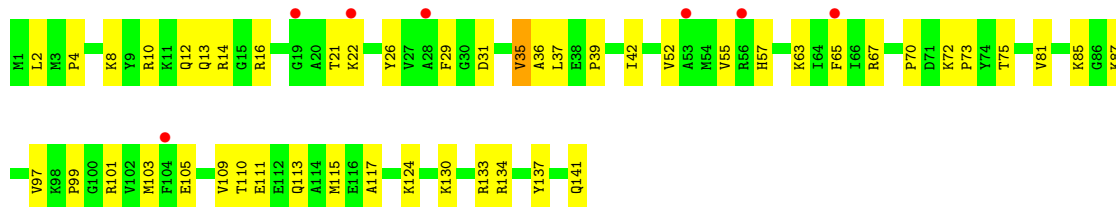




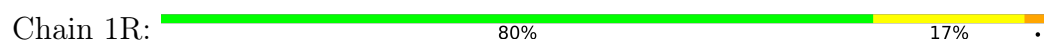
- Molecule 12: 50S ribosomal protein L16



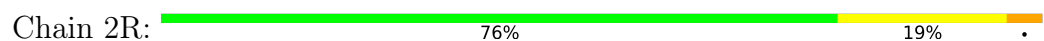
- Molecule 12: 50S ribosomal protein L16



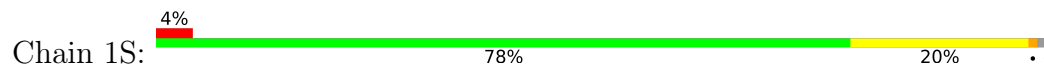
- Molecule 13: 50S ribosomal protein L17



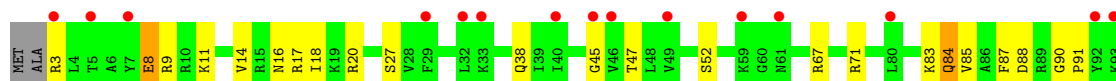
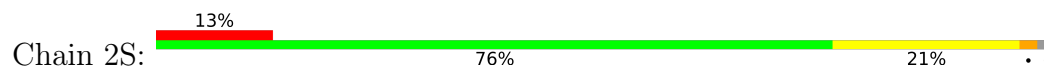
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

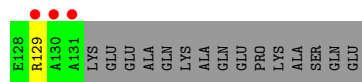


- Molecule 14: 50S ribosomal protein L18

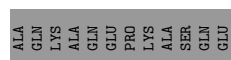
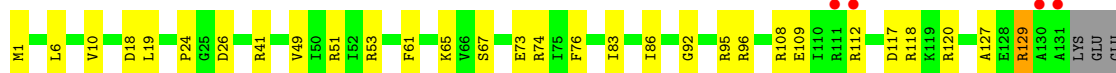




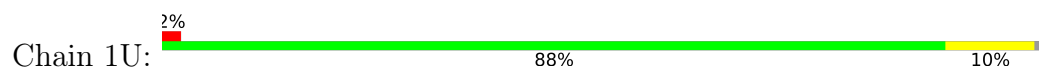
- Molecule 15: 50S ribosomal protein L19



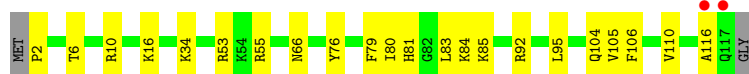
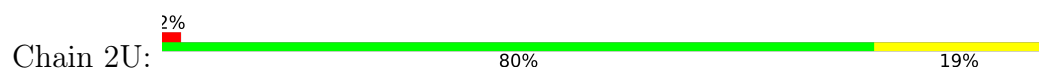
- Molecule 15: 50S ribosomal protein L19



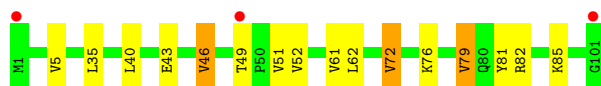
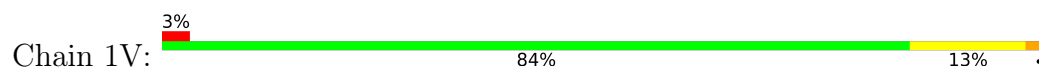
- Molecule 16: 50S ribosomal protein L20



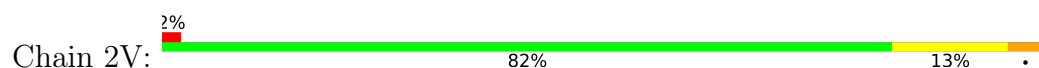
- Molecule 16: 50S ribosomal protein L20

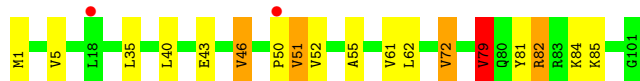


- Molecule 17: 50S ribosomal protein L21

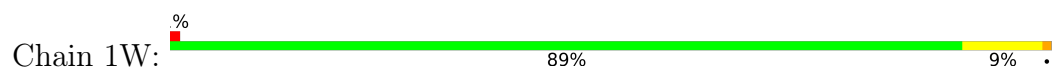


- Molecule 17: 50S ribosomal protein L21

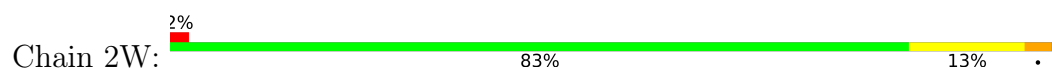




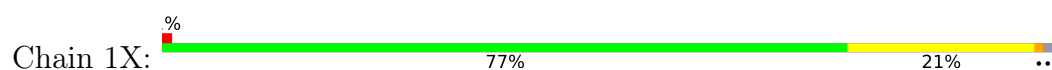
- Molecule 18: 50S ribosomal protein L22



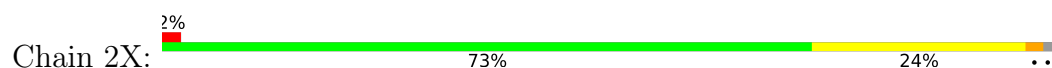
- Molecule 18: 50S ribosomal protein L22



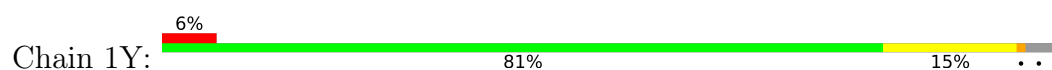
- Molecule 19: 50S ribosomal protein L23



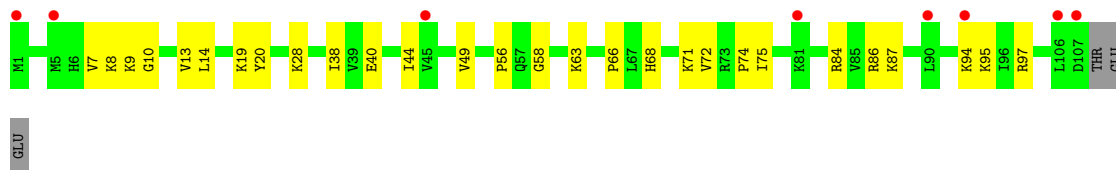
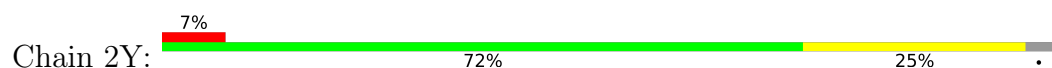
- Molecule 19: 50S ribosomal protein L23



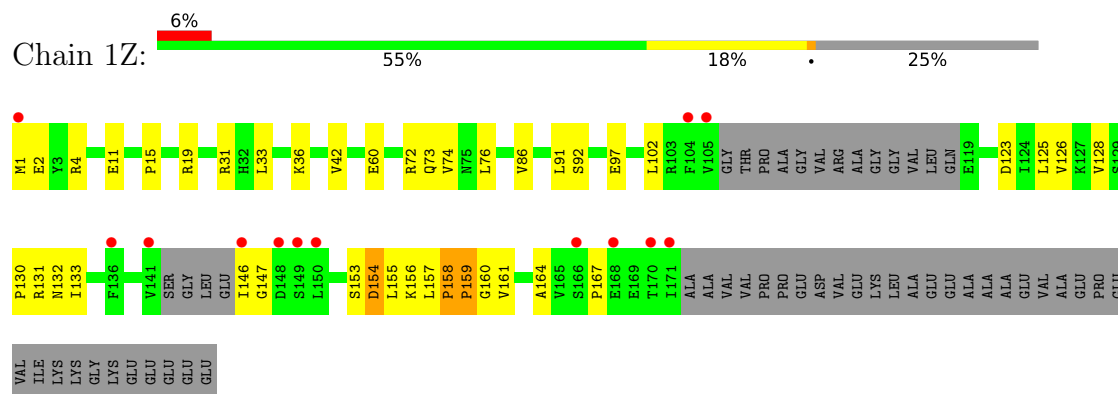
- Molecule 20: 50S ribosomal protein L24



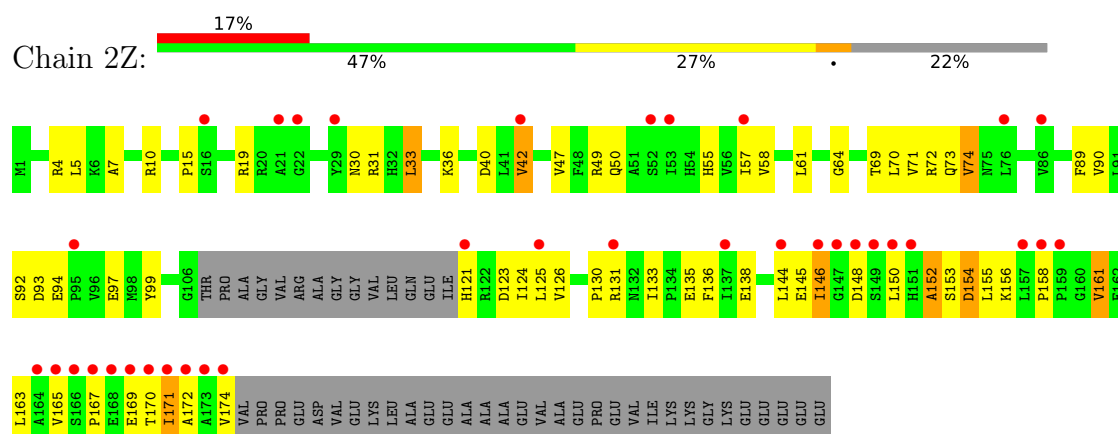
- Molecule 20: 50S ribosomal protein L24



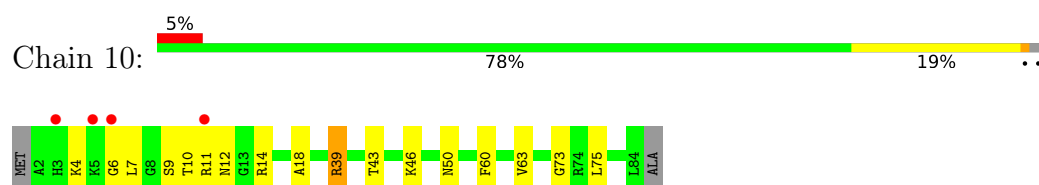
- Molecule 21: 50S ribosomal protein L25



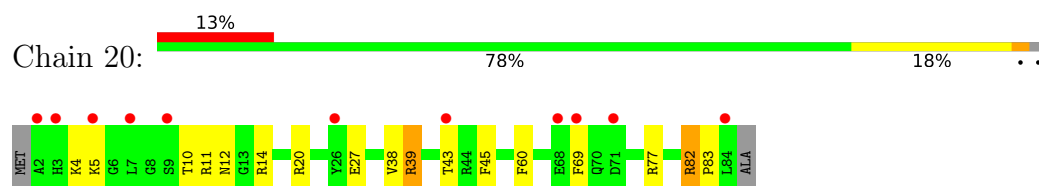
- Molecule 21: 50S ribosomal protein L25



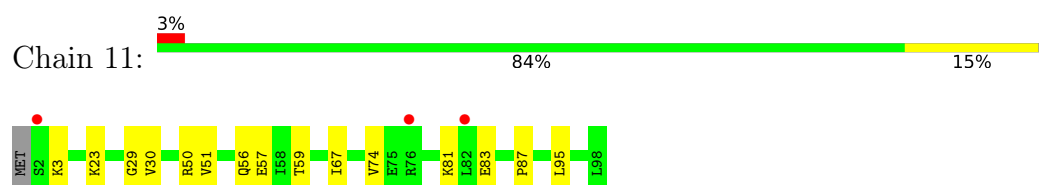
- Molecule 22: 50S ribosomal protein L27



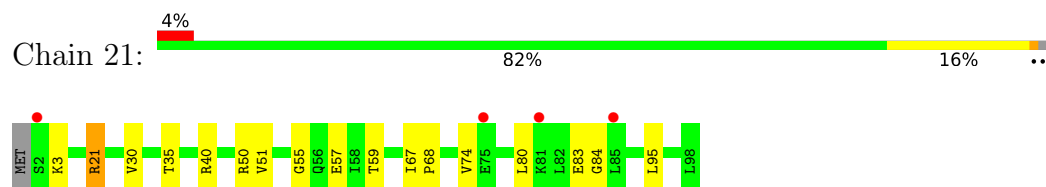
- Molecule 22: 50S ribosomal protein L27



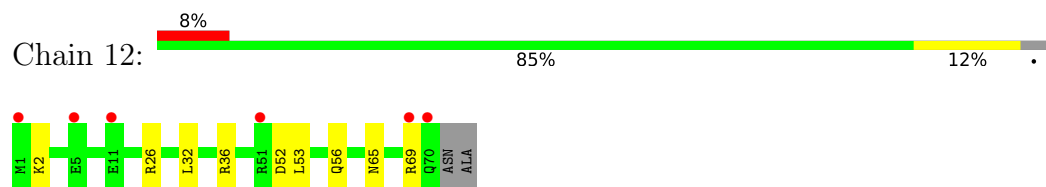
- Molecule 23: 50S ribosomal protein L28



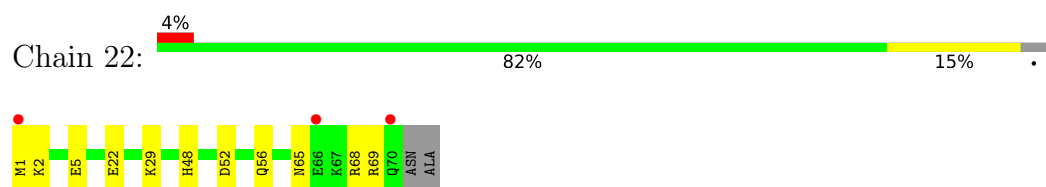
- Molecule 23: 50S ribosomal protein L28



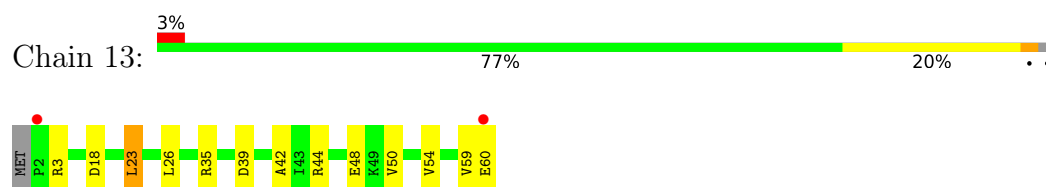
- Molecule 24: 50S ribosomal protein L29



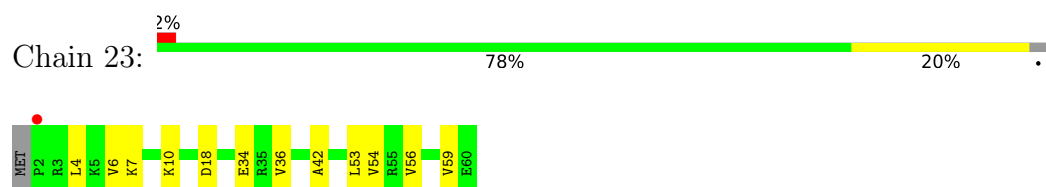
- Molecule 24: 50S ribosomal protein L29



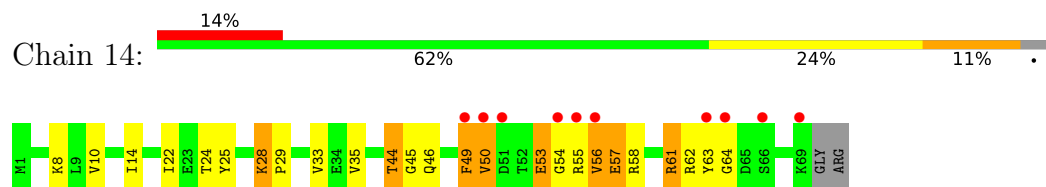
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31

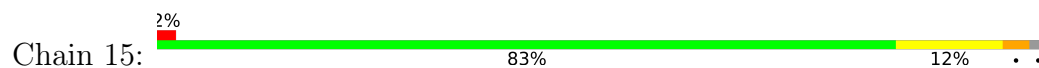


- Molecule 26: 50S ribosomal protein L31

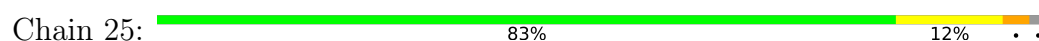




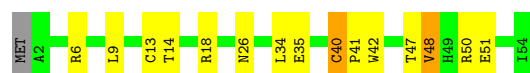
- Molecule 27: 50S ribosomal protein L32



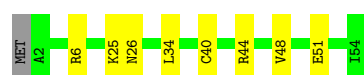
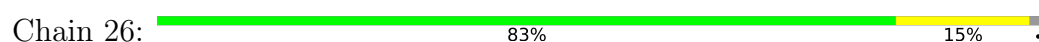
- Molecule 27: 50S ribosomal protein L32



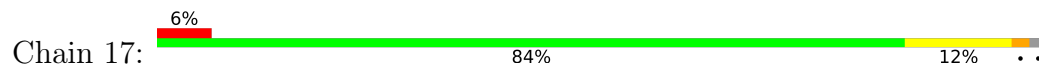
- Molecule 28: 50S ribosomal protein L33



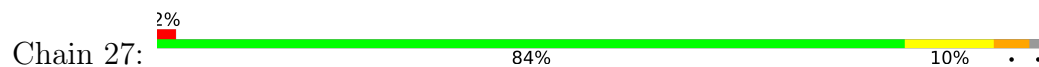
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



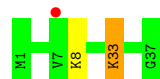
- Molecule 30: 50S ribosomal protein L35



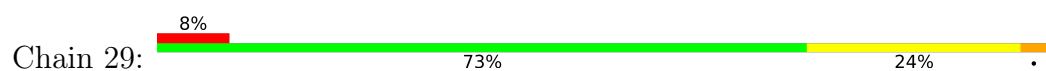
- Molecule 30: 50S ribosomal protein L35



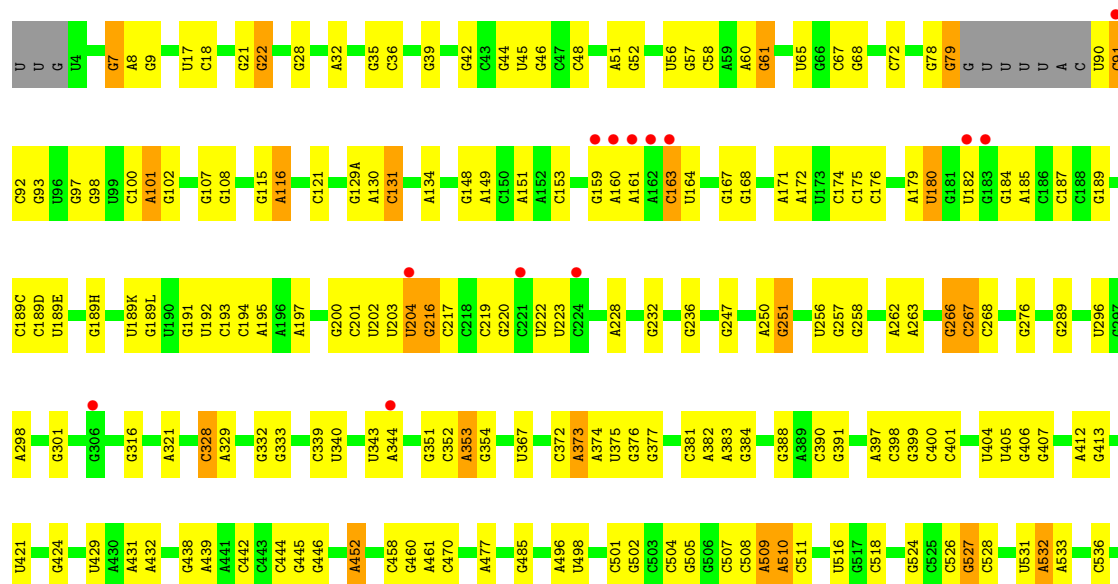
- Molecule 31: 50S ribosomal protein L36

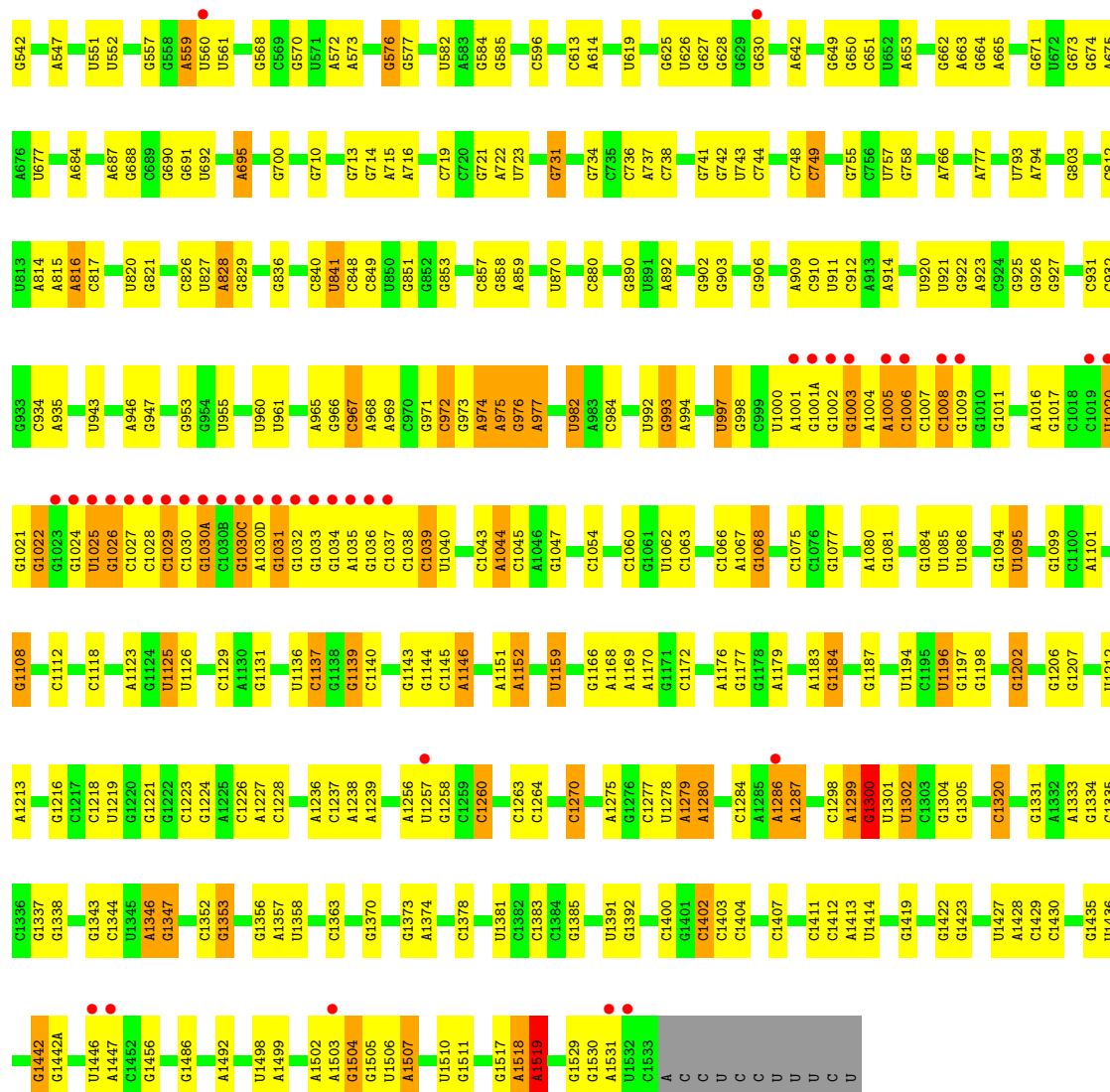


- Molecule 31: 50S ribosomal protein L36

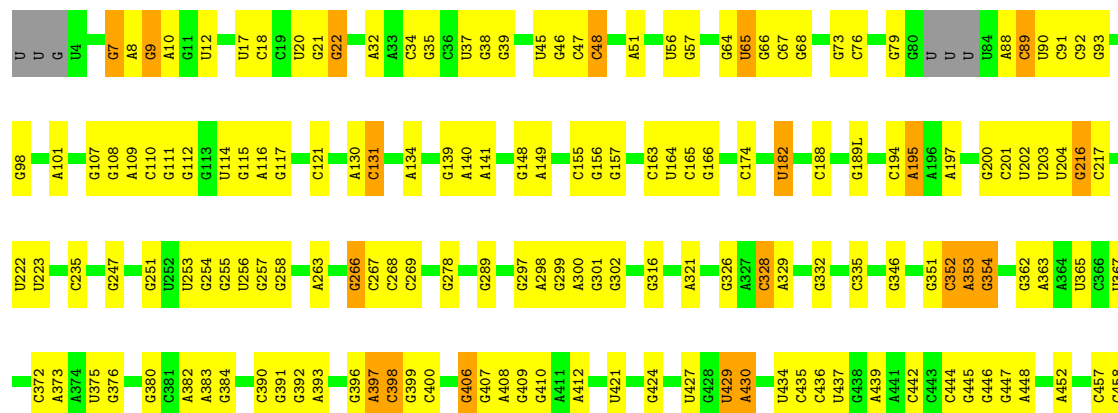


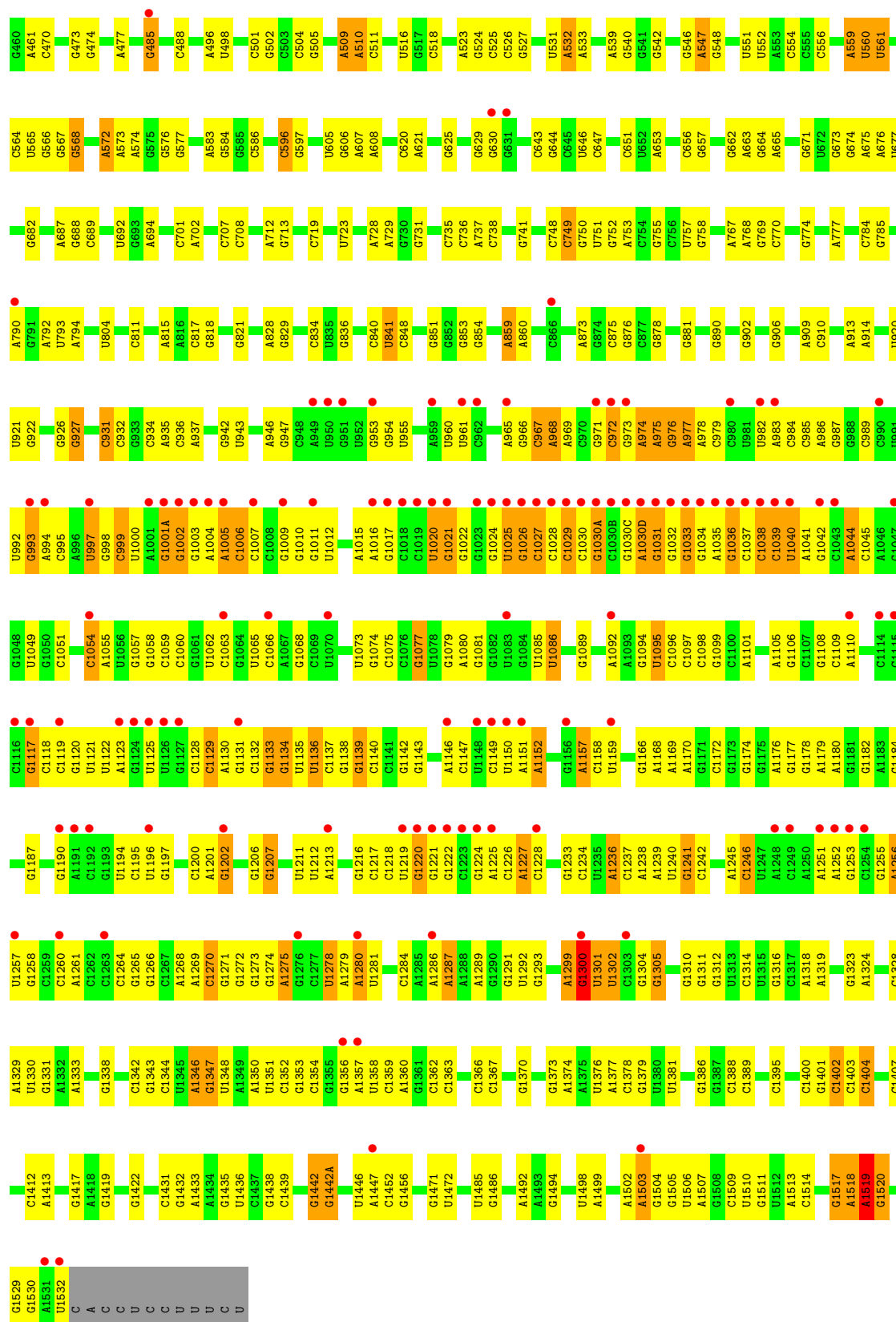
- Molecule 32: 16S ribosomal RNA

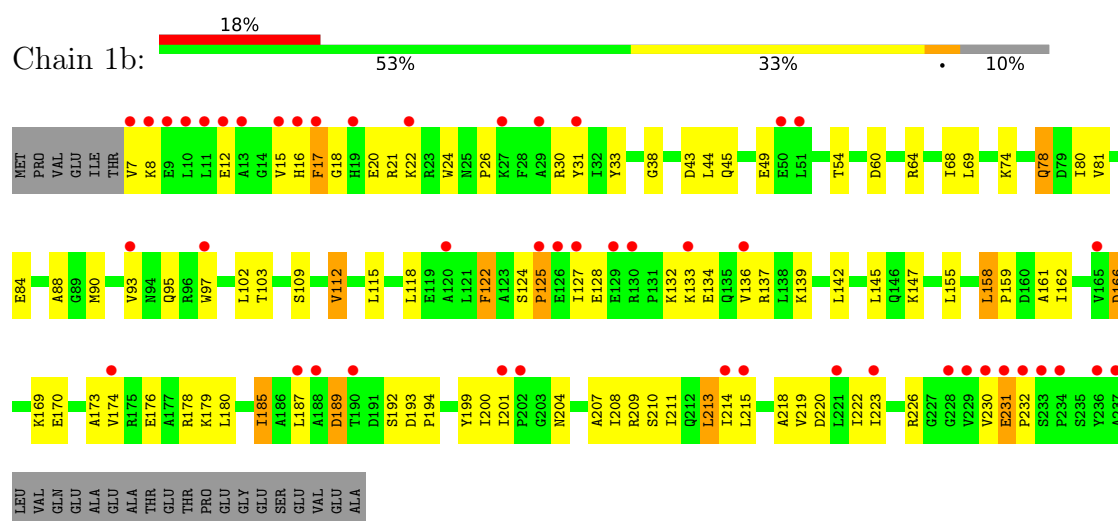




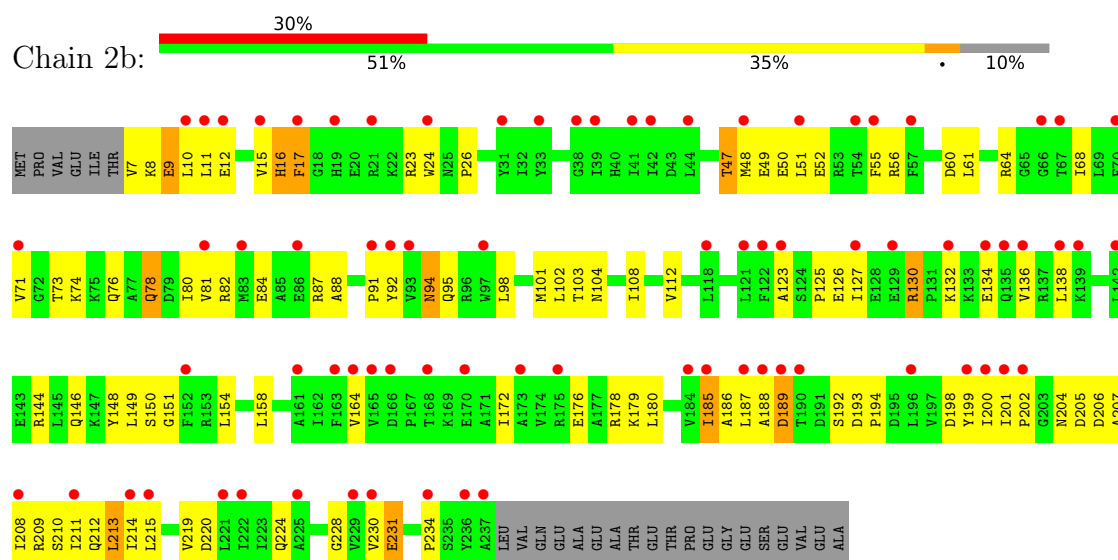
• Molecule 32: 16S ribosomal RNA



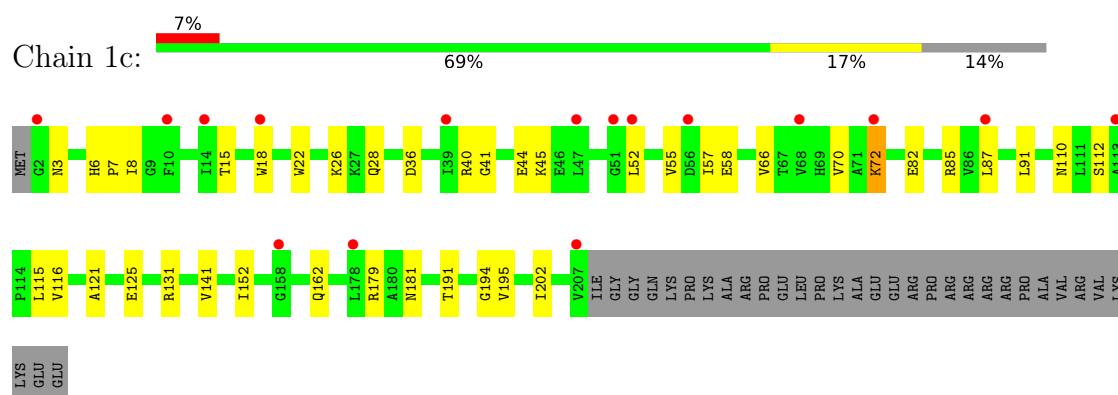




• Molecule 33: 30S ribosomal protein S2

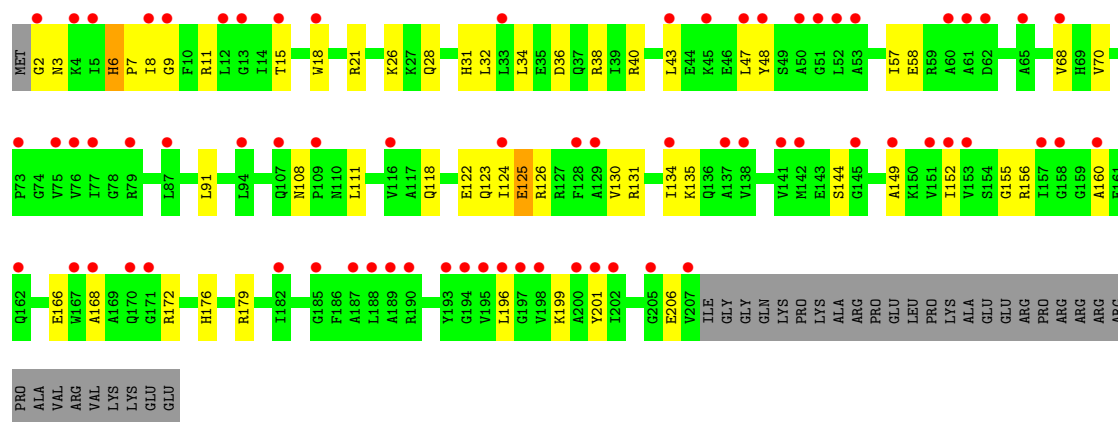


• Molecule 34: 30S ribosomal protein S3

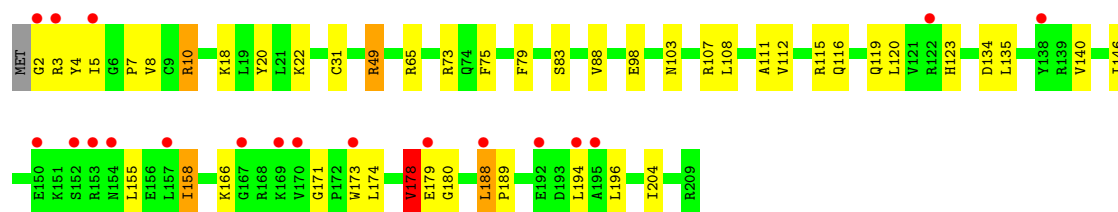
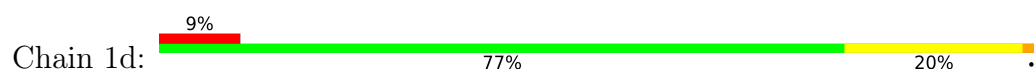


• Molecule 34: 30S ribosomal protein S3

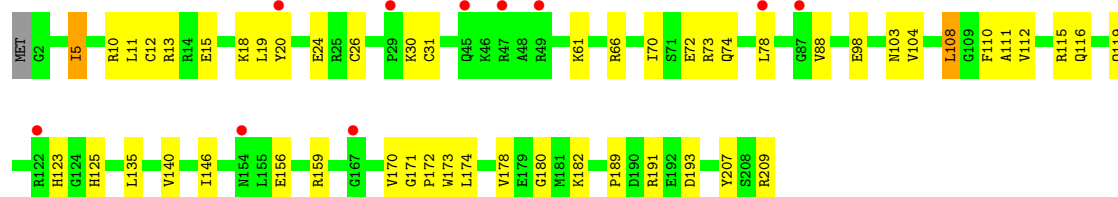
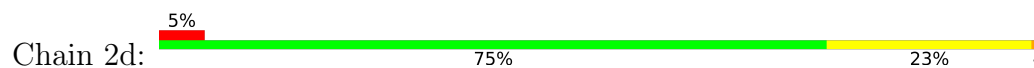




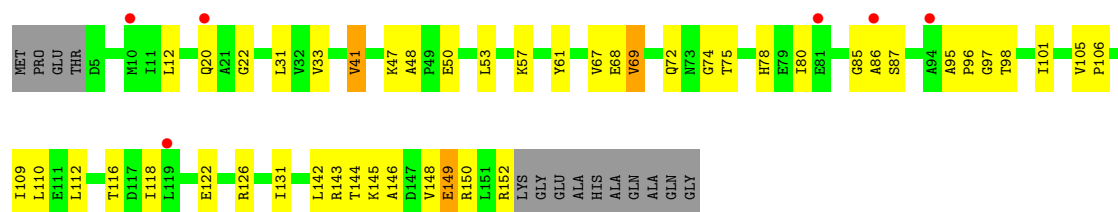
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

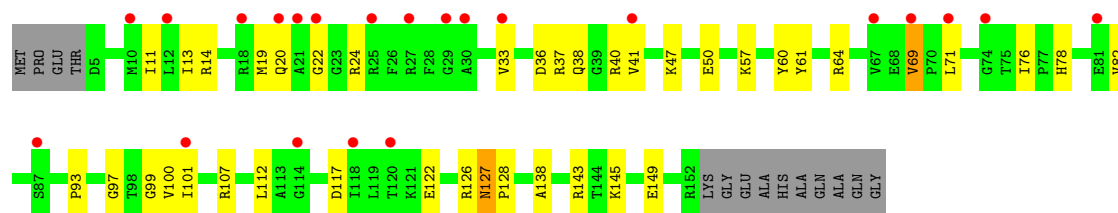


- Molecule 36: 30S ribosomal protein S5

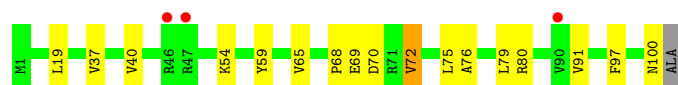
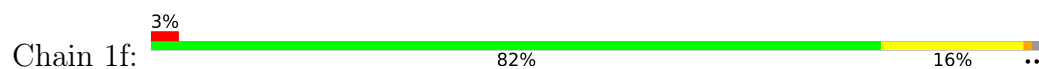


- Molecule 36: 30S ribosomal protein S5

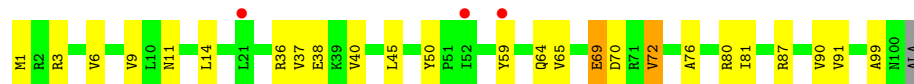
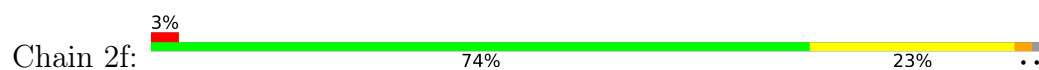




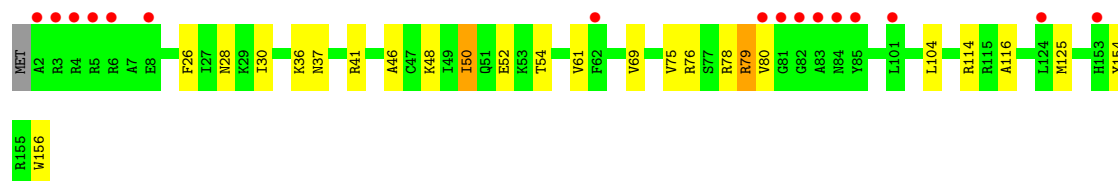
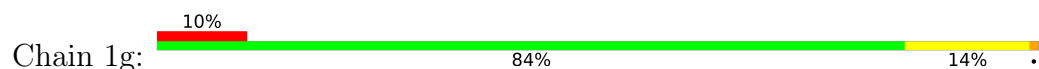
• Molecule 37: 30S ribosomal protein S6



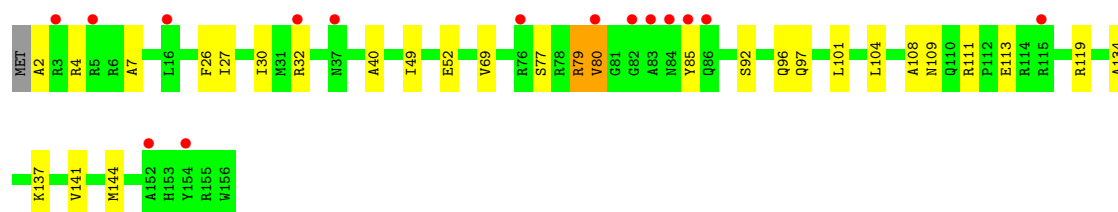
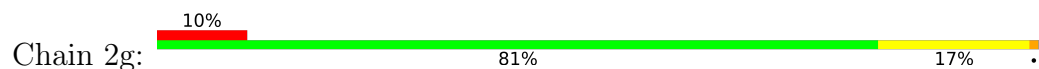
• Molecule 37: 30S ribosomal protein S6



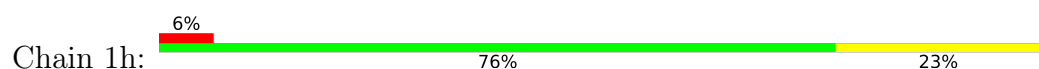
• Molecule 38: 30S ribosomal protein S7

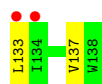


• Molecule 38: 30S ribosomal protein S7

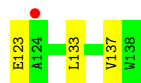
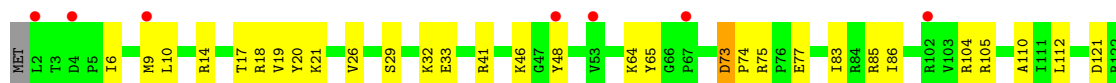
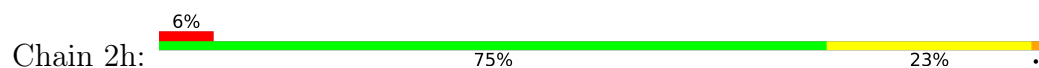


• Molecule 39: 30S ribosomal protein S8

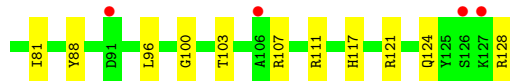




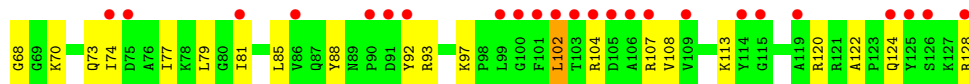
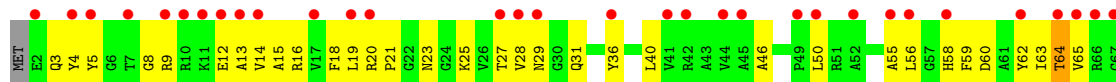
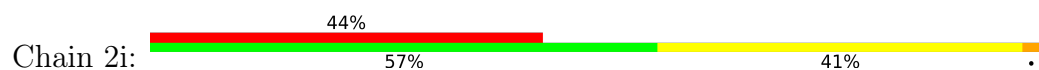
- Molecule 39: 30S ribosomal protein S8



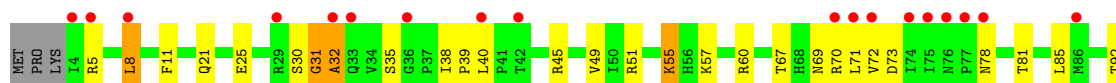
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

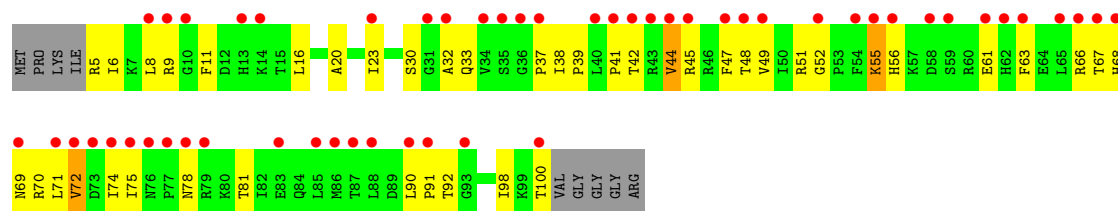


- Molecule 41: 30S ribosomal protein S10

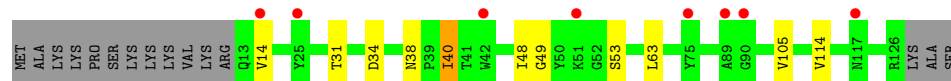
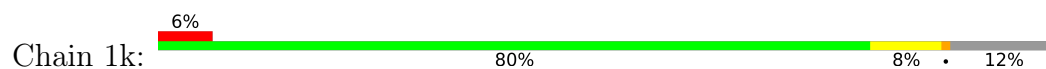


- Molecule 41: 30S ribosomal protein S10

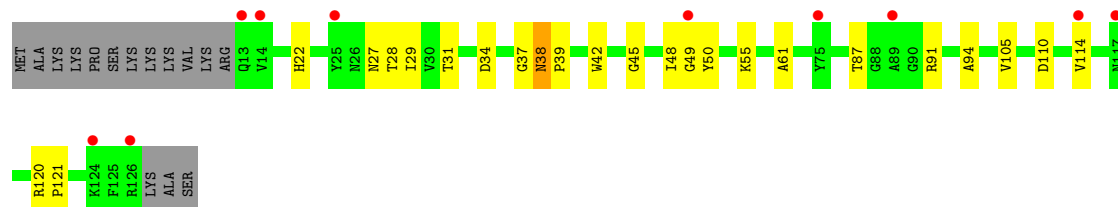




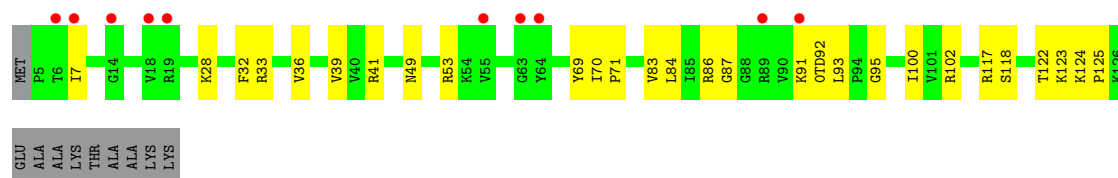
• Molecule 42: 30S ribosomal protein S11



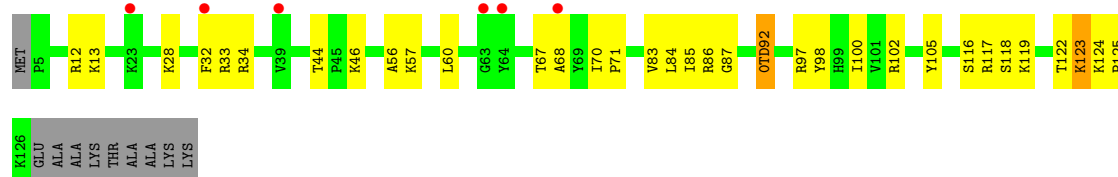
• Molecule 42: 30S ribosomal protein S11



• Molecule 43: 30S ribosomal protein S12

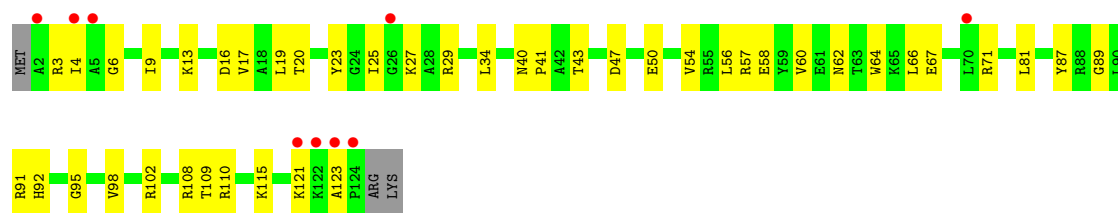


• Molecule 43: 30S ribosomal protein S12

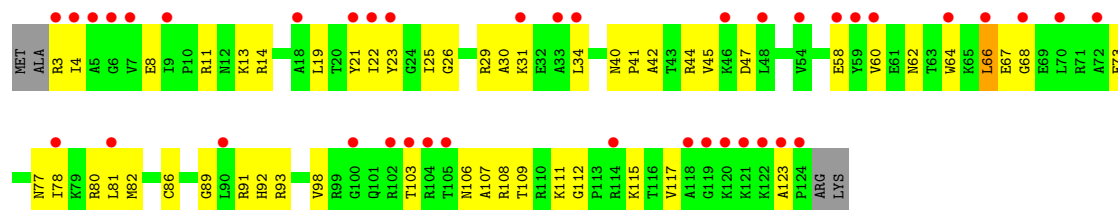


• Molecule 44: 30S ribosomal protein S13

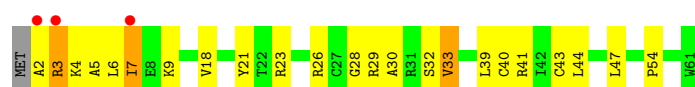




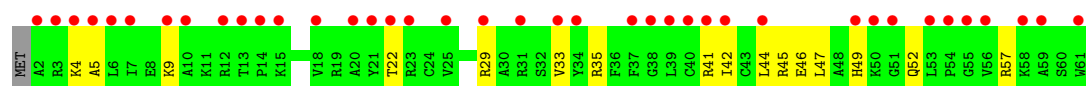
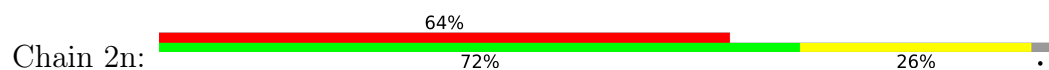
• Molecule 44: 30S ribosomal protein S13



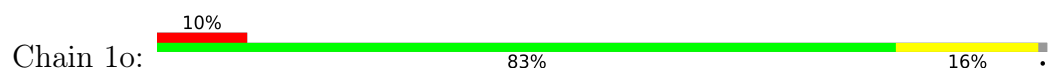
• Molecule 45: 30S ribosomal protein S14 type Z



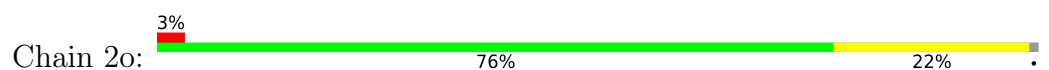
• Molecule 45: 30S ribosomal protein S14 type Z



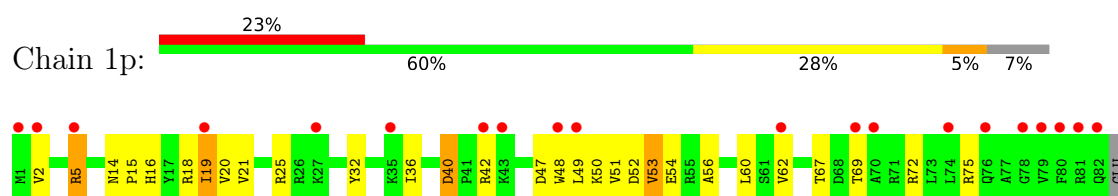
• Molecule 46: 30S ribosomal protein S15



• Molecule 46: 30S ribosomal protein S15

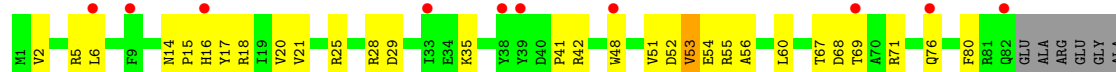


• Molecule 47: 30S ribosomal protein S16

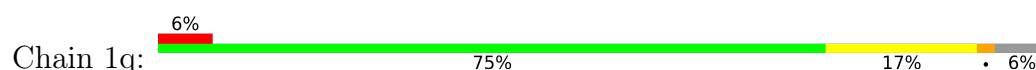


ALA
ARG
GLU
GLY
ALA

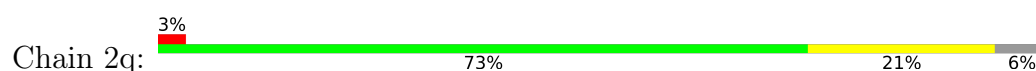
- Molecule 47: 30S ribosomal protein S16



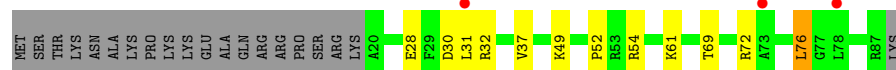
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

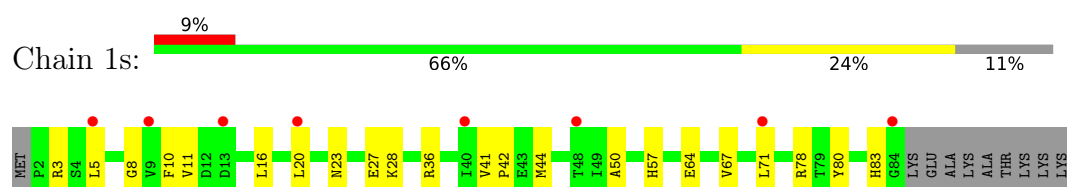


- Molecule 49: 30S ribosomal protein S18

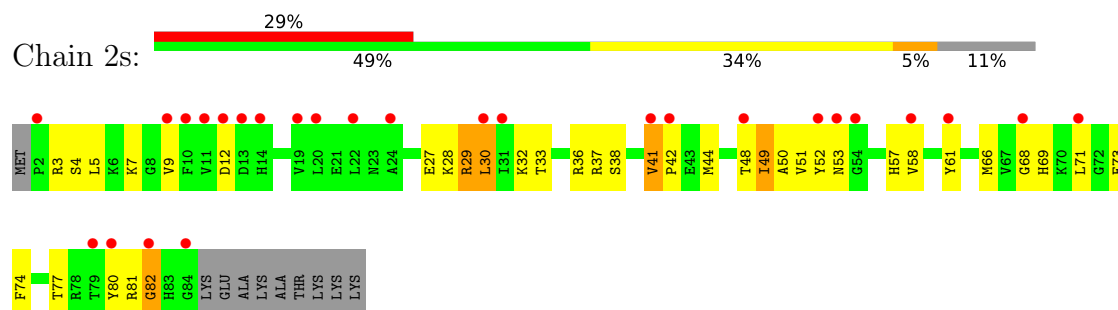


L85
V86
R87
LYS

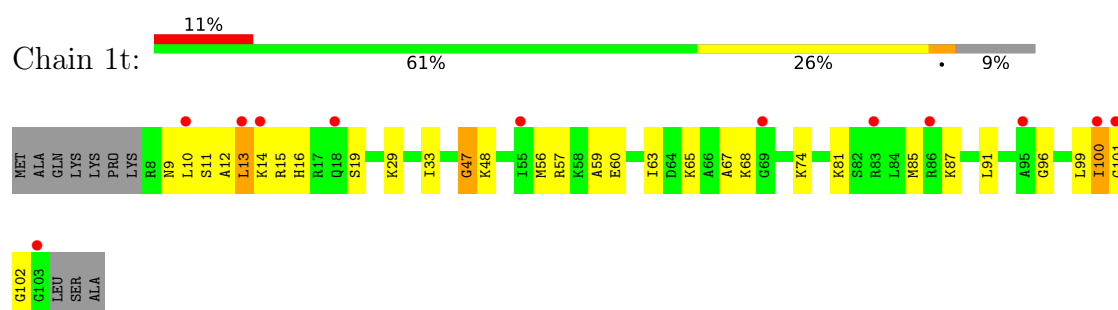
- Molecule 50: 30S ribosomal protein S19



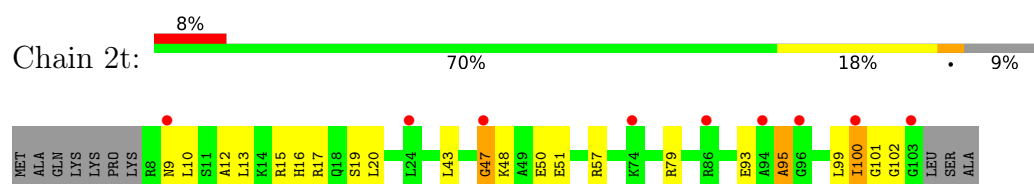
- Molecule 50: 30S ribosomal protein S19



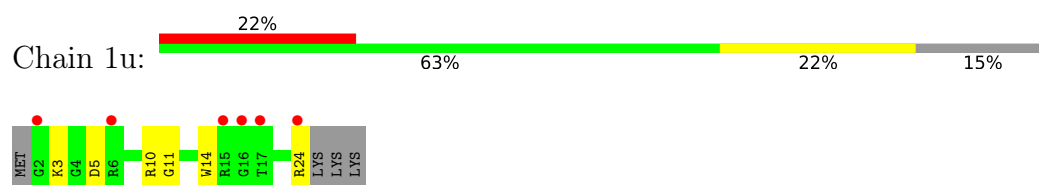
- Molecule 51: 30S ribosomal protein S20



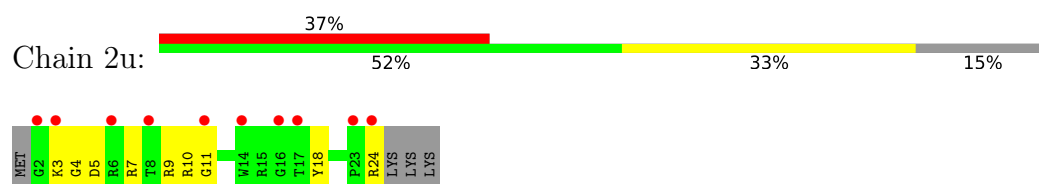
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



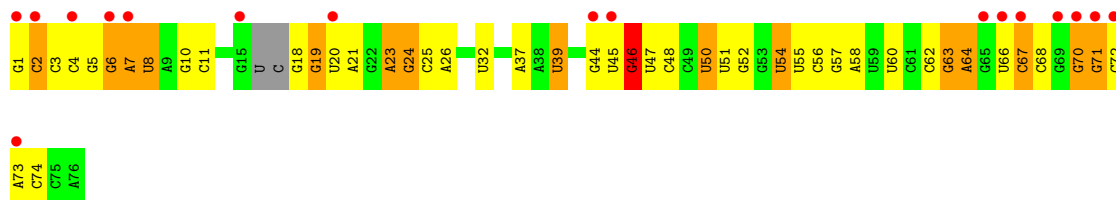
- Molecule 53: mRNA



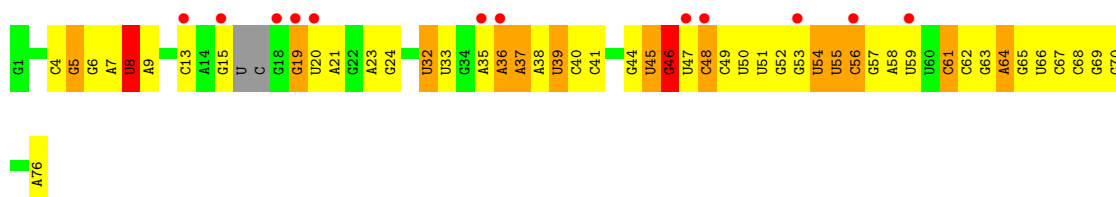
- Molecule 53: mRNA



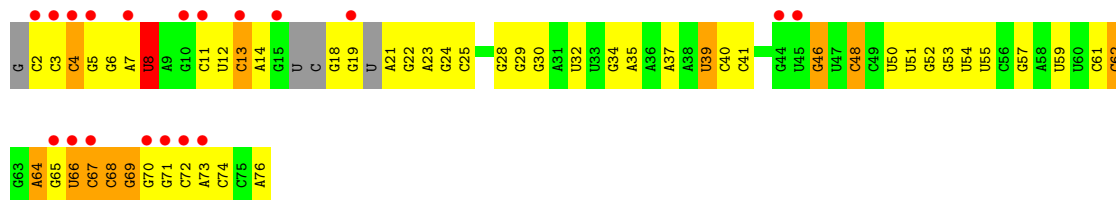
- Molecule 54: A-site and E-site tRNAs



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

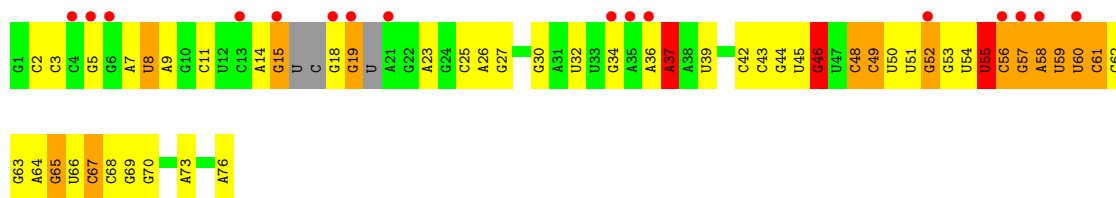


- Molecule 54: A-site and E-site tRNAs

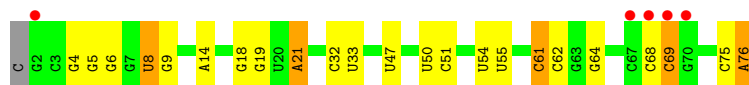


- Molecule 54: A-site and E-site tRNAs

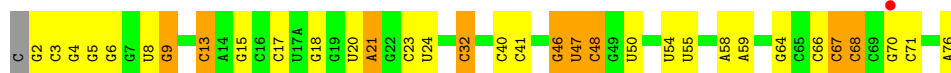




• Molecule 55: P-site tRNA



• Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 450.36Å 625.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.68 – 2.60 147.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (147.68-2.60) 99.3 (147.68-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.217 , 0.264 (Not available) , 0.251	Depositor DCC
R_{free} test set	89454 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	301328	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 7MG, SF4, M2G, UR3, MA6, 4OC, 4SU, PSU, MG, 2MA, 0TD, 5MU, 2MU, K, OMG, 2MG, CPT, MIA, ZN

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	0.27	0/69035	0.45	8/107753 (0.0%)
1	2A	0.23	0/67293	0.43	6/105034 (0.0%)
2	1B	0.20	0/2882	0.37	0/4494
2	2B	0.22	0/2879	0.40	0/4487
3	1D	0.46	0/2186	0.85	2/2944 (0.1%)
3	2D	0.41	0/2186	0.84	1/2944 (0.0%)
4	1E	0.48	0/1592	0.91	4/2149 (0.2%)
4	2E	0.39	0/1592	0.90	6/2149 (0.3%)
5	1F	0.45	0/1619	0.85	3/2193 (0.1%)
5	2F	0.39	0/1615	0.90	3/2188 (0.1%)
6	1G	0.39	0/1448	0.88	4/1957 (0.2%)
6	2G	0.38	0/1453	0.92	5/1963 (0.3%)
7	1H	0.41	0/1347	0.88	5/1823 (0.3%)
7	2H	0.41	0/1347	0.89	4/1823 (0.2%)
8	1I	0.36	0/1112	0.86	4/1514 (0.3%)
8	2I	0.36	0/1079	0.83	0/1475
9	1N	0.44	0/1144	0.82	2/1543 (0.1%)
9	2N	0.38	0/1144	0.89	4/1543 (0.3%)
10	1O	0.45	0/943	0.83	0/1269
10	2O	0.36	0/943	0.78	0/1269
11	1P	0.46	0/1152	0.84	2/1533 (0.1%)
11	2P	0.38	0/1152	0.95	5/1533 (0.3%)
12	1Q	0.46	0/1143	0.77	0/1527
12	2Q	0.39	0/1143	0.88	0/1527
13	1R	0.46	0/982	0.82	0/1312
13	2R	0.40	0/982	0.78	0/1312
14	1S	0.40	0/883	0.79	0/1176
14	2S	0.37	0/880	0.85	0/1172
15	1T	0.42	0/1105	0.79	0/1477
15	2T	0.37	0/1097	0.82	3/1468 (0.2%)
16	1U	0.52	0/977	0.82	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.40	0/977	0.80	0/1301
17	1V	0.46	0/782	0.79	0/1049
17	2V	0.40	0/782	0.80	0/1049
18	1W	0.51	0/897	0.81	2/1205 (0.2%)
18	2W	0.42	0/897	0.80	0/1205
19	1X	0.42	0/764	0.82	0/1025
19	2X	0.39	0/764	0.80	0/1025
20	1Y	0.42	0/819	0.84	0/1095
20	2Y	0.36	0/819	0.86	0/1095
21	1Z	0.39	0/1267	0.93	2/1717 (0.1%)
21	2Z	0.39	0/1299	0.97	4/1763 (0.2%)
22	10	0.42	0/662	0.88	2/881 (0.2%)
22	20	0.36	0/662	0.87	2/881 (0.2%)
23	11	0.42	0/762	0.84	2/1014 (0.2%)
23	21	0.39	0/762	0.80	0/1014
24	12	0.42	0/590	0.76	0/781
24	22	0.35	0/590	0.73	0/781
25	13	0.44	0/474	0.81	0/635
25	23	0.35	0/469	0.84	0/630
26	14	0.41	0/565	1.04	3/761 (0.4%)
26	24	0.44	0/545	0.97	3/737 (0.4%)
27	15	0.52	0/469	0.78	0/635
27	25	0.44	0/469	0.81	1/635 (0.2%)
28	16	0.45	0/460	0.75	2/613 (0.3%)
28	26	0.36	0/456	0.72	0/608
29	17	0.48	0/426	0.82	0/561
29	27	0.49	0/426	0.90	0/561
30	18	0.47	0/525	0.80	0/691
30	28	0.40	0/525	0.78	0/691
31	19	0.41	0/310	0.79	0/407
31	29	0.34	0/310	0.88	2/407 (0.5%)
32	1a	0.19	0/35795	0.39	2/55864 (0.0%)
32	2a	0.19	0/35886	0.37	2/56005 (0.0%)
33	1b	0.37	0/1881	0.91	9/2542 (0.4%)
33	2b	0.38	0/1860	0.96	8/2518 (0.3%)
34	1c	0.35	0/1572	0.85	3/2126 (0.1%)
34	2c	0.37	0/1566	0.89	5/2119 (0.2%)
35	1d	0.37	0/1685	0.85	5/2262 (0.2%)
35	2d	0.37	0/1704	0.86	2/2284 (0.1%)
36	1e	0.39	0/1145	0.87	3/1543 (0.2%)
36	2e	0.40	0/1149	0.95	3/1548 (0.2%)
37	1f	0.38	0/823	0.77	0/1115
37	2f	0.36	0/829	0.71	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.36	0/1250	0.81	1/1679 (0.1%)
38	2g	0.34	0/1254	0.85	0/1683
39	1h	0.36	0/1108	0.84	0/1494
39	2h	0.34	0/1108	0.84	0/1494
40	1i	0.38	0/1002	0.86	1/1346 (0.1%)
40	2i	0.37	0/997	0.86	0/1343
41	1j	0.39	0/722	0.92	0/982
41	2j	0.39	0/727	1.01	5/988 (0.5%)
42	1k	0.37	0/844	0.79	1/1145 (0.1%)
42	2k	0.38	0/848	0.84	2/1149 (0.2%)
43	1l	0.38	0/937	0.81	0/1260
43	2l	0.36	0/937	0.94	5/1260 (0.4%)
44	1m	0.37	0/969	0.83	0/1302
44	2m	0.37	0/961	0.92	4/1291 (0.3%)
45	1n	0.35	0/501	0.86	0/664
45	2n	0.34	0/501	0.83	1/664 (0.2%)
46	1o	0.35	0/739	0.78	1/985 (0.1%)
46	2o	0.36	0/739	0.80	0/985
47	1p	0.38	0/697	0.83	3/939 (0.3%)
47	2p	0.37	0/693	0.77	0/935
48	1q	0.34	0/836	0.81	0/1117
48	2q	0.33	0/836	0.83	2/1117 (0.2%)
49	1r	0.36	0/560	0.75	0/746
49	2r	0.34	0/560	0.74	0/746
50	1s	0.36	0/667	0.87	1/900 (0.1%)
50	2s	0.44	0/661	1.04	4/893 (0.4%)
51	1t	0.33	0/730	0.84	1/965 (0.1%)
51	2t	0.36	0/729	0.82	1/965 (0.1%)
52	1u	0.31	0/203	0.69	0/266
52	2u	0.33	0/203	0.83	0/266
53	1v	0.19	0/310	0.39	0/480
53	2v	0.20	0/310	0.32	0/480
54	1w	0.27	1/1606 (0.1%)	0.43	0/2497
54	1y	0.25	1/1606 (0.1%)	0.39	0/2497
54	2w	0.27	1/1556 (0.1%)	0.39	0/2418
54	2y	0.27	1/1583 (0.1%)	0.43	0/2459
55	1x	0.27	0/1725	0.43	0/2689
55	2x	0.24	0/1725	0.38	0/2689
All	All	0.29	4/316694 (0.0%)	0.57	172/474132 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	8	4SU	O3'-P	5.49	1.61	1.56
54	1w	8	4SU	O3'-P	5.42	1.61	1.56
54	1y	8	4SU	O3'-P	5.25	1.61	1.56
54	2y	8	4SU	O3'-P	5.02	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1300	G	C2'-C3'-O3'	-13.38	93.62	113.70
1	2A	2221	G	C2'-C3'-O3'	-13.27	93.79	113.70
1	1A	2233	G	C2'-C3'-O3'	-13.24	93.84	113.70
32	2a	1300	G	C2'-C3'-O3'	-13.11	94.04	113.70
1	2A	1606	G	C2'-C3'-O3'	-11.97	95.75	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61875	0	31204	560	0
1	2A	60322	0	30425	722	0
2	1B	2577	0	1305	16	0
2	2B	2575	0	1303	39	0
3	1D	2136	0	2218	39	0
3	2D	2136	0	2218	48	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	28	0
5	1F	1584	0	1625	30	0
5	2F	1580	0	1619	44	0
6	1G	1423	0	1436	26	0
6	2G	1428	0	1438	49	0
7	1H	1321	0	1394	23	0
7	2H	1321	0	1394	33	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	18	0
9	1N	1117	0	1184	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2N	1117	0	1184	19	0
10	1O	933	0	996	15	0
10	2O	933	0	996	19	0
11	1P	1135	0	1212	24	0
11	2P	1135	0	1212	30	0
12	1Q	1122	0	1179	9	0
12	2Q	1122	0	1179	36	0
13	1R	968	0	1033	13	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	14	0
14	2S	870	0	923	18	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	9	0
16	2U	959	0	1019	18	0
17	1V	771	0	829	7	0
17	2V	771	0	830	13	0
18	1W	886	0	940	5	0
18	2W	886	0	940	9	0
19	1X	750	0	814	14	0
19	2X	750	0	814	21	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	17	0
21	1Z	1240	0	1240	22	0
21	2Z	1271	0	1273	47	0
22	10	653	0	674	13	0
22	20	653	0	674	12	0
23	11	755	0	826	10	0
23	21	755	0	826	11	0
24	12	588	0	643	7	0
24	22	588	0	643	9	0
25	13	469	0	518	8	0
25	23	464	0	514	6	0
26	14	552	0	533	17	0
26	24	532	0	503	30	0
27	15	455	0	465	7	0
27	25	455	0	465	7	0
28	16	453	0	473	9	0
28	26	449	0	469	9	0
29	17	418	0	467	5	0
29	27	418	0	467	7	0
30	18	517	0	582	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	28	517	0	582	13	0
31	19	307	0	335	2	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	346	0
32	2a	32327	0	16339	478	0
33	1b	1846	0	1867	77	0
33	2b	1825	0	1828	76	0
34	1c	1548	0	1535	25	0
34	2c	1542	0	1517	42	0
35	1d	1655	0	1672	33	0
35	2d	1674	0	1714	42	0
36	1e	1129	0	1185	32	0
36	2e	1133	0	1191	30	0
37	1f	810	0	804	12	0
37	2f	816	0	808	17	0
38	1g	1231	0	1238	15	0
38	2g	1235	0	1249	23	0
39	1h	1088	0	1126	23	0
39	2h	1088	0	1126	26	0
40	1i	983	0	986	29	0
40	2i	978	0	966	46	0
41	1j	709	0	650	22	0
41	2j	714	0	672	30	0
42	1k	829	0	825	4	0
42	2k	833	0	836	14	0
43	1l	932	0	981	18	0
43	2l	932	0	980	21	0
44	1m	958	0	1002	27	0
44	2m	950	0	988	39	0
45	1n	492	0	529	20	0
45	2n	492	0	529	17	0
46	1o	728	0	760	7	0
46	2o	728	0	760	13	0
47	1p	681	0	697	20	0
47	2p	677	0	686	21	0
48	1q	823	0	891	15	0
48	2q	823	0	891	14	0
49	1r	555	0	618	8	0
49	2r	555	0	618	17	0
50	1s	652	0	662	15	0
50	2s	646	0	644	27	0
51	1t	728	0	798	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	2t	727	0	796	16	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	277	0	140	1	0
53	2v	277	0	140	3	0
54	1w	1592	0	819	37	0
54	1y	1585	0	804	36	0
54	2w	1544	0	788	40	0
54	2y	1565	0	795	48	0
55	1x	1625	0	829	13	0
55	2x	1625	0	829	23	0
56	10	6	0	0	0	0
56	11	5	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	2	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1220	0	0	0	0
56	1B	36	0	0	0	0
56	1D	12	0	0	0	0
56	1E	11	0	0	0	0
56	1F	7	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	6	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	8	0	0	0	0
56	1V	2	0	0	0	0
56	1W	4	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	4	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	284	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1b	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1n	3	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	18	0	0	0	0
56	1y	5	0	0	0	0
56	20	2	0	0	0	0
56	23	2	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	937	0	0	0	0
56	2B	20	0	0	0	0
56	2D	5	0	0	0	0
56	2E	9	0	0	0	0
56	2F	7	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	3	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	3	0	0	0	0
56	2S	1	0	0	0	0
56	2T	2	0	0	0	0
56	2U	3	0	0	0	0
56	2V	1	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	256	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	3	0	0	0	0
56	2n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2p	1	0	0	0	0
56	2q	4	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	4	0	0	0	0
56	2w	8	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
57	2A	1	0	0	0	0
58	1A	23	0	0	3	0
58	1I	4	0	0	0	0
58	1a	8	0	0	2	0
58	2A	23	0	0	2	0
58	2I	4	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	10	0	0	1	0
61	11	11	0	0	0	0
61	12	4	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	6	0	0	0	0
61	16	3	0	0	0	0
61	17	10	0	0	0	0
61	18	11	0	0	1	0
61	1A	2299	0	0	82	0
61	1B	68	0	0	2	0
61	1D	29	0	0	1	0
61	1E	30	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1F	17	0	0	0	0
61	1G	8	0	0	4	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	5	0	0	0	0
61	1O	7	0	0	1	0
61	1P	21	0	0	2	0
61	1Q	13	0	0	0	0
61	1R	13	0	0	2	0
61	1S	5	0	0	0	0
61	1T	8	0	0	1	0
61	1U	14	0	0	0	0
61	1V	12	0	0	0	0
61	1W	7	0	0	0	0
61	1X	8	0	0	0	0
61	1Y	9	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	516	0	0	27	0
61	1b	1	0	0	0	0
61	1c	1	0	0	0	0
61	1d	3	0	0	0	0
61	1e	2	0	0	0	0
61	1g	2	0	0	0	0
61	1i	1	0	0	0	0
61	1l	8	0	0	0	0
61	1m	2	0	0	0	0
61	1o	1	0	0	0	0
61	1p	1	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	1	0
61	1v	6	0	0	0	0
61	1w	21	0	0	0	0
61	1x	14	0	0	1	0
61	1y	3	0	0	0	0
61	20	6	0	0	0	0
61	21	12	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	3	0	0	0	0
61	27	4	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2A	1402	0	0	76	0
61	2B	27	0	0	0	0
61	2D	26	0	0	0	0
61	2E	17	0	0	0	0
61	2F	17	0	0	0	0
61	2I	4	0	0	0	0
61	2N	3	0	0	0	0
61	2O	1	0	0	0	0
61	2P	15	0	0	2	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	6	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	2	0	0	0	0
61	2Y	1	0	0	1	0
61	2Z	2	0	0	0	0
61	2a	380	0	0	26	0
61	2c	1	0	0	0	0
61	2d	4	0	0	0	0
61	2e	2	0	0	0	0
61	2f	1	0	0	0	0
61	2g	2	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	2	0
61	2l	7	0	0	2	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2t	3	0	0	0	0
61	2u	2	0	0	0	0
61	2v	2	0	0	0	0
61	2w	2	0	0	0	0
61	2x	7	0	0	0	0
61	2y	20	0	0	1	0
All	All	301328	0	196675	3844	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 8.

The worst 5 of 3844 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:997:U:H3	32:2a:1044:A:N6	1.36	1.20
1:2A:2138:C:N4	1:2A:2153:G:H1	1.42	1.17
54:1w:6:G:H1	54:1w:67:C:N4	1.43	1.15
1:1A:1128:U:H3	1:1A:1132:A:N6	1.53	1.05
54:2y:26:A:N1	54:2y:44:G:C6	2.26	1.02

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%)	263 (96%)	10 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	46
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	46
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	46
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	28
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	42
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	7	15
7	1H	171/180 (95%)	161 (94%)	9 (5%)	1 (1%)	21	42
7	2H	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	21	42
8	1I	144/148 (97%)	134 (93%)	9 (6%)	1 (1%)	18	38
8	2I	144/148 (97%)	132 (92%)	11 (8%)	1 (1%)	18	38
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	38
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	18	38
11	2P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9	19
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	30
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	28
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	28
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	25
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	18	38
21	2Z	156/206 (76%)	137 (88%)	17 (11%)	2 (1%)	9	21
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	78 (96%)	2 (2%)	1 (1%)	10	23
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	14
26	14	67/71 (94%)	54 (81%)	7 (10%)	6 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	5	10
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	199 (87%)	24 (10%)	6 (3%)	4	7
33	2b	229/256 (90%)	195 (85%)	26 (11%)	8 (4%)	3	4
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	24	46
34	2c	204/239 (85%)	186 (91%)	17 (8%)	1 (0%)	24	46
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	46
35	2d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	46
36	1e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	9	19
36	2e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	9	19
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	4 (3%)	3 (2%)	6	12
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	6	12
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	18	38
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	2	3
41	2j	94/105 (90%)	83 (88%)	7 (7%)	4 (4%)	2	2
42	1k	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	6	14
42	2k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	6	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	10 (8%)	1 (1%)	16	34
44	2m	120/126 (95%)	111 (92%)	8 (7%)	1 (1%)	16	34
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	21
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9	21
48	1q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	6 (7%)	3 (4%)	2	3
51	1t	94/106 (89%)	88 (94%)	2 (2%)	4 (4%)	2	2
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	2
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10722 (94%)	551 (5%)	95 (1%)	16	34

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
26	14	53	GLU
26	14	61	ARG
26	14	62	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%)	205 (95%)	10 (5%)	23	48
3	2D	215/218 (99%)	209 (97%)	6 (3%)	38	66
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9	19
4	2E	164/166 (99%)	145 (88%)	19 (12%)	5	11
5	1F	160/166 (96%)	149 (93%)	11 (7%)	14	32
5	2F	159/166 (96%)	149 (94%)	10 (6%)	16	36
6	1G	143/156 (92%)	138 (96%)	5 (4%)	32	59
6	2G	143/156 (92%)	136 (95%)	7 (5%)	22	47
7	1H	143/148 (97%)	139 (97%)	4 (3%)	38	66
7	2H	143/148 (97%)	140 (98%)	3 (2%)	47	73
8	1I	113/124 (91%)	103 (91%)	10 (9%)	9	21
8	2I	105/124 (85%)	98 (93%)	7 (7%)	15	33
9	1N	118/119 (99%)	112 (95%)	6 (5%)	21	45
9	2N	118/119 (99%)	114 (97%)	4 (3%)	32	60
10	1O	100/100 (100%)	98 (98%)	2 (2%)	48	74
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	74
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	51
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	59
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	51	76
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	50
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	13
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	20
14	1S	86/88 (98%)	81 (94%)	5 (6%)	18	39
14	2S	85/88 (97%)	82 (96%)	3 (4%)	32	59
15	1T	115/127 (91%)	114 (99%)	1 (1%)	70	87
15	2T	113/127 (89%)	111 (98%)	2 (2%)	51	76
16	1U	93/94 (99%)	91 (98%)	2 (2%)	45	72
16	2U	93/94 (99%)	92 (99%)	1 (1%)	65	84
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	21
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	40
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	26
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	68
19	2X	77/78 (99%)	76 (99%)	1 (1%)	61	82
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	23	48
20	2Y	85/91 (93%)	82 (96%)	3 (4%)	32	59
21	1Z	135/179 (75%)	129 (96%)	6 (4%)	25	50
21	2Z	137/179 (76%)	132 (96%)	5 (4%)	31	58
22	10	65/67 (97%)	64 (98%)	1 (2%)	57	80
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	80
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	69
23	21	80/83 (96%)	76 (95%)	4 (5%)	22	46
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	55
25	23	50/52 (96%)	49 (98%)	1 (2%)	48	74
26	14	59/63 (94%)	57 (97%)	2 (3%)	32	60
26	24	53/63 (84%)	52 (98%)	1 (2%)	50	75
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	37
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	37
28	16	51/52 (98%)	50 (98%)	1 (2%)	48	74
28	26	50/52 (96%)	49 (98%)	1 (2%)	48	74
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	29
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	38
33	1b	192/220 (87%)	185 (96%)	7 (4%)	31	58
33	2b	187/220 (85%)	179 (96%)	8 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	139 (98%)	3 (2%)	47	73
34	2c	140/188 (74%)	137 (98%)	3 (2%)	47	73
35	1d	169/181 (93%)	160 (95%)	9 (5%)	20	43
35	2d	173/181 (96%)	168 (97%)	5 (3%)	37	65
36	1e	113/123 (92%)	111 (98%)	2 (2%)	51	76
36	2e	114/123 (93%)	112 (98%)	2 (2%)	51	76
37	1f	84/90 (93%)	82 (98%)	2 (2%)	43	70
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	59
38	1g	119/127 (94%)	118 (99%)	1 (1%)	73	88
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	112 (98%)	2 (2%)	51	76
39	2h	114/119 (96%)	113 (99%)	1 (1%)	70	87
40	1i	90/99 (91%)	88 (98%)	2 (2%)	45	72
40	2i	89/99 (90%)	85 (96%)	4 (4%)	24	50
41	1j	66/92 (72%)	63 (96%)	3 (4%)	24	50
41	2j	69/92 (75%)	67 (97%)	2 (3%)	37	65
42	1k	82/99 (83%)	79 (96%)	3 (4%)	30	57
42	2k	83/99 (84%)	82 (99%)	1 (1%)	63	83
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	73
43	2l	96/108 (89%)	94 (98%)	2 (2%)	47	73
44	1m	93/101 (92%)	89 (96%)	4 (4%)	26	51
44	2m	92/101 (91%)	89 (97%)	3 (3%)	33	61
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	15
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	37
46	1o	78/80 (98%)	77 (99%)	1 (1%)	61	82
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	56
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	30
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18	38
48	1q	94/97 (97%)	92 (98%)	2 (2%)	47	73
48	2q	94/97 (97%)	92 (98%)	2 (2%)	47	73
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	45
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59	81
50	2s	67/80 (84%)	64 (96%)	3 (4%)	24	50
51	1t	70/82 (85%)	69 (99%)	1 (1%)	59	81
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9301/10064 (92%)	8935 (96%)	366 (4%)	28	55

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	2G	159	VAL
19	2X	76	ARG
8	2I	92	VAL
13	2R	54	LEU
25	23	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
51	1t	42	GLN
47	2p	76	GLN
14	2S	38	GLN
46	2o	28	GLN
37	2f	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	432 (15%)	39 (1%)
1	2A	2791/2915 (95%)	480 (17%)	27 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	26 (22%)	0
32	1a	1497/1521 (98%)	212 (14%)	0
32	2a	1501/1521 (98%)	235 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	1 (8%)	0
54	1w	72/76 (94%)	24 (33%)	0
54	1y	72/76 (94%)	21 (29%)	0
54	2w	69/76 (90%)	20 (28%)	0
54	2y	70/76 (92%)	24 (34%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	11 (14%)	0
All	All	9347/9620 (97%)	1508 (16%)	67 (0%)

5 of 1508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	27	G
1	1A	28	A
1	1A	34	C

5 of 67 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1606	G
1	2A	1913	A
1	2A	2689	U
1	1A	1466	U
1	1A	1425	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.99	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	21,30,33	2.19	4 (19%)
32	MA6	1a	1519	32	23,26,27	1.54	4 (17%)	33,38,41	2.26	11 (33%)
1	PSU	1A	1939	1	18,21,22	1.40	4 (22%)	21,30,33	2.16	4 (19%)
55	5MU	1x	54	56,55	19,22,23	1.43	6 (31%)	27,32,35	1.92	7 (25%)
54	5MU	2y	54	54	19,22,23	1.48	4 (21%)	27,32,35	2.07	8 (29%)
1	2MU	2A	2552	1,56	19,22,24	1.26	2 (10%)	25,31,36	1.86	6 (24%)
1	4OC	1A	1942	1	19,22,24	0.80	0	25,31,35	0.91	0
1	5MU	1A	1937	1	19,22,23	1.39	5 (26%)	27,32,35	2.19	7 (25%)
54	4SU	2w	8	54	18,21,22	1.65	4 (22%)	25,30,33	2.54	6 (24%)
43	0TD	2l	92	43	8,9,10	4.61	1 (12%)	6,11,13	3.39	3 (50%)
1	4OC	2A	1920	1	19,22,24	0.75	0	25,31,35	0.84	0
54	4SU	2y	8	54	18,21,22	1.79	4 (22%)	25,30,33	2.56	6 (24%)
54	PSU	1y	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.91	3 (14%)
54	5MU	1y	54	54	19,22,23	1.50	6 (31%)	27,32,35	1.87	6 (22%)
32	4OC	1a	1402	32	20,23,24	0.70	0	25,32,35	0.98	1 (4%)
54	4SU	1y	8	54	18,21,22	1.77	4 (22%)	25,30,33	1.90	5 (20%)
1	5MC	1A	1964	1,56	19,22,23	1.53	3 (15%)	26,32,35	1.21	2 (7%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.93	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.15	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.71	3 (11%)
32	M2G	2a	966	32	24,27,28	1.27	3 (12%)	33,40,43	1.87	6 (18%)
54	7MG	1w	46	54	23,26,27	1.38	4 (17%)	27,39,42	2.62	7 (25%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	3.67	3 (50%)
32	5MC	2a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.22	3 (11%)
54	PSU	2w	55	54	18,21,22	1.42	2 (11%)	21,30,33	2.01	3 (14%)
1	PSU	2A	1917	1,56	18,21,22	1.35	2 (11%)	21,30,33	1.91	3 (14%)
32	5MC	1a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.23	3 (11%)
1	5MU	2A	1939	1,56	19,22,23	1.43	6 (31%)	27,32,35	2.26	6 (22%)
54	5MU	1w	54	54	19,22,23	1.44	6 (31%)	27,32,35	1.98	8 (29%)
54	PSU	2y	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.99	5 (23%)
1	PSU	1A	2617	1,56	18,21,22	1.35	3 (16%)	21,30,33	2.27	4 (19%)
54	7MG	2y	46	54	23,26,27	1.37	3 (13%)	27,39,42	2.81	8 (29%)
1	5MC	2A	1942	1	19,22,23	1.67	3 (15%)	26,32,35	1.14	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.82	3 (15%)	26,32,35	1.25	4 (15%)
32	MA6	2a	1519	32	23,26,27	1.60	4 (17%)	33,38,41	2.29	12 (36%)

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	1.77	4 (22%)	25,30,33	1.98	5 (20%)
32	7MG	2a	527	32,56	23,26,27	1.35	4 (17%)	27,39,42	2.58	6 (22%)
1	5MC	1A	1984	1	19,22,23	1.63	3 (15%)	26,32,35	1.10	2 (7%)
54	7MG	2w	46	54	23,26,27	1.37	2 (8%)	27,39,42	2.53	8 (29%)
55	5MC	1x	32	55	19,22,23	1.55	3 (15%)	26,32,35	1.22	3 (11%)
1	5MU	1A	1961	1,56	19,22,23	1.41	5 (26%)	27,32,35	2.33	6 (22%)
1	2MU	1A	2564	1,56	19,22,24	1.24	3 (15%)	25,31,36	1.94	5 (20%)
1	2MA	1A	2515	1,56	22,25,26	1.44	3 (13%)	32,37,40	2.40	8 (25%)
1	5MC	2A	1962	1	19,22,23	1.64	3 (15%)	26,32,35	1.18	2 (7%)
55	PSU	1x	55	56,55	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
1	OMG	1A	2263	1,56,55	23,26,27	1.21	3 (13%)	32,38,41	2.07	7 (21%)
54	7MG	1y	46	54	23,26,27	1.36	4 (17%)	27,39,42	2.70	6 (22%)
54	PSU	2y	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.02	4 (19%)
55	4SU	2x	8	56,55	18,21,22	2.02	6 (33%)	25,30,33	1.59	5 (20%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.22	9 (27%)
55	5MU	2x	54	55	19,22,23	1.38	4 (21%)	27,32,35	2.07	6 (22%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.17	4 (15%)
1	PSU	1A	1933	1	18,21,22	1.39	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	1a	1518	32	23,26,27	1.50	5 (21%)	33,38,41	2.28	14 (42%)
32	5MC	1a	967	32	19,22,23	1.70	3 (15%)	26,32,35	1.17	3 (11%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.74	12 (31%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.88	3 (14%)
1	OMG	2A	2251	1,56,55	23,26,27	1.19	2 (8%)	32,38,41	2.09	7 (21%)
1	2MA	2A	2503	1,56	22,25,26	1.49	4 (18%)	32,37,40	2.31	8 (25%)
32	2MG	2a	1207	32,56	23,26,27	1.22	2 (8%)	33,38,41	2.20	7 (21%)
32	7MG	1a	527	32,56	23,26,27	1.40	4 (17%)	27,39,42	2.48	7 (25%)
54	PSU	1w	55	54	18,21,22	1.42	2 (11%)	21,30,33	2.04	4 (19%)
54	PSU	1y	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.81	4 (15%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.94	3 (14%)
54	5MU	2w	54	54	19,22,23	1.37	5 (26%)	27,32,35	2.02	7 (25%)
54	MIA	2y	37	54	21,24,32	1.63	4 (19%)	30,35,47	2.06	7 (23%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.17	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	1x	8	55	18,21,22	2.13	5 (27%)	25,30,33	1.59	6 (24%)
54	PSU	1y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.95	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.44	2 (10%)	26,32,35	1.10	3 (11%)
54	MIA	1y	37	54	21,24,32	1.60	3 (14%)	30,35,47	2.00	8 (26%)
32	PSU	1a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.99	5 (23%)
54	PSU	1w	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.03	4 (19%)
54	MIA	2w	37	54	24,27,32	2.04	5 (20%)	32,39,47	2.44	10 (31%)
32	5MC	2a	1407	32,56	19,22,23	1.56	3 (15%)	26,32,35	1.12	2 (7%)
32	PSU	2a	516	32	18,21,22	1.30	2 (11%)	21,30,33	1.98	4 (19%)
54	PSU	2y	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.87	3 (14%)
55	5MC	2x	32	55	19,22,23	1.57	3 (15%)	26,32,35	1.24	4 (15%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.04	2 (8%)
32	MA6	2a	1518	32	23,26,27	1.61	5 (21%)	33,38,41	2.30	11 (33%)

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	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
1	4OC	1A	1942	1	-	2/9/27/30	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	4/7/12/14	-
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	3/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	4SU	1y	8	54	-	5/7/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1,56	-	1/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/11/29/30	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	2/7/37/38	0/3/3/3
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
1	2MA	1A	2515	1,56	-	1/7/25/26	0/3/3/3
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	56,55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,56,55	-	0/9/27/28	0/3/3/3
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	56,55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	0/9/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	1/7/25/26	0/3/3/3
32	2MG	2a	1207	32,56	-	0/9/27/28	0/3/3/3
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	3/7/25/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.65	1.69	1.82
43	1l	92	0TD	CB-SB	-12.48	1.69	1.82
54	1w	37	MIA	C13-C14	6.83	1.52	1.32
32	2a	1404	5MC	C5-C4	6.70	1.49	1.44
54	1w	37	MIA	C2-S10	-6.68	1.70	1.75

The worst 5 of 432 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N9-C4-N3	9.86	139.91	125.46
54	1y	46	7MG	N9-C4-N3	9.50	139.38	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	46	7MG	N9-C4-N3	9.19	138.93	125.46
54	1w	37	MIA	C12-C13-C14	-9.06	110.76	127.01
32	2a	527	7MG	N9-C4-N3	8.67	138.16	125.46

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
32	2a	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

39 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1519	MA6	2	0
1	2A	2552	2MU	1	0
1	1A	1942	4OC	1	0
54	2w	8	4SU	2	0
43	2l	92	0TD	1	0
1	2A	1920	4OC	1	0
54	2y	8	4SU	2	0
54	1y	39	PSU	1	0
32	1a	1402	4OC	1	0
54	1y	8	4SU	1	0
54	1w	46	7MG	1	0
1	2A	1917	PSU	1	0
1	2A	1939	5MU	1	0
54	1w	54	5MU	1	0
54	2y	55	PSU	6	0
1	1A	2617	PSU	1	0
54	2y	46	7MG	1	0
32	2a	1404	5MC	1	0
32	2a	1519	MA6	4	0
1	1A	1961	5MU	1	0
1	1A	2564	2MU	1	0
1	1A	2515	2MA	1	0
54	1y	46	7MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	967	5MC	1	0
32	1a	1518	MA6	2	0
54	2w	39	PSU	3	0
1	2A	2251	OMG	1	0
1	2A	2503	2MA	1	0
32	2a	1207	2MG	1	0
54	1y	55	PSU	1	0
54	2y	37	MIA	1	0
1	2A	1915	5MU	1	0
55	1x	8	4SU	2	0
54	1y	32	PSU	1	0
54	1y	37	MIA	1	0
54	1w	39	PSU	1	0
55	2x	32	5MC	1	0
32	2a	1402	4OC	2	0
32	2a	1518	MA6	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3049 ligands modelled in this entry, 3031 are monoatomic - leaving 18 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	CPT	2A	3919	1	0,3,4	-	-	-		
58	CPT	1I	3002	8	0,3,4	-	-	-		
58	CPT	2A	3915	1	0,3,4	-	-	-		
58	CPT	1A	4182	1	0,3,4	-	-	-		
60	SF4	1d	501	35	0,12,12	-	-	-		
58	CPT	1A	4178	1	0,3,4	-	-	-		
58	CPT	1a	1883	32	0,3,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	CPT	1A	4177	1	0,3,4	-	-	-		
58	CPT	1A	4179	1	0,3,4	-	-	-		
58	CPT	2A	3914	1	0,3,4	-	-	-		
58	CPT	2A	3917	1	0,3,4	-	-	-		
58	CPT	2A	3918	1	0,2,4	-	-	-		
58	CPT	1A	4181	1	0,2,4	-	-	-		
58	CPT	2A	3916	1	0,3,4	-	-	-		
58	CPT	2I	201	8	0,3,4	-	-	-		
60	SF4	2d	302	35	0,12,12	-	-	-		
58	CPT	1a	1882	32	0,3,4	-	-	-		
58	CPT	1A	4180	1	0,3,4	-	-	-		

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
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

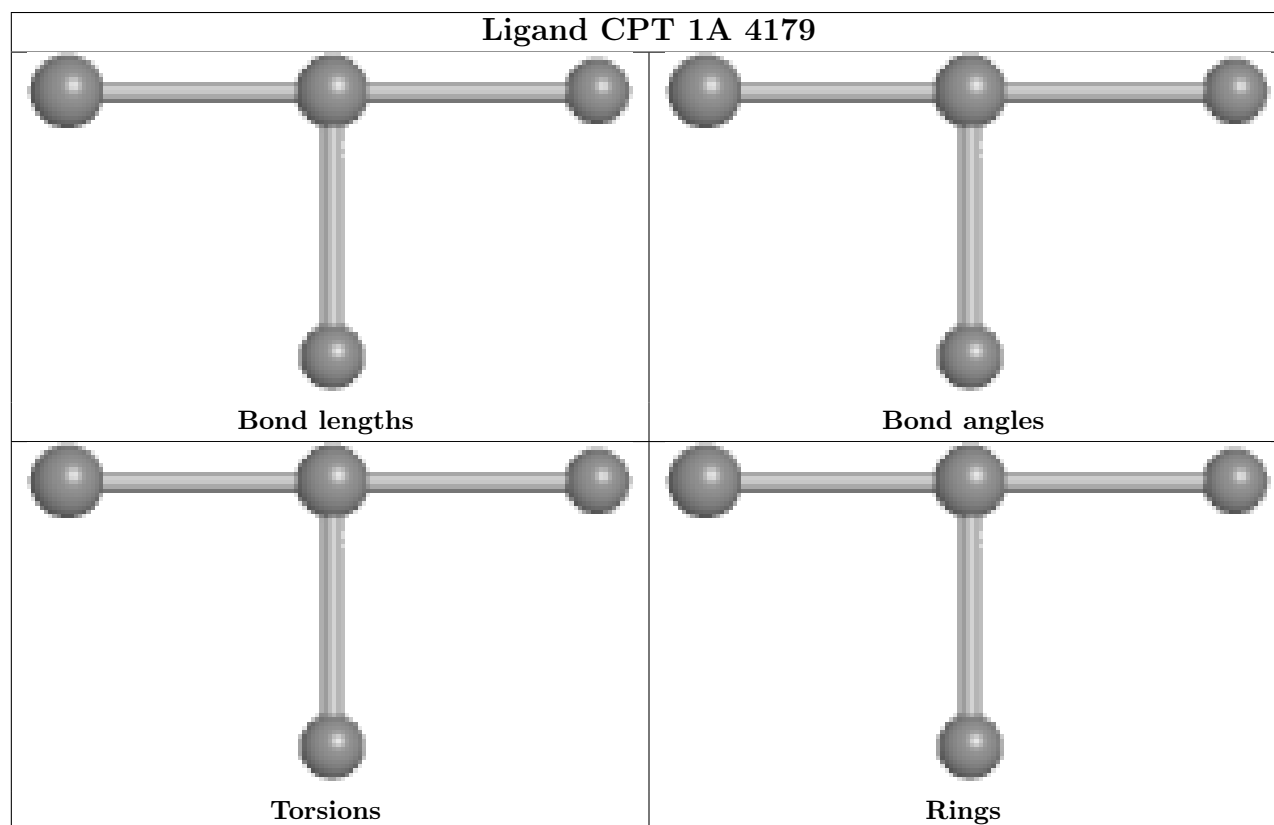
There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3919	CPT	1	0
58	1a	1883	CPT	2	0
58	1A	4179	CPT	1	0
58	2A	3917	CPT	1	0
58	1A	4181	CPT	1	0
58	2I	201	CPT	1	0
58	1A	4180	CPT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.13	164 (5%) 29 24	23, 44, 93, 105	1 (0%)
1	2A	2789/2915 (95%)	-0.09	98 (3%) 47 41	28, 48, 91, 104	0
2	1B	120/121 (99%)	0.28	0 100 100	39, 61, 73, 91	0
2	2B	120/121 (99%)	0.76	3 (2%) 58 52	46, 67, 77, 91	0
3	1D	275/276 (99%)	0.00	6 (2%) 62 57	24, 42, 58, 81	0
3	2D	275/276 (99%)	-0.00	3 (1%) 78 74	26, 44, 60, 80	0
4	1E	204/206 (99%)	0.27	4 (1%) 65 60	25, 48, 65, 80	0
4	2E	204/206 (99%)	0.12	2 (0%) 79 76	28, 51, 68, 80	0
5	1F	203/210 (96%)	0.31	4 (1%) 65 60	24, 53, 74, 86	0
5	2F	203/210 (96%)	0.34	2 (0%) 79 76	27, 57, 76, 86	0
6	1G	181/182 (99%)	0.97	19 (10%) 11 9	51, 70, 80, 92	0
6	2G	181/182 (99%)	1.29	27 (14%) 5 4	55, 73, 83, 93	0
7	1H	173/180 (96%)	1.05	13 (7%) 20 16	53, 66, 76, 84	0
7	2H	173/180 (96%)	1.32	25 (14%) 6 4	57, 71, 80, 84	0
8	1I	146/148 (98%)	0.79	3 (2%) 63 58	52, 74, 83, 90	0
8	2I	146/148 (98%)	0.86	5 (3%) 48 42	54, 74, 83, 86	0
9	1N	140/140 (100%)	0.50	2 (1%) 73 69	33, 50, 69, 76	0
9	2N	140/140 (100%)	0.57	4 (2%) 53 48	37, 54, 70, 77	0
10	1O	122/122 (100%)	-0.23	0 100 100	27, 40, 59, 66	0
10	2O	122/122 (100%)	0.41	2 (1%) 70 66	46, 61, 75, 78	0
11	1P	149/150 (99%)	0.48	5 (3%) 48 42	26, 56, 76, 82	0
11	2P	149/150 (99%)	0.48	3 (2%) 65 60	28, 60, 79, 83	0
12	1Q	141/141 (100%)	0.43	3 (2%) 63 58	37, 52, 69, 79	0
12	2Q	141/141 (100%)	0.76	7 (4%) 34 28	41, 58, 71, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.01	0 100 100	30, 41, 55, 63	0
13	2R	118/118 (100%)	-0.12	0 100 100	33, 44, 57, 66	0
14	1S	110/112 (98%)	0.68	5 (4%) 38 32	47, 60, 71, 75	0
14	2S	110/112 (98%)	1.09	15 (13%) 7 5	51, 64, 75, 79	0
15	1T	131/146 (89%)	0.55	10 (7%) 20 16	39, 52, 73, 80	0
15	2T	131/146 (89%)	0.45	4 (3%) 51 45	44, 55, 75, 80	0
16	1U	116/118 (98%)	0.25	2 (1%) 69 64	26, 42, 60, 72	0
16	2U	116/118 (98%)	0.33	2 (1%) 69 64	33, 47, 64, 74	0
17	1V	101/101 (100%)	0.41	3 (2%) 52 47	29, 52, 67, 76	0
17	2V	101/101 (100%)	0.60	2 (1%) 65 60	34, 58, 71, 76	0
18	1W	112/113 (99%)	-0.07	1 (0%) 81 78	26, 37, 61, 85	0
18	2W	112/113 (99%)	-0.14	2 (1%) 67 63	31, 40, 63, 87	0
19	1X	95/96 (98%)	0.26	1 (1%) 78 74	30, 45, 64, 83	0
19	2X	95/96 (98%)	0.46	2 (2%) 63 58	33, 49, 67, 83	0
20	1Y	107/110 (97%)	0.85	7 (6%) 25 19	41, 59, 74, 83	0
20	2Y	107/110 (97%)	0.84	8 (7%) 20 16	44, 63, 76, 85	0
21	1Z	154/206 (74%)	0.53	13 (8%) 17 13	37, 65, 87, 93	0
21	2Z	160/206 (77%)	1.46	36 (22%) 2 2	67, 83, 93, 102	0
22	10	83/85 (97%)	0.05	4 (4%) 35 30	26, 40, 64, 76	0
22	20	83/85 (97%)	1.20	11 (13%) 7 5	53, 66, 77, 84	0
23	11	97/98 (98%)	0.11	3 (3%) 51 45	27, 46, 72, 81	0
23	21	97/98 (98%)	0.57	4 (4%) 41 36	37, 57, 76, 82	0
24	12	70/72 (97%)	0.76	6 (8%) 16 12	41, 58, 69, 79	0
24	22	70/72 (97%)	0.70	3 (4%) 40 34	46, 63, 72, 79	0
25	13	59/60 (98%)	0.40	2 (3%) 48 42	33, 49, 67, 82	0
25	23	59/60 (98%)	0.34	1 (1%) 69 64	40, 54, 70, 84	0
26	14	69/71 (97%)	1.11	10 (14%) 6 4	65, 80, 89, 93	0
26	24	69/71 (97%)	1.52	17 (24%) 2 1	70, 81, 90, 94	0
27	15	59/60 (98%)	-0.14	1 (1%) 69 64	26, 37, 59, 70	0
27	25	59/60 (98%)	-0.19	0 100 100	30, 41, 62, 70	0
28	16	53/54 (98%)	0.25	0 100 100	39, 51, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.58	0	100 100	41, 55, 65, 72	0
29	17	48/49 (97%)	-0.05	3 (6%)	26 20	23, 32, 58, 71	0
29	27	48/49 (97%)	-0.21	1 (2%)	63 58	25, 35, 60, 72	0
30	18	64/65 (98%)	0.36	2 (3%)	51 45	33, 43, 54, 68	0
30	28	64/65 (98%)	0.35	0	100 100	37, 46, 57, 68	0
31	19	37/37 (100%)	0.70	1 (2%)	56 50	39, 52, 67, 71	0
31	29	37/37 (100%)	0.99	3 (8%)	18 14	46, 58, 69, 75	0
32	1a	1488/1521 (97%)	0.24	51 (3%)	48 42	35, 67, 91, 106	0
32	2a	1491/1521 (98%)	0.68	122 (8%)	17 14	49, 77, 95, 105	0
33	1b	231/256 (90%)	1.31	47 (20%)	3 2	65, 82, 89, 91	0
33	2b	231/256 (90%)	1.76	77 (33%)	1 1	67, 83, 90, 93	0
34	1c	206/239 (86%)	0.97	16 (7%)	19 15	67, 78, 85, 91	0
34	2c	206/239 (86%)	1.71	71 (34%)	1 1	69, 80, 87, 90	0
35	1d	208/209 (99%)	0.97	19 (9%)	15 11	59, 72, 80, 87	0
35	2d	208/209 (99%)	0.89	10 (4%)	35 30	60, 72, 80, 88	0
36	1e	148/162 (91%)	0.83	6 (4%)	41 36	58, 71, 81, 86	0
36	2e	148/162 (91%)	1.30	22 (14%)	5 4	62, 73, 82, 87	0
37	1f	100/101 (99%)	0.50	3 (3%)	52 47	52, 67, 77, 82	0
37	2f	100/101 (99%)	0.66	3 (3%)	52 47	59, 70, 80, 83	0
38	1g	155/156 (99%)	0.90	16 (10%)	12 9	65, 75, 84, 94	0
38	2g	155/156 (99%)	1.02	15 (9%)	13 10	66, 76, 85, 96	0
39	1h	137/138 (99%)	0.73	8 (5%)	29 23	60, 72, 78, 84	0
39	2h	137/138 (99%)	1.01	8 (5%)	29 23	62, 74, 80, 86	0
40	1i	127/128 (99%)	1.05	15 (11%)	9 7	52, 76, 85, 86	0
40	2i	127/128 (99%)	1.94	56 (44%)	0 0	67, 84, 90, 93	0
41	1j	97/105 (92%)	1.40	18 (18%)	3 3	57, 78, 87, 93	0
41	2j	96/105 (91%)	2.19	53 (55%)	0 0	73, 86, 92, 95	0
42	1k	114/129 (88%)	0.76	8 (7%)	22 18	52, 70, 80, 83	0
42	2k	114/129 (88%)	0.83	10 (8%)	15 12	53, 71, 81, 83	0
43	1l	121/132 (91%)	0.66	10 (8%)	17 13	51, 61, 73, 81	0
43	2l	121/132 (91%)	0.92	6 (4%)	34 28	53, 64, 74, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.79	9 (7%) 21 17	57, 70, 80, 88	0
44	2m	122/126 (96%)	1.74	40 (32%) 1 1	71, 84, 90, 92	0
45	1n	60/61 (98%)	0.93	3 (5%) 34 28	59, 68, 75, 78	0
45	2n	60/61 (98%)	2.32	39 (65%) 0 0	72, 84, 90, 93	0
46	1o	88/89 (98%)	0.93	9 (10%) 12 9	55, 69, 79, 82	0
46	2o	88/89 (98%)	0.74	3 (3%) 48 42	58, 70, 80, 83	0
47	1p	82/88 (93%)	1.49	20 (24%) 2 1	57, 71, 80, 83	0
47	2p	82/88 (93%)	1.24	10 (12%) 8 6	58, 71, 80, 83	0
48	1q	99/105 (94%)	1.01	6 (6%) 27 22	58, 71, 81, 84	0
48	2q	99/105 (94%)	0.85	3 (3%) 52 47	62, 72, 80, 85	0
49	1r	68/88 (77%)	0.62	3 (4%) 39 33	60, 69, 80, 81	0
49	2r	68/88 (77%)	0.55	1 (1%) 72 68	61, 70, 80, 83	0
50	1s	83/93 (89%)	1.07	8 (9%) 13 10	68, 79, 85, 91	0
50	2s	83/93 (89%)	1.84	27 (32%) 1 1	71, 81, 87, 91	0
51	1t	96/106 (90%)	1.11	12 (12%) 8 6	61, 71, 82, 84	0
51	2t	96/106 (90%)	0.98	9 (9%) 14 11	61, 71, 82, 85	0
52	1u	23/27 (85%)	1.38	6 (26%) 1 1	69, 73, 77, 79	0
52	2u	23/27 (85%)	1.80	10 (43%) 0 0	73, 75, 79, 81	0
53	1v	13/24 (54%)	0.85	2 (15%) 5 4	56, 67, 85, 95	0
53	2v	13/24 (54%)	1.49	4 (30%) 1 1	60, 72, 88, 95	0
54	1w	67/76 (88%)	1.35	17 (25%) 1 1	51, 88, 97, 101	0
54	1y	67/76 (88%)	1.30	12 (17%) 3 3	37, 92, 99, 103	0
54	2w	65/76 (85%)	1.66	19 (29%) 1 1	63, 94, 101, 103	0
54	2y	66/76 (86%)	1.54	16 (24%) 2 1	50, 96, 100, 102	0
55	1x	72/77 (93%)	0.47	5 (6%) 23 18	33, 67, 85, 91	0
55	2x	72/77 (93%)	0.83	1 (1%) 73 69	53, 81, 90, 95	0
All	All	20873/21748 (95%)	0.49	1553 (7%) 20 16	23, 63, 89, 106	1 (0%)

The worst 5 of 1553 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	931	C	7.3
1	1A	932	C	7.0

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Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	6.8
45	1n	2	ALA	6.6
7	1H	2	SER	6.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	7MG	1y	46	24/25	0.51	0.18	79,97,103,116	0
54	7MG	2w	46	24/25	0.53	0.16	85,97,104,130	0
54	4SU	2y	8	20/21	0.62	0.17	82,99,109,121	0
54	7MG	2y	46	24/25	0.67	0.17	83,97,105,122	0
54	5MU	2y	54	21/22	0.67	0.16	83,92,101,129	0
54	PSU	2y	55	20/21	0.67	0.16	88,97,113,114	0
54	4SU	1y	8	20/21	0.68	0.14	80,95,102,108	0
54	7MG	1w	46	24/25	0.69	0.17	74,88,107,126	0
54	PSU	1y	55	20/21	0.72	0.15	86,96,105,118	0
54	4SU	2w	8	20/21	0.72	0.14	85,97,111,115	0
54	MIA	2y	37	22/30	0.73	0.13	66,89,94,118	0
54	5MU	1y	54	21/22	0.76	0.15	84,90,99,116	0
54	PSU	2y	32	20/21	0.76	0.14	67,90,100,108	0
54	MIA	1y	37	22/30	0.79	0.15	77,86,92,97	0
54	PSU	1y	32	20/21	0.79	0.14	76,91,99,99	0
54	4SU	1w	8	20/21	0.80	0.15	80,86,108,116	0
54	5MU	2w	54	21/22	0.82	0.11	71,81,87,95	0
54	PSU	2y	39	20/21	0.83	0.12	83,88,96,110	0
55	PSU	2x	55	20/21	0.84	0.12	77,86,93,98	0
55	5MU	2x	54	21/22	0.85	0.14	72,87,94,102	0
55	4SU	2x	8	20/21	0.85	0.13	72,85,92,94	0
32	2MG	2a	1207	24/25	0.86	0.12	73,86,90,101	0
54	PSU	2w	55	20/21	0.86	0.11	73,84,98,98	0
1	5MU	2A	1915	21/22	0.87	0.13	62,69,75,82	0
54	PSU	1y	39	20/21	0.87	0.12	77,83,87,97	0
54	PSU	1w	55	20/21	0.88	0.10	64,78,85,90	0
55	PSU	1x	55	20/21	0.89	0.10	54,69,89,90	0
55	5MU	1x	54	21/22	0.90	0.11	59,70,77,78	0
32	5MC	2a	967	21/22	0.90	0.13	66,74,80,89	0
43	0TD	1l	92	10/11	0.90	0.14	56,62,65,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	M2G	2a	966	25/26	0.90	0.16	55,70,86,91	0
32	PSU	2a	516	20/21	0.91	0.11	63,75,81,88	0
32	4OC	2a	1402	22/23	0.91	0.12	50,64,75,79	0
54	PSU	2w	32	20/21	0.91	0.12	66,80,98,99	0
32	5MC	2a	1404	21/22	0.91	0.12	53,58,65,72	0
43	0TD	2l	92	10/11	0.92	0.11	62,64,70,87	0
32	7MG	2a	527	24/25	0.92	0.11	52,60,75,82	0
54	PSU	2w	39	20/21	0.92	0.11	72,83,93,94	0
1	PSU	2A	1917	20/21	0.92	0.10	56,65,69,73	0
55	5MC	2x	32	21/22	0.93	0.12	68,77,83,89	0
54	PSU	1w	32	20/21	0.93	0.11	58,70,78,82	0
54	MIA	2w	37	25/30	0.93	0.11	61,76,85,87	0
55	4SU	1x	8	20/21	0.93	0.11	58,70,80,91	0
1	PSU	2A	1911	20/21	0.93	0.09	53,61,67,68	0
1	5MU	1A	1937	21/22	0.94	0.11	57,65,71,73	0
32	5MC	2a	1407	21/22	0.94	0.12	40,56,69,76	0
32	UR3	2a	1498	21/22	0.94	0.12	51,59,70,72	0
1	5MC	2A	1962	21/22	0.94	0.10	28,44,54,61	0
54	MIA	1w	37	29/30	0.95	0.13	46,57,69,76	0
1	5MC	2A	1942	21/22	0.95	0.11	49,54,59,64	0
32	7MG	1a	527	24/25	0.95	0.08	33,46,53,62	0
54	5MU	1w	54	21/22	0.95	0.08	43,64,74,80	0
32	2MG	1a	1207	24/25	0.95	0.09	60,68,75,76	0
32	MA6	2a	1518	24/25	0.95	0.12	53,67,75,80	0
32	MA6	2a	1519	24/25	0.95	0.13	44,68,73,79	0
32	5MC	2a	1400	21/22	0.95	0.11	66,70,79,87	0
1	4OC	2A	1920	21/23	0.95	0.10	45,57,62,65	0
32	MA6	1a	1519	24/25	0.96	0.09	38,45,51,54	0
1	5MC	1A	1964	21/22	0.96	0.10	45,50,57,58	0
1	OMG	2A	2251	24/25	0.96	0.08	29,35,40,47	0
32	PSU	1a	516	20/21	0.96	0.08	48,58,65,70	0
55	5MC	1x	32	21/22	0.96	0.10	49,54,65,69	0
54	PSU	1w	39	20/21	0.96	0.09	55,68,77,79	0
1	PSU	1A	1933	20/21	0.96	0.10	50,57,63,64	0
32	M2G	1a	966	25/26	0.96	0.10	44,57,68,77	0
1	PSU	1A	1939	20/21	0.96	0.09	54,61,64,67	0
1	5MU	2A	1939	21/22	0.96	0.09	29,36,40,43	0
32	5MC	1a	967	21/22	0.97	0.08	44,52,68,72	0
1	4OC	1A	1942	21/23	0.97	0.09	39,56,58,62	0
32	5MC	1a	1400	21/22	0.97	0.10	41,53,58,62	0
1	2MA	2A	2503	23/24	0.97	0.07	24,29,34,40	0
1	PSU	2A	2605	20/21	0.97	0.07	29,35,43,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.09	38,47,55,64	0
32	5MC	1a	1404	21/22	0.97	0.09	37,44,49,52	0
32	5MC	1a	1407	21/22	0.97	0.07	34,42,47,48	0
32	MA6	1a	1518	24/25	0.97	0.10	30,41,50,51	0
1	2MA	1A	2515	23/24	0.98	0.06	19,26,31,32	0
1	2MU	1A	2564	21/23	0.98	0.07	26,35,40,42	0
1	PSU	1A	2617	20/21	0.98	0.06	27,32,41,41	0
1	5MU	1A	1961	21/22	0.98	0.08	28,34,41,42	0
1	5MC	1A	1984	21/22	0.98	0.06	27,41,49,56	0
1	2MU	2A	2552	21/23	0.98	0.06	32,36,44,51	0
1	OMG	1A	2263	24/25	0.98	0.06	26,30,36,39	0
32	UR3	1a	1498	21/22	0.98	0.07	35,46,50,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1833	1/1	0.47	0.26	79,79,79,79	0
56	MG	1A	4123	1/1	0.48	0.22	79,79,79,79	0
56	MG	1a	1712	1/1	0.55	0.30	83,83,83,83	0
56	MG	1A	3779	1/1	0.56	0.21	80,80,80,80	0
56	MG	2y	3004	1/1	0.56	0.29	86,86,86,86	0
56	MG	2a	1813	1/1	0.57	0.32	78,78,78,78	0
56	MG	1B	3028	1/1	0.58	0.30	82,82,82,82	0
56	MG	1A	3762	1/1	0.59	0.24	56,56,56,56	0
56	MG	2A	3700	1/1	0.60	0.26	68,68,68,68	0
56	MG	1B	3027	1/1	0.60	0.11	87,87,87,87	0
56	MG	2a	1623	1/1	0.61	0.19	81,81,81,81	0
56	MG	1A	3740	1/1	0.62	0.21	71,71,71,71	0
56	MG	1a	1658	1/1	0.64	0.29	79,79,79,79	0
56	MG	1a	1821	1/1	0.65	0.13	81,81,81,81	0
56	MG	2A	3725	1/1	0.65	0.15	76,76,76,76	0
56	MG	17	102	1/1	0.66	0.47	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	2j	8002	1/1	0.66	0.15	74,74,74,74	0
56	MG	2A	3673	1/1	0.66	0.18	59,59,59,59	0
56	MG	2y	3005	1/1	0.66	0.18	94,94,94,94	0
56	MG	1a	1791	1/1	0.67	0.29	88,88,88,88	0
56	MG	1A	4139	1/1	0.67	0.14	70,70,70,70	0
56	MG	2A	3340	1/1	0.67	0.22	74,74,74,74	0
56	MG	1A	3541	1/1	0.67	0.15	58,58,58,58	0
56	MG	1A	3263	1/1	0.68	0.28	76,76,76,76	0
56	MG	2A	3766	1/1	0.68	0.14	58,58,58,58	0
56	MG	2A	3506	1/1	0.69	0.26	61,61,61,61	0
56	MG	2B	3011	1/1	0.69	0.16	69,69,69,69	0
56	MG	1A	3933	1/1	0.70	0.18	56,56,56,56	0
56	MG	1a	1879	1/1	0.70	0.22	82,82,82,82	0
56	MG	1A	3558	1/1	0.70	0.26	75,75,75,75	0
56	MG	2x	102	1/1	0.70	0.42	88,88,88,88	0
56	MG	1A	3825	1/1	0.70	0.13	24,24,24,24	0
56	MG	1a	1816	1/1	0.70	0.26	72,72,72,72	0
56	MG	2a	1764	1/1	0.71	0.18	89,89,89,89	0
56	MG	1w	110	1/1	0.71	0.27	85,85,85,85	0
56	MG	1E	308	1/1	0.71	0.22	69,69,69,69	0
56	MG	2a	1849	1/1	0.71	0.44	82,82,82,82	0
56	MG	1A	4038	1/1	0.71	0.20	97,97,97,97	0
56	MG	2a	1629	1/1	0.71	0.29	88,88,88,88	0
56	MG	2a	1656	1/1	0.71	0.26	86,86,86,86	0
56	MG	2a	1725	1/1	0.71	0.38	75,75,75,75	0
56	MG	1y	105	1/1	0.72	0.13	88,88,88,88	0
56	MG	2A	3202	1/1	0.72	0.19	56,56,56,56	0
56	MG	2A	3805	1/1	0.72	0.32	54,54,54,54	0
56	MG	2A	3910	1/1	0.72	0.16	76,76,76,76	0
56	MG	1A	3266	1/1	0.72	0.26	64,64,64,64	0
56	MG	2B	3016	1/1	0.72	0.21	70,70,70,70	0
56	MG	1A	3454	1/1	0.72	0.36	55,55,55,55	0
56	MG	1A	4084	1/1	0.72	0.20	94,94,94,94	0
56	MG	1A	3862	1/1	0.72	0.24	73,73,73,73	0
56	MG	1a	1743	1/1	0.73	0.39	77,77,77,77	0
56	MG	1w	103	1/1	0.73	0.31	79,79,79,79	0
56	MG	1A	3534	1/1	0.73	0.17	92,92,92,92	0
56	MG	2A	3718	1/1	0.73	0.16	61,61,61,61	0
56	MG	2A	3368	1/1	0.73	0.22	69,69,69,69	0
56	MG	2a	1603	1/1	0.73	0.16	70,70,70,70	0
56	MG	1a	1795	1/1	0.74	0.23	75,75,75,75	0
56	MG	1a	1640	1/1	0.74	0.38	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3460	1/1	0.74	0.24	65,65,65,65	0
56	MG	2A	3492	1/1	0.74	0.30	68,68,68,68	0
56	MG	1A	3422	1/1	0.74	0.21	63,63,63,63	0
56	MG	2A	3669	1/1	0.74	0.15	70,70,70,70	0
56	MG	2a	1752	1/1	0.74	0.19	101,101,101,101	0
56	MG	1a	1691	1/1	0.74	0.41	69,69,69,69	0
56	MG	1B	3034	1/1	0.74	0.16	82,82,82,82	0
56	MG	1a	1725	1/1	0.74	0.41	72,72,72,72	0
56	MG	1x	112	1/1	0.74	0.24	77,77,77,77	0
56	MG	1B	3011	1/1	0.74	0.24	78,78,78,78	0
56	MG	2A	3115	1/1	0.74	0.17	56,56,56,56	0
56	MG	1A	3892	1/1	0.74	0.18	55,55,55,55	0
56	MG	2A	3215	1/1	0.74	0.20	78,78,78,78	0
56	MG	2y	3007	1/1	0.74	0.14	82,82,82,82	0
56	MG	1A	3936	1/1	0.75	0.33	77,77,77,77	0
56	MG	2B	3015	1/1	0.75	0.24	70,70,70,70	0
56	MG	1Z	303	1/1	0.75	0.14	73,73,73,73	0
56	MG	1w	106	1/1	0.75	0.15	81,81,81,81	0
56	MG	2A	3469	1/1	0.75	0.21	67,67,67,67	0
56	MG	2a	1625	1/1	0.75	0.29	86,86,86,86	0
56	MG	2A	3476	1/1	0.75	0.27	70,70,70,70	0
56	MG	1A	4027	1/1	0.75	0.18	66,66,66,66	0
56	MG	1w	111	1/1	0.75	0.17	74,74,74,74	0
56	MG	2a	1730	1/1	0.75	0.22	76,76,76,76	0
56	MG	1a	1755	1/1	0.75	0.43	83,83,83,83	0
56	MG	1A	3845	1/1	0.75	0.24	81,81,81,81	0
56	MG	2A	3677	1/1	0.75	0.15	57,57,57,57	0
56	MG	2A	3064	1/1	0.75	0.22	74,74,74,74	0
56	MG	1a	1654	1/1	0.75	0.28	81,81,81,81	0
56	MG	1A	3922	1/1	0.75	0.21	54,54,54,54	0
56	MG	2A	3213	1/1	0.75	0.14	58,58,58,58	0
56	MG	2y	3002	1/1	0.75	0.30	79,79,79,79	0
56	MG	2A	3796	1/1	0.75	0.26	71,71,71,71	0
56	MG	1A	3438	1/1	0.75	0.16	52,52,52,52	0
56	MG	2A	3257	1/1	0.75	0.28	69,69,69,69	0
56	MG	1A	3694	1/1	0.76	0.21	65,65,65,65	0
56	MG	1a	1693	1/1	0.76	0.28	63,63,63,63	0
56	MG	2a	1658	1/1	0.76	0.16	81,81,81,81	0
56	MG	2A	3339	1/1	0.76	0.15	64,64,64,64	0
56	MG	1y	104	1/1	0.76	0.32	79,79,79,79	0
56	MG	1A	3329	1/1	0.76	0.21	59,59,59,59	0
56	MG	2A	3370	1/1	0.76	0.18	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	3937	1/1	0.76	0.24	45,45,45,45	0
56	MG	2A	3099	1/1	0.76	0.36	71,71,71,71	0
56	MG	1A	4132	1/1	0.76	0.30	62,62,62,62	0
56	MG	2A	3193	1/1	0.76	0.37	70,70,70,70	0
56	MG	1A	3537	1/1	0.76	0.14	67,67,67,67	0
56	MG	2A	3605	1/1	0.76	0.17	70,70,70,70	0
56	MG	2a	1621	1/1	0.76	0.19	77,77,77,77	0
56	MG	1a	1665	1/1	0.76	0.36	69,69,69,69	0
56	MG	2A	3214	1/1	0.76	0.17	64,64,64,64	0
58	CPT	1A	4179	4/5	0.76	0.52	54,72,88,231	4
58	CPT	2A	3918	3/5	0.76	0.29	62,62,65,108	3
56	MG	1a	1713	1/1	0.77	0.37	73,73,73,73	0
56	MG	2A	3694	1/1	0.77	0.20	63,63,63,63	0
56	MG	1a	1622	1/1	0.77	0.39	79,79,79,79	0
56	MG	2v	104	1/1	0.77	0.20	70,70,70,70	0
56	MG	2w	102	1/1	0.77	0.24	81,81,81,81	0
56	MG	2w	103	1/1	0.77	0.19	75,75,75,75	0
56	MG	2x	101	1/1	0.77	0.42	82,82,82,82	0
56	MG	2A	3551	1/1	0.77	0.20	63,63,63,63	0
56	MG	2A	3291	1/1	0.77	0.12	53,53,53,53	0
56	MG	20	101	1/1	0.77	0.22	71,71,71,71	0
56	MG	2a	1731	1/1	0.77	0.35	80,80,80,80	0
56	MG	1A	3423	1/1	0.77	0.17	59,59,59,59	0
56	MG	2A	3768	1/1	0.77	0.19	46,46,46,46	0
56	MG	1a	1746	1/1	0.77	0.26	70,70,70,70	0
56	MG	2A	3272	1/1	0.78	0.20	68,68,68,68	0
56	MG	2A	3278	1/1	0.78	0.18	64,64,64,64	0
56	MG	1G	3005	1/1	0.78	0.20	69,69,69,69	0
56	MG	1A	3575	1/1	0.78	0.22	63,63,63,63	0
56	MG	1A	3611	1/1	0.78	0.23	61,61,61,61	0
56	MG	1A	3208	1/1	0.78	0.21	67,67,67,67	0
56	MG	1A	3359	1/1	0.78	0.13	66,66,66,66	0
56	MG	2A	3385	1/1	0.78	0.12	70,70,70,70	0
56	MG	2A	3429	1/1	0.78	0.12	69,69,69,69	0
56	MG	1a	1886	1/1	0.78	0.15	71,71,71,71	0
56	MG	1A	3755	1/1	0.78	0.13	34,34,34,34	0
56	MG	1A	3513	1/1	0.78	0.27	74,74,74,74	0
56	MG	1A	3520	1/1	0.78	0.19	61,61,61,61	0
56	MG	1a	1670	1/1	0.78	0.35	72,72,72,72	0
56	MG	1A	4124	1/1	0.78	0.16	86,86,86,86	0
56	MG	1y	103	1/1	0.78	0.26	89,89,89,89	0
56	MG	1A	3788	1/1	0.78	0.14	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	2a	1831	1/1	0.78	0.21	75,75,75,75	0
56	MG	1A	3377	1/1	0.78	0.23	68,68,68,68	0
56	MG	1A	3259	1/1	0.78	0.21	54,54,54,54	0
56	MG	1a	1719	1/1	0.78	0.27	73,73,73,73	0
56	MG	1A	3854	1/1	0.78	0.16	64,64,64,64	0
56	MG	2A	3174	1/1	0.78	0.28	77,77,77,77	0
56	MG	1A	3313	1/1	0.78	0.19	60,60,60,60	0
56	MG	2w	108	1/1	0.78	0.23	70,70,70,70	0
56	MG	1A	3556	1/1	0.78	0.11	63,63,63,63	0
56	MG	1a	1747	1/1	0.78	0.46	70,70,70,70	0
56	MG	2x	103	1/1	0.78	0.23	77,77,77,77	0
56	MG	2A	3774	1/1	0.78	0.22	62,62,62,62	0
56	MG	2A	3780	1/1	0.78	0.25	63,63,63,63	0
56	MG	1a	1751	1/1	0.78	0.18	70,70,70,70	0
56	MG	1A	3424	1/1	0.78	0.20	68,68,68,68	0
56	MG	2A	3823	1/1	0.78	0.15	54,54,54,54	0
56	MG	1a	1760	1/1	0.78	0.32	75,75,75,75	0
56	MG	2a	1670	1/1	0.79	0.22	71,71,71,71	0
56	MG	2a	1719	1/1	0.79	0.27	77,77,77,77	0
56	MG	2a	1723	1/1	0.79	0.24	87,87,87,87	0
56	MG	1A	3738	1/1	0.79	0.11	36,36,36,36	0
56	MG	1a	1716	1/1	0.79	0.35	75,75,75,75	0
56	MG	2A	3769	1/1	0.79	0.12	58,58,58,58	0
56	MG	2a	1743	1/1	0.79	0.36	72,72,72,72	0
56	MG	1A	3385	1/1	0.79	0.42	74,74,74,74	0
56	MG	2A	3197	1/1	0.79	0.14	60,60,60,60	0
56	MG	2a	1812	1/1	0.79	0.17	66,66,66,66	0
56	MG	1A	3863	1/1	0.79	0.20	51,51,51,51	0
56	MG	1a	1740	1/1	0.79	0.32	72,72,72,72	0
56	MG	1A	3870	1/1	0.79	0.23	67,67,67,67	0
56	MG	2A	3536	1/1	0.79	0.20	63,63,63,63	0
56	MG	2j	8001	1/1	0.79	0.15	66,66,66,66	0
56	MG	1A	3312	1/1	0.79	0.31	63,63,63,63	0
56	MG	2l	201	1/1	0.79	0.18	76,76,76,76	0
56	MG	1A	3480	1/1	0.79	0.24	64,64,64,64	0
56	MG	2A	3663	1/1	0.79	0.16	68,68,68,68	0
56	MG	2F	302	1/1	0.79	0.17	58,58,58,58	0
56	MG	2w	104	1/1	0.79	0.14	73,73,73,73	0
56	MG	2U	3001	1/1	0.79	0.17	56,56,56,56	0
56	MG	1a	1749	1/1	0.79	0.20	61,61,61,61	0
56	MG	1A	3776	1/1	0.79	0.20	78,78,78,78	0
56	MG	1A	3505	1/1	0.79	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3254	1/1	0.79	0.28	61,61,61,61	0
56	MG	1A	3327	1/1	0.79	0.38	65,65,65,65	0
56	MG	2A	3087	1/1	0.79	0.13	53,53,53,53	0
56	MG	2a	1646	1/1	0.79	0.31	67,67,67,67	0
56	MG	1A	3429	1/1	0.79	0.16	59,59,59,59	0
56	MG	2A	3749	1/1	0.79	0.23	70,70,70,70	0
56	MG	2A	3463	1/1	0.80	0.33	65,65,65,65	0
56	MG	1A	4087	1/1	0.80	0.14	81,81,81,81	0
56	MG	1A	3617	1/1	0.80	0.35	80,80,80,80	0
56	MG	2A	3789	1/1	0.80	0.13	49,49,49,49	0
56	MG	2A	3481	1/1	0.80	0.27	68,68,68,68	0
56	MG	2a	1747	1/1	0.80	0.18	73,73,73,73	0
56	MG	1Y	204	1/1	0.80	0.12	71,71,71,71	0
56	MG	1x	104	1/1	0.80	0.33	65,65,65,65	0
56	MG	1x	111	1/1	0.80	0.16	73,73,73,73	0
56	MG	1a	1759	1/1	0.80	0.22	79,79,79,79	0
56	MG	1y	102	1/1	0.80	0.12	61,61,61,61	0
56	MG	2A	3629	1/1	0.80	0.12	33,33,33,33	0
56	MG	2a	1834	1/1	0.80	0.24	71,71,71,71	0
56	MG	1A	3638	1/1	0.80	0.31	70,70,70,70	0
56	MG	2R	203	1/1	0.80	0.15	54,54,54,54	0
56	MG	1A	3457	1/1	0.80	0.21	69,69,69,69	0
56	MG	1A	3956	1/1	0.80	0.20	62,62,62,62	0
56	MG	25	105	1/1	0.80	0.24	81,81,81,81	0
56	MG	1A	4196	1/1	0.80	0.29	64,64,64,64	0
56	MG	1A	3319	1/1	0.80	0.18	57,57,57,57	0
56	MG	2A	3695	1/1	0.80	0.11	58,58,58,58	0
56	MG	1a	1831	1/1	0.80	0.11	88,88,88,88	0
56	MG	2A	3376	1/1	0.80	0.17	68,68,68,68	0
56	MG	1A	3315	1/1	0.80	0.30	68,68,68,68	0
56	MG	2a	1647	1/1	0.80	0.29	63,63,63,63	0
56	MG	2A	3726	1/1	0.80	0.14	67,67,67,67	0
56	MG	1A	4063	1/1	0.80	0.17	41,41,41,41	0
56	MG	2A	3445	1/1	0.80	0.20	49,49,49,49	0
56	MG	2a	1673	1/1	0.80	0.41	79,79,79,79	0
56	MG	2a	1682	1/1	0.80	0.34	70,70,70,70	0
56	MG	1A	3613	1/1	0.80	0.15	56,56,56,56	0
56	MG	1A	3265	1/1	0.81	0.18	64,64,64,64	0
56	MG	2A	3290	1/1	0.81	0.10	59,59,59,59	0
56	MG	1A	3464	1/1	0.81	0.22	69,69,69,69	0
56	MG	2A	3834	1/1	0.81	0.12	49,49,49,49	0
56	MG	2A	3846	1/1	0.81	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	2A	3537	1/1	0.81	0.18	51,51,51,51	0
56	MG	2A	3913	1/1	0.81	0.18	68,68,68,68	0
56	MG	2A	3302	1/1	0.81	0.14	67,67,67,67	0
56	MG	2A	3330	1/1	0.81	0.20	66,66,66,66	0
56	MG	1A	4057	1/1	0.81	0.19	90,90,90,90	0
56	MG	1A	3479	1/1	0.81	0.17	72,72,72,72	0
56	MG	1A	3211	1/1	0.81	0.19	76,76,76,76	0
56	MG	2S	201	1/1	0.81	0.20	83,83,83,83	0
56	MG	1A	3698	1/1	0.81	0.17	64,64,64,64	0
56	MG	1A	3414	1/1	0.81	0.29	62,62,62,62	0
56	MG	1A	3416	1/1	0.81	0.27	78,78,78,78	0
56	MG	2A	3392	1/1	0.81	0.19	67,67,67,67	0
56	MG	2q	204	1/1	0.81	0.22	79,79,79,79	0
56	MG	2A	3424	1/1	0.81	0.16	68,68,68,68	0
56	MG	1a	1703	1/1	0.81	0.39	81,81,81,81	0
56	MG	1A	3063	1/1	0.81	0.50	69,69,69,69	0
56	MG	2A	3453	1/1	0.81	0.37	64,64,64,64	0
56	MG	2A	3729	1/1	0.81	0.24	66,66,66,66	0
56	MG	16	101	1/1	0.81	0.31	62,62,62,62	0
56	MG	1A	4002	1/1	0.81	0.21	55,55,55,55	0
56	MG	2A	3248	1/1	0.81	0.19	54,54,54,54	0
56	MG	2x	105	1/1	0.81	0.20	63,63,63,63	0
56	MG	2a	1669	1/1	0.81	0.17	75,75,75,75	0
56	MG	2A	3470	1/1	0.81	0.34	63,63,63,63	0
56	MG	2A	3472	1/1	0.81	0.28	61,61,61,61	0
56	MG	1a	1801	1/1	0.81	0.27	67,67,67,67	0
56	MG	2a	1691	1/1	0.81	0.24	72,72,72,72	0
56	MG	1a	1606	1/1	0.81	0.25	61,61,61,61	0
56	MG	2a	1662	1/1	0.82	0.29	81,81,81,81	0
56	MG	1A	3463	1/1	0.82	0.31	66,66,66,66	0
56	MG	1A	3545	1/1	0.82	0.14	53,53,53,53	0
56	MG	1A	3415	1/1	0.82	0.24	68,68,68,68	0
56	MG	1A	3867	1/1	0.82	0.18	57,57,57,57	0
56	MG	2a	1684	1/1	0.82	0.31	67,67,67,67	0
56	MG	1A	4116	1/1	0.82	0.34	47,47,47,47	0
56	MG	1A	3356	1/1	0.82	0.16	65,65,65,65	0
56	MG	2A	3458	1/1	0.82	0.18	57,57,57,57	0
56	MG	1A	3523	1/1	0.82	0.17	72,72,72,72	0
56	MG	1a	1815	1/1	0.82	0.19	74,74,74,74	0
56	MG	2A	3212	1/1	0.82	0.24	74,74,74,74	0
56	MG	1A	3908	1/1	0.82	0.16	67,67,67,67	0
56	MG	1A	3759	1/1	0.82	0.18	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	3531	1/1	0.82	0.19	66,66,66,66	0
56	MG	2a	1756	1/1	0.82	0.15	95,95,95,95	0
56	MG	1B	3002	1/1	0.82	0.22	58,58,58,58	0
56	MG	1a	1702	1/1	0.82	0.18	92,92,92,92	0
56	MG	2A	3261	1/1	0.82	0.17	72,72,72,72	0
56	MG	2a	1822	1/1	0.82	0.28	66,66,66,66	0
56	MG	2B	3006	1/1	0.82	0.23	71,71,71,71	0
56	MG	2A	3533	1/1	0.82	0.11	48,48,48,48	0
56	MG	2B	3014	1/1	0.82	0.14	75,75,75,75	0
56	MG	2a	1848	1/1	0.82	0.17	75,75,75,75	0
56	MG	1A	3357	1/1	0.82	0.13	59,59,59,59	0
56	MG	1B	3015	1/1	0.82	0.14	55,55,55,55	0
56	MG	2A	3284	1/1	0.82	0.17	64,64,64,64	0
56	MG	1B	3019	1/1	0.82	0.13	58,58,58,58	0
56	MG	1A	3535	1/1	0.82	0.21	75,75,75,75	0
56	MG	2A	3645	1/1	0.82	0.17	68,68,68,68	0
56	MG	2A	3300	1/1	0.82	0.20	68,68,68,68	0
56	MG	1A	3786	1/1	0.82	0.11	70,70,70,70	0
56	MG	1A	3960	1/1	0.82	0.24	74,74,74,74	0
56	MG	2a	1611	1/1	0.82	0.26	75,75,75,75	0
56	MG	2a	1613	1/1	0.82	0.24	67,67,67,67	0
56	MG	1A	3961	1/1	0.82	0.17	59,59,59,59	0
56	MG	1F	301	1/1	0.82	0.16	78,78,78,78	0
56	MG	1A	3504	1/1	0.82	0.14	66,66,66,66	0
56	MG	1A	3656	1/1	0.82	0.17	70,70,70,70	0
56	MG	2A	3704	1/1	0.82	0.21	69,69,69,69	0
56	MG	2A	3708	1/1	0.82	0.13	42,42,42,42	0
56	MG	2a	1649	1/1	0.82	0.31	69,69,69,69	0
56	MG	2A	3372	1/1	0.82	0.12	68,68,68,68	0
56	MG	1A	3665	1/1	0.82	0.14	39,39,39,39	0
56	MG	2A	3750	1/1	0.83	0.21	81,81,81,81	0
56	MG	2A	3755	1/1	0.83	0.14	76,76,76,76	0
56	MG	2A	3756	1/1	0.83	0.18	66,66,66,66	0
56	MG	1A	3358	1/1	0.83	0.29	66,66,66,66	0
56	MG	2A	3265	1/1	0.83	0.20	70,70,70,70	0
56	MG	1A	3629	1/1	0.83	0.28	72,72,72,72	0
56	MG	1A	3945	1/1	0.83	0.16	43,43,43,43	0
56	MG	2A	3279	1/1	0.83	0.09	60,60,60,60	0
56	MG	2A	3785	1/1	0.83	0.12	59,59,59,59	0
56	MG	2A	3056	1/1	0.83	0.13	56,56,56,56	0
56	MG	2a	1701	1/1	0.83	0.25	84,84,84,84	0
56	MG	2a	1708	1/1	0.83	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3434	1/1	0.83	0.26	56,56,56,56	0
56	MG	1A	4110	1/1	0.83	0.15	54,54,54,54	0
56	MG	2A	3808	1/1	0.83	0.10	44,44,44,44	0
56	MG	2A	3482	1/1	0.83	0.17	71,71,71,71	0
56	MG	2A	3830	1/1	0.83	0.24	71,71,71,71	0
56	MG	2a	1736	1/1	0.83	0.40	69,69,69,69	0
56	MG	2A	3089	1/1	0.83	0.19	62,62,62,62	0
56	MG	2A	3096	1/1	0.83	0.12	52,52,52,52	0
56	MG	2A	3310	1/1	0.83	0.25	57,57,57,57	0
56	MG	2A	3326	1/1	0.83	0.17	69,69,69,69	0
56	MG	1a	1875	1/1	0.83	0.12	83,83,83,83	0
56	MG	2a	1804	1/1	0.83	0.21	77,77,77,77	0
56	MG	2A	3337	1/1	0.83	0.54	69,69,69,69	0
56	MG	1A	3958	1/1	0.83	0.17	51,51,51,51	0
56	MG	1A	3411	1/1	0.83	0.23	67,67,67,67	0
56	MG	2A	3347	1/1	0.83	0.13	58,58,58,58	0
56	MG	2B	3020	1/1	0.83	0.25	76,76,76,76	0
56	MG	2A	3348	1/1	0.83	0.40	75,75,75,75	0
56	MG	2a	1847	1/1	0.83	0.14	74,74,74,74	0
56	MG	2N	8001	1/1	0.83	0.11	55,55,55,55	0
56	MG	1A	3901	1/1	0.83	0.14	71,71,71,71	0
56	MG	1A	3977	1/1	0.83	0.19	77,77,77,77	0
56	MG	1T	202	1/1	0.83	0.15	59,59,59,59	0
56	MG	2A	3689	1/1	0.83	0.17	52,52,52,52	0
56	MG	1A	3190	1/1	0.83	0.44	67,67,67,67	0
56	MG	1A	3681	1/1	0.83	0.23	55,55,55,55	0
56	MG	2a	1604	1/1	0.83	0.20	80,80,80,80	0
56	MG	2a	1607	1/1	0.83	0.32	77,77,77,77	0
56	MG	1a	1783	1/1	0.83	0.15	69,69,69,69	0
56	MG	2A	3420	1/1	0.83	0.11	60,60,60,60	0
56	MG	2a	1615	1/1	0.83	0.34	73,73,73,73	0
56	MG	2a	1617	1/1	0.83	0.17	71,71,71,71	0
56	MG	2A	3422	1/1	0.83	0.12	67,67,67,67	0
56	MG	1l	104	1/1	0.83	0.29	66,66,66,66	0
56	MG	1x	113	1/1	0.83	0.14	66,66,66,66	0
56	MG	1A	3334	1/1	0.83	0.18	65,65,65,65	0
56	MG	2a	1633	1/1	0.83	0.38	76,76,76,76	0
56	MG	2a	1644	1/1	0.83	0.36	70,70,70,70	0
56	MG	2A	3258	1/1	0.83	0.10	59,59,59,59	0
56	MG	2A	3456	1/1	0.83	0.36	62,62,62,62	0
56	MG	2a	1661	1/1	0.84	0.20	69,69,69,69	0
56	MG	1A	3856	1/1	0.84	0.19	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	1a	1673	1/1	0.84	0.27	74,74,74,74	0
56	MG	1A	3963	1/1	0.84	0.15	67,67,67,67	0
56	MG	1A	3970	1/1	0.84	0.19	54,54,54,54	0
56	MG	2A	3067	1/1	0.84	0.21	59,59,59,59	0
56	MG	2A	3822	1/1	0.84	0.12	73,73,73,73	0
56	MG	2A	3521	1/1	0.84	0.13	56,56,56,56	0
56	MG	2A	3522	1/1	0.84	0.17	33,33,33,33	0
56	MG	1A	3932	1/1	0.84	0.22	55,55,55,55	0
56	MG	2a	1711	1/1	0.84	0.21	69,69,69,69	0
56	MG	1A	3364	1/1	0.84	0.16	70,70,70,70	0
56	MG	2A	3886	1/1	0.84	0.19	67,67,67,67	0
56	MG	2A	3908	1/1	0.84	0.23	71,71,71,71	0
56	MG	2a	1729	1/1	0.84	0.32	75,75,75,75	0
56	MG	1a	1706	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3297	1/1	0.84	0.30	58,58,58,58	0
56	MG	2A	3557	1/1	0.84	0.10	34,34,34,34	0
56	MG	2a	1740	1/1	0.84	0.24	67,67,67,67	0
56	MG	2A	3103	1/1	0.84	0.17	58,58,58,58	0
56	MG	2a	1746	1/1	0.84	0.18	71,71,71,71	0
56	MG	1A	4162	1/1	0.84	0.12	42,42,42,42	0
56	MG	1A	4033	1/1	0.84	0.17	80,80,80,80	0
56	MG	2A	3656	1/1	0.84	0.17	45,45,45,45	0
56	MG	2A	3363	1/1	0.84	0.10	71,71,71,71	0
56	MG	1A	3059	1/1	0.84	0.15	65,65,65,65	0
56	MG	2a	1811	1/1	0.84	0.16	83,83,83,83	0
56	MG	1A	3517	1/1	0.84	0.14	58,58,58,58	0
56	MG	1a	1728	1/1	0.84	0.38	77,77,77,77	0
56	MG	2A	3375	1/1	0.84	0.12	66,66,66,66	0
56	MG	2a	1828	1/1	0.84	0.20	69,69,69,69	0
56	MG	1n	102	1/1	0.84	0.38	69,69,69,69	0
56	MG	1r	101	1/1	0.84	0.20	71,71,71,71	0
56	MG	1w	102	1/1	0.84	0.21	78,78,78,78	0
56	MG	2a	1840	1/1	0.84	0.17	73,73,73,73	0
56	MG	2a	1844	1/1	0.84	0.14	72,72,72,72	0
56	MG	1a	1730	1/1	0.84	0.36	72,72,72,72	0
56	MG	1A	3397	1/1	0.84	0.16	63,63,63,63	0
56	MG	2A	3255	1/1	0.84	0.33	64,64,64,64	0
56	MG	1a	1628	1/1	0.84	0.30	75,75,75,75	0
56	MG	1a	1637	1/1	0.84	0.29	62,62,62,62	0
56	MG	2A	3447	1/1	0.84	0.34	61,61,61,61	0
56	MG	2A	3732	1/1	0.84	0.21	65,65,65,65	0
56	MG	1A	4075	1/1	0.84	0.11	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	2A	3264	1/1	0.84	0.21	63,63,63,63	0
56	MG	1A	3004	1/1	0.84	0.18	41,41,41,41	0
56	MG	1A	3771	1/1	0.84	0.14	59,59,59,59	0
56	MG	2a	1630	1/1	0.84	0.30	70,70,70,70	0
56	MG	2A	3757	1/1	0.84	0.20	54,54,54,54	0
56	MG	2A	3763	1/1	0.84	0.12	64,64,64,64	0
56	MG	1a	1753	1/1	0.84	0.41	73,73,73,73	0
56	MG	1A	4092	1/1	0.84	0.10	76,76,76,76	0
56	MG	2y	3001	1/1	0.84	0.18	77,77,77,77	0
56	MG	2A	3283	1/1	0.84	0.10	57,57,57,57	0
56	MG	2a	1655	1/1	0.84	0.38	79,79,79,79	0
56	MG	2A	3471	1/1	0.84	0.21	58,58,58,58	0
56	MG	1a	1756	1/1	0.84	0.45	75,75,75,75	0
56	MG	2a	1659	1/1	0.84	0.10	80,80,80,80	0
56	MG	2a	1660	1/1	0.84	0.16	64,64,64,64	0
56	MG	1A	4042	1/1	0.85	0.20	74,74,74,74	0
56	MG	2A	3068	1/1	0.85	0.14	39,39,39,39	0
56	MG	2A	3706	1/1	0.85	0.16	51,51,51,51	0
56	MG	2A	3354	1/1	0.85	0.12	63,63,63,63	0
56	MG	2a	1648	1/1	0.85	0.34	80,80,80,80	0
56	MG	2A	3081	1/1	0.85	0.22	59,59,59,59	0
56	MG	2A	3724	1/1	0.85	0.12	55,55,55,55	0
56	MG	2A	3367	1/1	0.85	0.12	62,62,62,62	0
56	MG	1A	3679	1/1	0.85	0.25	57,57,57,57	0
56	MG	1a	1763	1/1	0.85	0.07	67,67,67,67	0
56	MG	1a	1766	1/1	0.85	0.27	67,67,67,67	0
56	MG	2A	3741	1/1	0.85	0.22	59,59,59,59	0
56	MG	2A	3748	1/1	0.85	0.11	51,51,51,51	0
56	MG	2a	1664	1/1	0.85	0.16	78,78,78,78	0
56	MG	1A	4058	1/1	0.85	0.14	74,74,74,74	0
56	MG	1A	3400	1/1	0.85	0.14	68,68,68,68	0
56	MG	1A	3522	1/1	0.85	0.17	64,64,64,64	0
56	MG	2A	3150	1/1	0.85	0.25	64,64,64,64	0
56	MG	2A	3395	1/1	0.85	0.23	65,65,65,65	0
56	MG	2a	1688	1/1	0.85	0.17	72,72,72,72	0
56	MG	2A	3399	1/1	0.85	0.23	60,60,60,60	0
56	MG	1D	302	1/1	0.85	0.25	53,53,53,53	0
56	MG	1a	1807	1/1	0.85	0.15	85,85,85,85	0
56	MG	1a	1694	1/1	0.85	0.30	57,57,57,57	0
56	MG	1D	312	1/1	0.85	0.20	46,46,46,46	0
56	MG	1A	3328	1/1	0.85	0.32	62,62,62,62	0
56	MG	2A	3782	1/1	0.85	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1827	1/1	0.85	0.16	92,92,92,92	0
56	MG	1A	3576	1/1	0.85	0.33	69,69,69,69	0
56	MG	1a	1833	1/1	0.85	0.13	73,73,73,73	0
56	MG	2A	3801	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3223	1/1	0.85	0.21	62,62,62,62	0
56	MG	2A	3231	1/1	0.85	0.23	58,58,58,58	0
56	MG	1a	1873	1/1	0.85	0.11	69,69,69,69	0
56	MG	2A	3468	1/1	0.85	0.31	56,56,56,56	0
56	MG	2a	1749	1/1	0.85	0.25	68,68,68,68	0
56	MG	2A	3250	1/1	0.85	0.13	71,71,71,71	0
56	MG	2A	3253	1/1	0.85	0.35	67,67,67,67	0
56	MG	1A	4090	1/1	0.85	0.20	77,77,77,77	0
56	MG	2a	1780	1/1	0.85	0.12	75,75,75,75	0
56	MG	2A	3851	1/1	0.85	0.13	46,46,46,46	0
56	MG	1A	3492	1/1	0.85	0.12	62,62,62,62	0
56	MG	1U	202	1/1	0.85	0.51	88,88,88,88	0
56	MG	1A	3498	1/1	0.85	0.15	52,52,52,52	0
56	MG	1a	1723	1/1	0.85	0.19	65,65,65,65	0
56	MG	2a	1823	1/1	0.85	0.21	68,68,68,68	0
56	MG	2A	3923	1/1	0.85	0.15	39,39,39,39	0
56	MG	1A	4114	1/1	0.85	0.16	41,41,41,41	0
56	MG	1a	1726	1/1	0.85	0.20	63,63,63,63	0
56	MG	10	105	1/1	0.85	0.19	63,63,63,63	0
56	MG	2a	1838	1/1	0.85	0.25	58,58,58,58	0
56	MG	1A	3221	1/1	0.85	0.20	52,52,52,52	0
56	MG	1A	3622	1/1	0.85	0.32	57,57,57,57	0
56	MG	1A	3884	1/1	0.85	0.26	64,64,64,64	0
56	MG	2E	301	1/1	0.85	0.18	69,69,69,69	0
56	MG	2E	302	1/1	0.85	0.19	54,54,54,54	0
56	MG	1a	1744	1/1	0.85	0.34	67,67,67,67	0
56	MG	2A	3545	1/1	0.85	0.12	52,52,52,52	0
56	MG	1a	1603	1/1	0.85	0.27	74,74,74,74	0
56	MG	1A	3296	1/1	0.85	0.21	51,51,51,51	0
56	MG	2r	3001	1/1	0.85	0.24	81,81,81,81	0
56	MG	2A	3592	1/1	0.85	0.15	52,52,52,52	0
56	MG	1A	3984	1/1	0.85	0.16	37,37,37,37	0
56	MG	2A	3303	1/1	0.85	0.27	63,63,63,63	0
56	MG	2A	3635	1/1	0.85	0.26	73,73,73,73	0
56	MG	2A	3307	1/1	0.85	0.14	59,59,59,59	0
56	MG	1A	3355	1/1	0.85	0.22	62,62,62,62	0
56	MG	1A	3478	1/1	0.85	0.21	71,71,71,71	0
56	MG	1A	3548	1/1	0.85	0.29	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3331	1/1	0.85	0.17	67,67,67,67	0
56	MG	2A	3334	1/1	0.85	0.15	65,65,65,65	0
56	MG	2A	3681	1/1	0.85	0.11	45,45,45,45	0
56	MG	2y	3003	1/1	0.85	0.19	80,80,80,80	0
56	MG	2a	1622	1/1	0.85	0.14	65,65,65,65	0
56	MG	2A	3038	1/1	0.85	0.15	61,61,61,61	0
56	MG	2A	3691	1/1	0.85	0.09	43,43,43,43	0
56	MG	1A	3787	1/1	0.85	0.15	53,53,53,53	0
56	MG	1a	1758	1/1	0.85	0.33	76,76,76,76	0
56	MG	1A	3072	1/1	0.86	0.22	58,58,58,58	0
56	MG	2a	1651	1/1	0.86	0.24	71,71,71,71	0
56	MG	2A	3299	1/1	0.86	0.13	62,62,62,62	0
56	MG	1B	3008	1/1	0.86	0.22	51,51,51,51	0
56	MG	2a	1657	1/1	0.86	0.31	67,67,67,67	0
56	MG	1A	3264	1/1	0.86	0.14	56,56,56,56	0
56	MG	1a	1826	1/1	0.86	0.10	89,89,89,89	0
56	MG	2A	3773	1/1	0.86	0.38	48,48,48,48	0
56	MG	18	101	1/1	0.86	0.14	84,84,84,84	0
56	MG	2A	3776	1/1	0.86	0.15	70,70,70,70	0
56	MG	2a	1663	1/1	0.86	0.22	79,79,79,79	0
56	MG	2A	3777	1/1	0.86	0.20	65,65,65,65	0
56	MG	2a	1665	1/1	0.86	0.29	90,90,90,90	0
56	MG	1B	3013	1/1	0.86	0.11	62,62,62,62	0
56	MG	2A	3497	1/1	0.86	0.19	53,53,53,53	0
56	MG	2a	1672	1/1	0.86	0.13	74,74,74,74	0
56	MG	2A	3313	1/1	0.86	0.19	61,61,61,61	0
56	MG	1a	1604	1/1	0.86	0.23	68,68,68,68	0
56	MG	1A	4065	1/1	0.86	0.19	32,32,32,32	0
56	MG	2a	1687	1/1	0.86	0.38	76,76,76,76	0
56	MG	1A	3132	1/1	0.86	0.17	54,54,54,54	0
56	MG	2A	3534	1/1	0.86	0.17	63,63,63,63	0
56	MG	2a	1693	1/1	0.86	0.19	73,73,73,73	0
56	MG	2a	1694	1/1	0.86	0.21	72,72,72,72	0
56	MG	1a	1733	1/1	0.86	0.39	74,74,74,74	0
56	MG	2a	1702	1/1	0.86	0.23	72,72,72,72	0
56	MG	2A	3192	1/1	0.86	0.11	59,59,59,59	0
56	MG	2a	1709	1/1	0.86	0.21	57,57,57,57	0
56	MG	1A	3718	1/1	0.86	0.13	60,60,60,60	0
56	MG	2a	1712	1/1	0.86	0.23	69,69,69,69	0
56	MG	1l	203	1/1	0.86	0.08	57,57,57,57	0
56	MG	1a	1629	1/1	0.86	0.25	61,61,61,61	0
56	MG	2A	3588	1/1	0.86	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1726	1/1	0.86	0.24	76,76,76,76	0
56	MG	2A	3849	1/1	0.86	0.14	51,51,51,51	0
56	MG	1a	1630	1/1	0.86	0.14	65,65,65,65	0
56	MG	2A	3871	1/1	0.86	0.15	53,53,53,53	0
56	MG	2a	1732	1/1	0.86	0.45	74,74,74,74	0
56	MG	2A	3881	1/1	0.86	0.12	86,86,86,86	0
56	MG	2A	3885	1/1	0.86	0.21	53,53,53,53	0
56	MG	2A	3594	1/1	0.86	0.16	60,60,60,60	0
56	MG	1A	3721	1/1	0.86	0.17	30,30,30,30	0
56	MG	2A	3622	1/1	0.86	0.15	60,60,60,60	0
56	MG	2A	3356	1/1	0.86	0.11	58,58,58,58	0
56	MG	1A	3173	1/1	0.86	0.21	66,66,66,66	0
56	MG	2A	3929	1/1	0.86	0.12	53,53,53,53	0
56	MG	2B	3003	1/1	0.86	0.35	75,75,75,75	0
56	MG	2A	3640	1/1	0.86	0.17	59,59,59,59	0
56	MG	2A	3644	1/1	0.86	0.20	31,31,31,31	0
56	MG	2a	1810	1/1	0.86	0.13	74,74,74,74	0
56	MG	1w	105	1/1	0.86	0.24	75,75,75,75	0
56	MG	1A	3793	1/1	0.86	0.11	54,54,54,54	0
56	MG	1D	311	1/1	0.86	0.26	78,78,78,78	0
56	MG	2A	3236	1/1	0.86	0.17	56,56,56,56	0
56	MG	2D	302	1/1	0.86	0.10	58,58,58,58	0
56	MG	2A	3374	1/1	0.86	0.12	70,70,70,70	0
56	MG	2A	3242	1/1	0.86	0.13	61,61,61,61	0
56	MG	2A	3245	1/1	0.86	0.19	56,56,56,56	0
56	MG	2A	3684	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3811	1/1	0.86	0.26	58,58,58,58	0
56	MG	1A	3912	1/1	0.86	0.17	57,57,57,57	0
56	MG	2A	3252	1/1	0.86	0.27	63,63,63,63	0
56	MG	2U	3003	1/1	0.86	0.23	48,48,48,48	0
56	MG	2A	3398	1/1	0.86	0.22	58,58,58,58	0
56	MG	2A	3698	1/1	0.86	0.15	49,49,49,49	0
56	MG	2a	1602	1/1	0.86	0.25	75,75,75,75	0
56	MG	1A	3820	1/1	0.86	0.14	36,36,36,36	0
56	MG	2A	3415	1/1	0.86	0.12	61,61,61,61	0
56	MG	1a	1684	1/1	0.86	0.19	73,73,73,73	0
56	MG	2a	1608	1/1	0.86	0.38	72,72,72,72	0
56	MG	1a	1690	1/1	0.86	0.23	51,51,51,51	0
56	MG	2a	1612	1/1	0.86	0.48	79,79,79,79	0
56	MG	2A	3715	1/1	0.86	0.14	70,70,70,70	0
56	MG	2A	3423	1/1	0.86	0.16	77,77,77,77	0
56	MG	1x	117	1/1	0.86	0.19	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4013	1/1	0.86	0.18	53,53,53,53	0
56	MG	1O	3005	1/1	0.86	0.12	66,66,66,66	0
56	MG	1A	3929	1/1	0.86	0.14	52,52,52,52	0
56	MG	2A	3731	1/1	0.86	0.14	57,57,57,57	0
56	MG	2a	1626	1/1	0.86	0.17	71,71,71,71	0
56	MG	1a	1700	1/1	0.86	0.19	62,62,62,62	0
56	MG	1A	3655	1/1	0.86	0.14	69,69,69,69	0
56	MG	2A	3040	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3398	1/1	0.86	0.46	49,49,49,49	0
56	MG	1A	3481	1/1	0.86	0.11	61,61,61,61	0
56	MG	2A	3287	1/1	0.86	0.08	54,54,54,54	0
56	MG	1A	3270	1/1	0.86	0.20	67,67,67,67	0
56	MG	2A	3714	1/1	0.87	0.21	60,60,60,60	0
56	MG	2A	3382	1/1	0.87	0.13	52,52,52,52	0
56	MG	1A	3580	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3180	1/1	0.87	0.17	60,60,60,60	0
56	MG	2a	1634	1/1	0.87	0.14	67,67,67,67	0
56	MG	1A	3381	1/1	0.87	0.21	50,50,50,50	0
56	MG	1A	3507	1/1	0.87	0.17	52,52,52,52	0
56	MG	2A	3194	1/1	0.87	0.10	63,63,63,63	0
56	MG	2A	3400	1/1	0.87	0.12	52,52,52,52	0
56	MG	2A	3412	1/1	0.87	0.20	48,48,48,48	0
56	MG	2A	3738	1/1	0.87	0.12	57,57,57,57	0
56	MG	2a	1654	1/1	0.87	0.09	83,83,83,83	0
56	MG	2A	3413	1/1	0.87	0.11	56,56,56,56	0
56	MG	1a	1626	1/1	0.87	0.29	62,62,62,62	0
56	MG	1A	3940	1/1	0.87	0.18	49,49,49,49	0
56	MG	1A	3944	1/1	0.87	0.14	34,34,34,34	0
56	MG	2A	3751	1/1	0.87	0.18	62,62,62,62	0
56	MG	2A	3754	1/1	0.87	0.11	54,54,54,54	0
56	MG	1A	3430	1/1	0.87	0.26	60,60,60,60	0
56	MG	1A	4151	1/1	0.87	0.14	51,51,51,51	0
56	MG	1A	4152	1/1	0.87	0.10	46,46,46,46	0
56	MG	2A	3431	1/1	0.87	0.13	70,70,70,70	0
56	MG	2A	3440	1/1	0.87	0.23	47,47,47,47	0
56	MG	1a	1642	1/1	0.87	0.15	67,67,67,67	0
56	MG	2A	3226	1/1	0.87	0.21	55,55,55,55	0
56	MG	1a	1646	1/1	0.87	0.29	71,71,71,71	0
56	MG	1A	3954	1/1	0.87	0.16	58,58,58,58	0
56	MG	1A	4166	1/1	0.87	0.09	56,56,56,56	0
56	MG	1a	1659	1/1	0.87	0.14	65,65,65,65	0
56	MG	2a	1686	1/1	0.87	0.18	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	4185	1/1	0.87	0.13	30,30,30,30	0
56	MG	2A	3781	1/1	0.87	0.15	66,66,66,66	0
56	MG	1A	3256	1/1	0.87	0.10	61,61,61,61	0
56	MG	1A	3625	1/1	0.87	0.24	70,70,70,70	0
56	MG	1a	1677	1/1	0.87	0.21	72,72,72,72	0
56	MG	1a	1682	1/1	0.87	0.37	72,72,72,72	0
56	MG	1A	3791	1/1	0.87	0.09	53,53,53,53	0
56	MG	2A	3803	1/1	0.87	0.16	52,52,52,52	0
56	MG	1A	3390	1/1	0.87	0.10	51,51,51,51	0
56	MG	1A	3343	1/1	0.87	0.15	65,65,65,65	0
56	MG	1a	1692	1/1	0.87	0.41	57,57,57,57	0
56	MG	1A	3023	1/1	0.87	0.20	59,59,59,59	0
56	MG	2A	3826	1/1	0.87	0.18	56,56,56,56	0
56	MG	1A	3048	1/1	0.87	0.08	43,43,43,43	0
56	MG	2A	3500	1/1	0.87	0.21	59,59,59,59	0
56	MG	2A	3845	1/1	0.87	0.09	54,54,54,54	0
56	MG	1a	1697	1/1	0.87	0.25	71,71,71,71	0
56	MG	1B	3023	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3145	1/1	0.87	0.17	52,52,52,52	0
56	MG	2A	3532	1/1	0.87	0.11	57,57,57,57	0
56	MG	1A	3469	1/1	0.87	0.14	60,60,60,60	0
56	MG	1A	3149	1/1	0.87	0.23	51,51,51,51	0
56	MG	1x	105	1/1	0.87	0.18	65,65,65,65	0
56	MG	2A	3896	1/1	0.87	0.17	59,59,59,59	0
56	MG	2A	3901	1/1	0.87	0.09	57,57,57,57	0
56	MG	1A	3215	1/1	0.87	0.16	51,51,51,51	0
56	MG	1A	3150	1/1	0.87	0.22	44,44,44,44	0
56	MG	1A	3715	1/1	0.87	0.09	33,33,33,33	0
56	MG	1a	1717	1/1	0.87	0.18	53,53,53,53	0
56	MG	1A	3420	1/1	0.87	0.23	65,65,65,65	0
56	MG	2A	3944	1/1	0.87	0.13	58,58,58,58	0
56	MG	1A	3873	1/1	0.87	0.13	60,60,60,60	0
56	MG	2A	3593	1/1	0.87	0.09	48,48,48,48	0
56	MG	1F	307	1/1	0.87	0.15	67,67,67,67	0
56	MG	2a	1816	1/1	0.87	0.30	71,71,71,71	0
56	MG	2B	3012	1/1	0.87	0.25	65,65,65,65	0
56	MG	1A	3484	1/1	0.87	0.22	73,73,73,73	0
56	MG	2A	3315	1/1	0.87	0.10	53,53,53,53	0
56	MG	1N	201	1/1	0.87	0.32	58,58,58,58	0
56	MG	2A	3630	1/1	0.87	0.09	49,49,49,49	0
56	MG	1O	3001	1/1	0.87	0.11	70,70,70,70	0
56	MG	1A	4060	1/1	0.87	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3060	1/1	0.87	0.23	55,55,55,55	0
56	MG	2a	1841	1/1	0.87	0.31	72,72,72,72	0
56	MG	2F	301	1/1	0.87	0.12	66,66,66,66	0
56	MG	1Q	203	1/1	0.87	0.13	64,64,64,64	0
56	MG	2A	3654	1/1	0.87	0.11	37,37,37,37	0
56	MG	2Q	3002	1/1	0.87	0.11	44,44,44,44	0
56	MG	1A	3371	1/1	0.87	0.17	62,62,62,62	0
56	MG	2A	3661	1/1	0.87	0.16	53,53,53,53	0
56	MG	1A	3563	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3666	1/1	0.87	0.17	47,47,47,47	0
56	MG	1A	3753	1/1	0.87	0.19	61,61,61,61	0
56	MG	2t	3001	1/1	0.87	0.20	54,54,54,54	0
56	MG	2v	102	1/1	0.87	0.31	69,69,69,69	0
56	MG	1A	3565	1/1	0.87	0.20	60,60,60,60	0
56	MG	26	101	1/1	0.87	0.25	61,61,61,61	0
56	MG	28	101	1/1	0.87	0.20	54,54,54,54	0
56	MG	2A	3353	1/1	0.87	0.10	61,61,61,61	0
56	MG	1A	3913	1/1	0.87	0.21	43,43,43,43	0
56	MG	2A	3090	1/1	0.87	0.13	57,57,57,57	0
56	MG	1A	3152	1/1	0.87	0.23	42,42,42,42	0
56	MG	1A	3378	1/1	0.87	0.19	68,68,68,68	0
56	MG	2x	104	1/1	0.87	0.17	56,56,56,56	0
56	MG	1A	4104	1/1	0.87	0.19	81,81,81,81	0
56	MG	1A	4107	1/1	0.87	0.22	64,64,64,64	0
56	MG	2A	3696	1/1	0.87	0.25	72,72,72,72	0
56	MG	2A	3121	1/1	0.87	0.16	56,56,56,56	0
56	MG	2A	3699	1/1	0.87	0.12	61,61,61,61	0
56	MG	2A	3128	1/1	0.87	0.20	49,49,49,49	0
56	MG	1A	3767	1/1	0.87	0.25	64,64,64,64	0
56	MG	2A	3166	1/1	0.87	0.31	58,58,58,58	0
56	MG	2A	3379	1/1	0.87	0.16	69,69,69,69	0
56	MG	1B	3033	1/1	0.88	0.16	82,82,82,82	0
56	MG	1A	3644	1/1	0.88	0.15	56,56,56,56	0
56	MG	2A	3701	1/1	0.88	0.11	51,51,51,51	0
56	MG	2a	1618	1/1	0.88	0.20	71,71,71,71	0
56	MG	1a	1767	1/1	0.88	0.41	66,66,66,66	0
56	MG	2A	3131	1/1	0.88	0.14	81,81,81,81	0
56	MG	2A	3146	1/1	0.88	0.19	59,59,59,59	0
56	MG	2A	3713	1/1	0.88	0.16	66,66,66,66	0
56	MG	1A	3777	1/1	0.88	0.13	59,59,59,59	0
56	MG	2A	3391	1/1	0.88	0.21	75,75,75,75	0
56	MG	2A	3153	1/1	0.88	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	1631	1/1	0.88	0.15	74,74,74,74	0
56	MG	2A	3722	1/1	0.88	0.13	39,39,39,39	0
56	MG	2A	3165	1/1	0.88	0.21	48,48,48,48	0
56	MG	2A	3396	1/1	0.88	0.21	58,58,58,58	0
56	MG	2a	1645	1/1	0.88	0.17	82,82,82,82	0
56	MG	1a	1671	1/1	0.88	0.17	72,72,72,72	0
56	MG	1a	1672	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	3920	1/1	0.88	0.11	52,52,52,52	0
56	MG	1a	1806	1/1	0.88	0.23	67,67,67,67	0
56	MG	1a	1674	1/1	0.88	0.30	74,74,74,74	0
56	MG	1a	1675	1/1	0.88	0.24	70,70,70,70	0
56	MG	2A	3746	1/1	0.88	0.13	58,58,58,58	0
56	MG	1A	3648	1/1	0.88	0.19	41,41,41,41	0
56	MG	2A	3421	1/1	0.88	0.08	65,65,65,65	0
56	MG	2A	3201	1/1	0.88	0.12	42,42,42,42	0
56	MG	1a	1681	1/1	0.88	0.18	56,56,56,56	0
56	MG	1E	307	1/1	0.88	0.24	73,73,73,73	0
56	MG	2A	3427	1/1	0.88	0.09	68,68,68,68	0
56	MG	1A	3399	1/1	0.88	0.18	52,52,52,52	0
56	MG	1A	3472	1/1	0.88	0.15	64,64,64,64	0
56	MG	2A	3434	1/1	0.88	0.30	49,49,49,49	0
56	MG	2A	3764	1/1	0.88	0.14	63,63,63,63	0
56	MG	2a	1667	1/1	0.88	0.13	70,70,70,70	0
56	MG	1A	4089	1/1	0.88	0.10	62,62,62,62	0
56	MG	1a	1836	1/1	0.88	0.10	75,75,75,75	0
56	MG	2A	3446	1/1	0.88	0.12	56,56,56,56	0
56	MG	1a	1840	1/1	0.88	0.16	61,61,61,61	0
56	MG	1a	1841	1/1	0.88	0.14	50,50,50,50	0
56	MG	2A	3233	1/1	0.88	0.24	61,61,61,61	0
56	MG	1a	1856	1/1	0.88	0.17	63,63,63,63	0
56	MG	2A	3238	1/1	0.88	0.26	56,56,56,56	0
56	MG	1A	3294	1/1	0.88	0.15	66,66,66,66	0
56	MG	2a	1690	1/1	0.88	0.14	65,65,65,65	0
56	MG	1a	1874	1/1	0.88	0.16	55,55,55,55	0
56	MG	2A	3783	1/1	0.88	0.13	46,46,46,46	0
56	MG	1A	3514	1/1	0.88	0.16	67,67,67,67	0
56	MG	1a	1877	1/1	0.88	0.09	76,76,76,76	0
56	MG	2A	3791	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3194	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3810	1/1	0.88	0.15	63,63,63,63	0
56	MG	1A	3379	1/1	0.88	0.31	65,65,65,65	0
56	MG	1A	3695	1/1	0.88	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1713	1/1	0.88	0.29	69,69,69,69	0
56	MG	2a	1718	1/1	0.88	0.28	66,66,66,66	0
56	MG	1A	3950	1/1	0.88	0.11	52,52,52,52	0
56	MG	2a	1720	1/1	0.88	0.21	72,72,72,72	0
56	MG	2A	3487	1/1	0.88	0.18	65,65,65,65	0
56	MG	1w	101	1/1	0.88	0.20	69,69,69,69	0
56	MG	1A	3234	1/1	0.88	0.18	61,61,61,61	0
56	MG	2A	3829	1/1	0.88	0.10	50,50,50,50	0
56	MG	1a	1707	1/1	0.88	0.29	68,68,68,68	0
56	MG	1A	3837	1/1	0.88	0.18	33,33,33,33	0
56	MG	2A	3839	1/1	0.88	0.10	62,62,62,62	0
56	MG	1A	3843	1/1	0.88	0.10	49,49,49,49	0
56	MG	1a	1715	1/1	0.88	0.28	62,62,62,62	0
56	MG	2A	3282	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3051	1/1	0.88	0.11	51,51,51,51	0
56	MG	2A	3867	1/1	0.88	0.10	66,66,66,66	0
56	MG	15	103	1/1	0.88	0.13	57,57,57,57	0
56	MG	1A	3717	1/1	0.88	0.09	30,30,30,30	0
56	MG	1a	1721	1/1	0.88	0.49	70,70,70,70	0
56	MG	1A	3578	1/1	0.88	0.17	54,54,54,54	0
56	MG	2a	1771	1/1	0.88	0.12	66,66,66,66	0
56	MG	2a	1778	1/1	0.88	0.11	83,83,83,83	0
56	MG	2A	3295	1/1	0.88	0.15	50,50,50,50	0
56	MG	2a	1795	1/1	0.88	0.09	81,81,81,81	0
56	MG	1A	3528	1/1	0.88	0.14	67,67,67,67	0
56	MG	2a	1805	1/1	0.88	0.20	84,84,84,84	0
56	MG	2A	3569	1/1	0.88	0.12	69,69,69,69	0
56	MG	2A	3909	1/1	0.88	0.23	72,72,72,72	0
56	MG	2A	3581	1/1	0.88	0.10	40,40,40,40	0
56	MG	1A	3974	1/1	0.88	0.11	38,38,38,38	0
56	MG	1x	118	1/1	0.88	0.13	72,72,72,72	0
56	MG	2a	1817	1/1	0.88	0.11	73,73,73,73	0
56	MG	2a	1821	1/1	0.88	0.14	74,74,74,74	0
56	MG	1A	4172	1/1	0.88	0.17	60,60,60,60	0
56	MG	2A	3931	1/1	0.88	0.27	44,44,44,44	0
56	MG	2a	1824	1/1	0.88	0.11	72,72,72,72	0
56	MG	2a	1827	1/1	0.88	0.16	74,74,74,74	0
56	MG	2A	3934	1/1	0.88	0.20	44,44,44,44	0
56	MG	1A	3087	1/1	0.88	0.10	59,59,59,59	0
56	MG	1A	3496	1/1	0.88	0.10	55,55,55,55	0
56	MG	2A	3621	1/1	0.88	0.17	57,57,57,57	0
56	MG	2a	1837	1/1	0.88	0.21	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	2B	3008	1/1	0.88	0.20	69,69,69,69	0
56	MG	1a	1738	1/1	0.88	0.11	64,64,64,64	0
56	MG	2A	3002	1/1	0.88	0.29	59,59,59,59	0
56	MG	2A	3320	1/1	0.88	0.21	64,64,64,64	0
56	MG	2a	1845	1/1	0.88	0.12	74,74,74,74	0
56	MG	1a	1739	1/1	0.88	0.14	70,70,70,70	0
56	MG	2A	3636	1/1	0.88	0.14	62,62,62,62	0
56	MG	1A	3497	1/1	0.88	0.10	55,55,55,55	0
56	MG	2a	1856	1/1	0.88	0.15	60,60,60,60	0
56	MG	2g	8001	1/1	0.88	0.17	82,82,82,82	0
56	MG	2A	3641	1/1	0.88	0.09	43,43,43,43	0
56	MG	1B	3006	1/1	0.88	0.23	70,70,70,70	0
56	MG	1A	3536	1/1	0.88	0.17	80,80,80,80	0
56	MG	2q	202	1/1	0.88	0.17	62,62,62,62	0
56	MG	2A	3647	1/1	0.88	0.13	67,67,67,67	0
56	MG	2A	3650	1/1	0.88	0.26	48,48,48,48	0
56	MG	2A	3061	1/1	0.88	0.10	50,50,50,50	0
56	MG	1A	3879	1/1	0.88	0.11	46,46,46,46	0
56	MG	2A	3660	1/1	0.88	0.12	66,66,66,66	0
56	MG	1a	1635	1/1	0.88	0.31	64,64,64,64	0
56	MG	1a	1636	1/1	0.88	0.24	70,70,70,70	0
56	MG	2A	3080	1/1	0.88	0.18	53,53,53,53	0
56	MG	2Z	8001	1/1	0.88	0.13	79,79,79,79	0
56	MG	1A	3338	1/1	0.88	0.22	60,60,60,60	0
56	MG	25	102	1/1	0.88	0.26	60,60,60,60	0
56	MG	1A	4035	1/1	0.88	0.09	79,79,79,79	0
56	MG	1A	3891	1/1	0.88	0.25	73,73,73,73	0
56	MG	2A	3360	1/1	0.88	0.08	55,55,55,55	0
56	MG	2A	3361	1/1	0.88	0.15	58,58,58,58	0
56	MG	1a	1645	1/1	0.88	0.20	63,63,63,63	0
56	MG	2A	3365	1/1	0.88	0.30	65,65,65,65	0
56	MG	1A	3538	1/1	0.88	0.19	79,79,79,79	0
56	MG	1A	3630	1/1	0.88	0.19	60,60,60,60	0
56	MG	2a	1610	1/1	0.88	0.16	92,92,92,92	0
56	MG	2A	3101	1/1	0.88	0.17	58,58,58,58	0
56	MG	1A	3053	1/1	0.88	0.15	61,61,61,61	0
56	MG	1a	1632	1/1	0.89	0.37	69,69,69,69	0
56	MG	2A	3373	1/1	0.89	0.10	60,60,60,60	0
56	MG	1a	1761	1/1	0.89	0.26	71,71,71,71	0
56	MG	2a	1620	1/1	0.89	0.20	68,68,68,68	0
56	MG	1A	3907	1/1	0.89	0.09	67,67,67,67	0
56	MG	1a	1765	1/1	0.89	0.28	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	3377	1/1	0.89	0.23	67,67,67,67	0
56	MG	1A	3185	1/1	0.89	0.11	56,56,56,56	0
56	MG	2A	3137	1/1	0.89	0.17	46,46,46,46	0
56	MG	2a	1627	1/1	0.89	0.30	74,74,74,74	0
56	MG	1A	3386	1/1	0.89	0.18	60,60,60,60	0
56	MG	2A	3711	1/1	0.89	0.07	65,65,65,65	0
56	MG	1A	3551	1/1	0.89	0.24	61,61,61,61	0
56	MG	1A	3186	1/1	0.89	0.09	72,72,72,72	0
56	MG	2A	3162	1/1	0.89	0.21	58,58,58,58	0
56	MG	2a	1643	1/1	0.89	0.16	79,79,79,79	0
56	MG	2A	3717	1/1	0.89	0.07	51,51,51,51	0
56	MG	1A	3392	1/1	0.89	0.13	58,58,58,58	0
56	MG	1A	3039	1/1	0.89	0.20	60,60,60,60	0
56	MG	2A	3723	1/1	0.89	0.12	62,62,62,62	0
56	MG	1a	1647	1/1	0.89	0.22	62,62,62,62	0
56	MG	1A	3082	1/1	0.89	0.23	46,46,46,46	0
56	MG	2A	3408	1/1	0.89	0.27	67,67,67,67	0
56	MG	2A	3188	1/1	0.89	0.22	66,66,66,66	0
56	MG	1A	3001	1/1	0.89	0.18	51,51,51,51	0
56	MG	2A	3414	1/1	0.89	0.13	58,58,58,58	0
56	MG	2A	3734	1/1	0.89	0.12	51,51,51,51	0
56	MG	1A	3342	1/1	0.89	0.19	58,58,58,58	0
56	MG	1a	1819	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	4175	1/1	0.89	0.12	72,72,72,72	0
56	MG	1A	3766	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3493	1/1	0.89	0.17	68,68,68,68	0
56	MG	2A	3204	1/1	0.89	0.19	68,68,68,68	0
56	MG	1a	1829	1/1	0.89	0.12	73,73,73,73	0
56	MG	2A	3752	1/1	0.89	0.15	73,73,73,73	0
56	MG	1A	3401	1/1	0.89	0.31	67,67,67,67	0
56	MG	1a	1832	1/1	0.89	0.13	65,65,65,65	0
56	MG	1B	3004	1/1	0.89	0.33	67,67,67,67	0
56	MG	2A	3437	1/1	0.89	0.29	55,55,55,55	0
56	MG	2A	3760	1/1	0.89	0.08	55,55,55,55	0
56	MG	2a	1675	1/1	0.89	0.17	67,67,67,67	0
56	MG	2A	3222	1/1	0.89	0.13	58,58,58,58	0
56	MG	1A	3599	1/1	0.89	0.11	48,48,48,48	0
56	MG	1a	1837	1/1	0.89	0.14	53,53,53,53	0
56	MG	1A	3601	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3451	1/1	0.89	0.16	59,59,59,59	0
56	MG	1a	1676	1/1	0.89	0.14	80,80,80,80	0
56	MG	1A	3606	1/1	0.89	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	1692	1/1	0.89	0.27	73,73,73,73	0
56	MG	1A	3610	1/1	0.89	0.16	63,63,63,63	0
56	MG	1A	3410	1/1	0.89	0.14	47,47,47,47	0
56	MG	2a	1695	1/1	0.89	0.18	67,67,67,67	0
56	MG	2a	1697	1/1	0.89	0.37	69,69,69,69	0
56	MG	2a	1700	1/1	0.89	0.24	59,59,59,59	0
56	MG	2A	3462	1/1	0.89	0.27	56,56,56,56	0
56	MG	1A	3098	1/1	0.89	0.25	74,74,74,74	0
56	MG	2a	1706	1/1	0.89	0.31	82,82,82,82	0
56	MG	2A	3464	1/1	0.89	0.16	69,69,69,69	0
56	MG	1B	3021	1/1	0.89	0.14	65,65,65,65	0
56	MG	1A	3347	1/1	0.89	0.19	51,51,51,51	0
56	MG	1B	3026	1/1	0.89	0.07	41,41,41,41	0
56	MG	1A	3292	1/1	0.89	0.32	61,61,61,61	0
56	MG	2a	1716	1/1	0.89	0.14	66,66,66,66	0
56	MG	2a	1717	1/1	0.89	0.20	58,58,58,58	0
56	MG	2A	3793	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3967	1/1	0.89	0.17	42,42,42,42	0
56	MG	2A	3473	1/1	0.89	0.20	63,63,63,63	0
56	MG	1A	3795	1/1	0.89	0.17	48,48,48,48	0
56	MG	1A	3971	1/1	0.89	0.16	48,48,48,48	0
56	MG	1A	3800	1/1	0.89	0.21	59,59,59,59	0
56	MG	2a	1728	1/1	0.89	0.15	63,63,63,63	0
56	MG	1A	3805	1/1	0.89	0.15	61,61,61,61	0
56	MG	2A	3488	1/1	0.89	0.32	50,50,50,50	0
56	MG	2A	3491	1/1	0.89	0.28	61,61,61,61	0
56	MG	2A	3827	1/1	0.89	0.14	40,40,40,40	0
56	MG	1A	3100	1/1	0.89	0.23	58,58,58,58	0
56	MG	2a	1739	1/1	0.89	0.30	71,71,71,71	0
56	MG	1A	3991	1/1	0.89	0.12	60,60,60,60	0
56	MG	2a	1741	1/1	0.89	0.51	69,69,69,69	0
56	MG	1a	1708	1/1	0.89	0.20	66,66,66,66	0
56	MG	2a	1745	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3504	1/1	0.89	0.20	69,69,69,69	0
56	MG	1A	3996	1/1	0.89	0.08	52,52,52,52	0
56	MG	1A	3626	1/1	0.89	0.10	49,49,49,49	0
56	MG	1A	3165	1/1	0.89	0.22	53,53,53,53	0
56	MG	2A	3523	1/1	0.89	0.22	57,57,57,57	0
56	MG	2a	1763	1/1	0.89	0.12	85,85,85,85	0
56	MG	2A	3524	1/1	0.89	0.14	56,56,56,56	0
56	MG	1x	106	1/1	0.89	0.20	67,67,67,67	0
56	MG	2A	3286	1/1	0.89	0.22	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	1x	110	1/1	0.89	0.28	71,71,71,71	0
56	MG	1A	3166	1/1	0.89	0.14	44,44,44,44	0
56	MG	2a	1801	1/1	0.89	0.20	64,64,64,64	0
56	MG	2a	1802	1/1	0.89	0.09	73,73,73,73	0
56	MG	1A	3303	1/1	0.89	0.26	38,38,38,38	0
56	MG	2A	3897	1/1	0.89	0.25	67,67,67,67	0
56	MG	1A	3362	1/1	0.89	0.17	62,62,62,62	0
56	MG	2A	3904	1/1	0.89	0.13	57,57,57,57	0
56	MG	2A	3550	1/1	0.89	0.15	47,47,47,47	0
56	MG	2A	3296	1/1	0.89	0.15	53,53,53,53	0
56	MG	2A	3553	1/1	0.89	0.09	42,42,42,42	0
56	MG	1x	114	1/1	0.89	0.29	76,76,76,76	0
56	MG	2a	1819	1/1	0.89	0.12	63,63,63,63	0
56	MG	2A	3562	1/1	0.89	0.09	40,40,40,40	0
56	MG	2A	3926	1/1	0.89	0.31	47,47,47,47	0
56	MG	1A	3245	1/1	0.89	0.25	66,66,66,66	0
56	MG	2A	3301	1/1	0.89	0.10	46,46,46,46	0
56	MG	1A	3847	1/1	0.89	0.18	59,59,59,59	0
56	MG	2A	3936	1/1	0.89	0.13	47,47,47,47	0
56	MG	1A	3366	1/1	0.89	0.16	61,61,61,61	0
56	MG	2B	3002	1/1	0.89	0.10	67,67,67,67	0
56	MG	1A	3367	1/1	0.89	0.18	66,66,66,66	0
56	MG	2a	1835	1/1	0.89	0.41	77,77,77,77	0
56	MG	2a	1836	1/1	0.89	0.15	70,70,70,70	0
56	MG	2B	3005	1/1	0.89	0.13	68,68,68,68	0
56	MG	1a	1727	1/1	0.89	0.10	62,62,62,62	0
56	MG	2A	3595	1/1	0.89	0.11	48,48,48,48	0
56	MG	2B	3010	1/1	0.89	0.11	71,71,71,71	0
56	MG	1A	3657	1/1	0.89	0.22	59,59,59,59	0
56	MG	2A	3619	1/1	0.89	0.12	50,50,50,50	0
56	MG	1a	1729	1/1	0.89	0.16	65,65,65,65	0
56	MG	2A	3318	1/1	0.89	0.18	64,64,64,64	0
56	MG	2A	3625	1/1	0.89	0.11	60,60,60,60	0
56	MG	2a	1854	1/1	0.89	0.10	58,58,58,58	0
56	MG	2A	3628	1/1	0.89	0.09	34,34,34,34	0
56	MG	2A	3023	1/1	0.89	0.14	60,60,60,60	0
56	MG	1A	3252	1/1	0.89	0.08	68,68,68,68	0
56	MG	2A	3634	1/1	0.89	0.12	39,39,39,39	0
56	MG	2E	303	1/1	0.89	0.11	44,44,44,44	0
56	MG	2l	203	1/1	0.89	0.19	76,76,76,76	0
56	MG	2p	101	1/1	0.89	0.25	65,65,65,65	0
56	MG	2q	201	1/1	0.89	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3328	1/1	0.89	0.15	66,66,66,66	0
56	MG	1A	3666	1/1	0.89	0.14	59,59,59,59	0
56	MG	2A	3637	1/1	0.89	0.21	66,66,66,66	0
56	MG	2A	3049	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3053	1/1	0.89	0.17	64,64,64,64	0
56	MG	1A	3451	1/1	0.89	0.13	46,46,46,46	0
56	MG	1A	502	1/1	0.89	0.30	73,73,73,73	0
56	MG	1A	3119	1/1	0.89	0.13	46,46,46,46	0
56	MG	2A	3344	1/1	0.89	0.13	62,62,62,62	0
56	MG	1A	3318	1/1	0.89	0.19	55,55,55,55	0
56	MG	1A	3881	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3458	1/1	0.89	0.23	64,64,64,64	0
56	MG	2A	3079	1/1	0.89	0.24	62,62,62,62	0
56	MG	2A	3355	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	3887	1/1	0.89	0.11	58,58,58,58	0
56	MG	1A	4095	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	4099	1/1	0.89	0.11	54,54,54,54	0
56	MG	1A	3184	1/1	0.89	0.24	65,65,65,65	0
56	MG	1A	3704	1/1	0.89	0.09	65,65,65,65	0
56	MG	1A	4108	1/1	0.89	0.14	60,60,60,60	0
56	MG	1A	3899	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	3321	1/1	0.89	0.12	58,58,58,58	0
56	MG	2A	3371	1/1	0.89	0.10	65,65,65,65	0
56	MG	1A	4020	1/1	0.90	0.12	34,34,34,34	0
56	MG	2A	3743	1/1	0.90	0.12	71,71,71,71	0
56	MG	1A	3743	1/1	0.90	0.14	32,32,32,32	0
56	MG	1a	1838	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3746	1/1	0.90	0.12	72,72,72,72	0
56	MG	2a	1653	1/1	0.90	0.20	66,66,66,66	0
56	MG	2A	3449	1/1	0.90	0.24	56,56,56,56	0
56	MG	2A	3227	1/1	0.90	0.13	66,66,66,66	0
56	MG	1a	1678	1/1	0.90	0.15	58,58,58,58	0
56	MG	1A	3345	1/1	0.90	0.30	61,61,61,61	0
56	MG	1a	1858	1/1	0.90	0.08	70,70,70,70	0
56	MG	1a	1871	1/1	0.90	0.09	72,72,72,72	0
56	MG	1A	3019	1/1	0.90	0.13	41,41,41,41	0
56	MG	1a	1683	1/1	0.90	0.13	69,69,69,69	0
56	MG	2A	3761	1/1	0.90	0.08	55,55,55,55	0
56	MG	2A	3247	1/1	0.90	0.12	57,57,57,57	0
56	MG	2A	3467	1/1	0.90	0.25	49,49,49,49	0
56	MG	1A	3882	1/1	0.90	0.18	56,56,56,56	0
56	MG	1a	1686	1/1	0.90	0.28	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	1a	1687	1/1	0.90	0.29	60,60,60,60	0
56	MG	1A	4055	1/1	0.90	0.22	81,81,81,81	0
56	MG	1b	3001	1/1	0.90	0.07	75,75,75,75	0
56	MG	1A	3757	1/1	0.90	0.14	45,45,45,45	0
56	MG	1A	3885	1/1	0.90	0.27	57,57,57,57	0
56	MG	2A	3778	1/1	0.90	0.08	42,42,42,42	0
56	MG	2A	3478	1/1	0.90	0.25	62,62,62,62	0
56	MG	1F	306	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3314	1/1	0.90	0.10	60,60,60,60	0
56	MG	1A	3255	1/1	0.90	0.12	67,67,67,67	0
56	MG	2a	1689	1/1	0.90	0.12	69,69,69,69	0
56	MG	2A	3268	1/1	0.90	0.20	75,75,75,75	0
56	MG	1A	3316	1/1	0.90	0.28	56,56,56,56	0
56	MG	1A	3532	1/1	0.90	0.12	56,56,56,56	0
56	MG	1A	3900	1/1	0.90	0.10	56,56,56,56	0
56	MG	1a	1704	1/1	0.90	0.27	59,59,59,59	0
56	MG	2A	3501	1/1	0.90	0.42	61,61,61,61	0
56	MG	1O	3006	1/1	0.90	0.11	83,83,83,83	0
56	MG	1P	203	1/1	0.90	0.16	53,53,53,53	0
56	MG	1A	3278	1/1	0.90	0.21	59,59,59,59	0
56	MG	1a	1709	1/1	0.90	0.31	62,62,62,62	0
56	MG	1x	108	1/1	0.90	0.15	58,58,58,58	0
56	MG	2a	1707	1/1	0.90	0.25	69,69,69,69	0
56	MG	1a	1710	1/1	0.90	0.17	66,66,66,66	0
56	MG	2A	3527	1/1	0.90	0.11	21,21,21,21	0
56	MG	2a	1710	1/1	0.90	0.24	47,47,47,47	0
56	MG	1R	203	1/1	0.90	0.18	44,44,44,44	0
56	MG	1T	201	1/1	0.90	0.23	62,62,62,62	0
56	MG	1A	3291	1/1	0.90	0.27	54,54,54,54	0
56	MG	1A	3470	1/1	0.90	0.24	63,63,63,63	0
56	MG	1A	3778	1/1	0.90	0.16	64,64,64,64	0
56	MG	1a	1718	1/1	0.90	0.31	51,51,51,51	0
56	MG	2A	3546	1/1	0.90	0.12	29,29,29,29	0
56	MG	2A	3548	1/1	0.90	0.19	53,53,53,53	0
56	MG	1A	3361	1/1	0.90	0.21	58,58,58,58	0
56	MG	2A	3868	1/1	0.90	0.11	61,61,61,61	0
56	MG	1A	3914	1/1	0.90	0.12	78,78,78,78	0
56	MG	2A	3308	1/1	0.90	0.10	54,54,54,54	0
56	MG	10	106	1/1	0.90	0.09	58,58,58,58	0
56	MG	2A	3561	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3312	1/1	0.90	0.09	60,60,60,60	0
56	MG	11	101	1/1	0.90	0.14	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	1733	1/1	0.90	0.11	48,48,48,48	0
56	MG	2a	1735	1/1	0.90	0.42	72,72,72,72	0
56	MG	1A	3639	1/1	0.90	0.35	63,63,63,63	0
56	MG	2a	1737	1/1	0.90	0.32	64,64,64,64	0
56	MG	2A	3007	1/1	0.90	0.16	48,48,48,48	0
56	MG	1A	3642	1/1	0.90	0.28	62,62,62,62	0
56	MG	2A	3325	1/1	0.90	0.22	53,53,53,53	0
56	MG	2a	1742	1/1	0.90	0.26	68,68,68,68	0
56	MG	2A	3035	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	3923	1/1	0.90	0.21	47,47,47,47	0
56	MG	1A	3122	1/1	0.90	0.24	60,60,60,60	0
56	MG	2A	3607	1/1	0.90	0.34	66,66,66,66	0
56	MG	2A	3612	1/1	0.90	0.22	58,58,58,58	0
56	MG	2A	3616	1/1	0.90	0.11	36,36,36,36	0
56	MG	16	103	1/1	0.90	0.10	69,69,69,69	0
56	MG	2A	3050	1/1	0.90	0.12	52,52,52,52	0
56	MG	1A	3363	1/1	0.90	0.21	66,66,66,66	0
56	MG	1A	3412	1/1	0.90	0.15	57,57,57,57	0
56	MG	19	103	1/1	0.90	0.23	64,64,64,64	0
56	MG	1A	3546	1/1	0.90	0.33	52,52,52,52	0
56	MG	2a	1793	1/1	0.90	0.11	71,71,71,71	0
56	MG	1A	3197	1/1	0.90	0.33	45,45,45,45	0
56	MG	2a	1800	1/1	0.90	0.13	74,74,74,74	0
56	MG	1a	1605	1/1	0.90	0.15	63,63,63,63	0
56	MG	2A	3352	1/1	0.90	0.08	67,67,67,67	0
56	MG	1A	3261	1/1	0.90	0.17	67,67,67,67	0
56	MG	1a	1610	1/1	0.90	0.31	60,60,60,60	0
56	MG	2a	1806	1/1	0.90	0.22	73,73,73,73	0
56	MG	2B	3013	1/1	0.90	0.18	77,77,77,77	0
56	MG	1a	1611	1/1	0.90	0.19	64,64,64,64	0
56	MG	1a	1615	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3643	1/1	0.90	0.09	49,49,49,49	0
56	MG	2B	3017	1/1	0.90	0.09	58,58,58,58	0
56	MG	2A	3358	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3555	1/1	0.90	0.20	46,46,46,46	0
56	MG	1A	4142	1/1	0.90	0.12	56,56,56,56	0
56	MG	1A	3081	1/1	0.90	0.33	46,46,46,46	0
56	MG	1A	3816	1/1	0.90	0.13	23,23,23,23	0
56	MG	2E	305	1/1	0.90	0.08	55,55,55,55	0
56	MG	2a	1826	1/1	0.90	0.09	77,77,77,77	0
56	MG	1A	3333	1/1	0.90	0.10	44,44,44,44	0
56	MG	1A	3822	1/1	0.90	0.12	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	2F	304	1/1	0.90	0.11	51,51,51,51	0
56	MG	2G	3001	1/1	0.90	0.20	60,60,60,60	0
56	MG	1A	3373	1/1	0.90	0.21	64,64,64,64	0
56	MG	2A	3108	1/1	0.90	0.09	57,57,57,57	0
56	MG	2A	3111	1/1	0.90	0.09	52,52,52,52	0
56	MG	2A	3668	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3113	1/1	0.90	0.18	56,56,56,56	0
56	MG	1A	3834	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3118	1/1	0.90	0.20	59,59,59,59	0
56	MG	2a	1843	1/1	0.90	0.08	64,64,64,64	0
56	MG	1A	3300	1/1	0.90	0.10	54,54,54,54	0
56	MG	25	101	1/1	0.90	0.10	49,49,49,49	0
56	MG	1A	3335	1/1	0.90	0.08	53,53,53,53	0
56	MG	1A	4212	1/1	0.90	0.20	53,53,53,53	0
56	MG	1a	1768	1/1	0.90	0.27	69,69,69,69	0
56	MG	2A	3384	1/1	0.90	0.11	64,64,64,64	0
56	MG	2A	3144	1/1	0.90	0.24	58,58,58,58	0
56	MG	1a	1773	1/1	0.90	0.30	64,64,64,64	0
56	MG	1A	3246	1/1	0.90	0.33	65,65,65,65	0
56	MG	2a	1605	1/1	0.90	0.32	64,64,64,64	0
56	MG	2a	1606	1/1	0.90	0.27	68,68,68,68	0
56	MG	1a	1788	1/1	0.90	0.10	78,78,78,78	0
56	MG	1A	3380	1/1	0.90	0.18	56,56,56,56	0
56	MG	1A	3850	1/1	0.90	0.18	30,30,30,30	0
56	MG	2A	3703	1/1	0.90	0.22	78,78,78,78	0
56	MG	1a	1653	1/1	0.90	0.21	63,63,63,63	0
56	MG	1A	3851	1/1	0.90	0.12	21,21,21,21	0
56	MG	1A	3309	1/1	0.90	0.35	59,59,59,59	0
56	MG	1A	3591	1/1	0.90	0.14	51,51,51,51	0
56	MG	2A	3191	1/1	0.90	0.15	63,63,63,63	0
56	MG	2w	101	1/1	0.90	0.28	66,66,66,66	0
56	MG	1a	1660	1/1	0.90	0.15	63,63,63,63	0
56	MG	1a	1818	1/1	0.90	0.11	87,87,87,87	0
56	MG	1a	1662	1/1	0.90	0.13	71,71,71,71	0
56	MG	2w	107	1/1	0.90	0.07	78,78,78,78	0
56	MG	1A	3988	1/1	0.90	0.10	65,65,65,65	0
56	MG	2a	1624	1/1	0.90	0.08	53,53,53,53	0
56	MG	2A	3199	1/1	0.90	0.17	56,56,56,56	0
56	MG	1a	1668	1/1	0.90	0.21	63,63,63,63	0
56	MG	1A	3437	1/1	0.90	0.11	60,60,60,60	0
56	MG	2A	3426	1/1	0.90	0.08	52,52,52,52	0
56	MG	1A	3172	1/1	0.90	0.35	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3208	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3864	1/1	0.90	0.10	51,51,51,51	0
56	MG	1A	3446	1/1	0.90	0.09	67,67,67,67	0
56	MG	2a	1639	1/1	0.90	0.29	68,68,68,68	0
56	MG	2A	3733	1/1	0.90	0.09	48,48,48,48	0
56	MG	1A	4017	1/1	0.90	0.12	53,53,53,53	0
56	MG	2A	3438	1/1	0.90	0.27	42,42,42,42	0
56	MG	2A	3697	1/1	0.91	0.07	43,43,43,43	0
56	MG	2A	3152	1/1	0.91	0.15	46,46,46,46	0
56	MG	1A	3697	1/1	0.91	0.11	59,59,59,59	0
56	MG	1A	3433	1/1	0.91	0.12	46,46,46,46	0
56	MG	1A	3702	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3597	1/1	0.91	0.08	48,48,48,48	0
56	MG	2A	3171	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3115	1/1	0.91	0.24	42,42,42,42	0
56	MG	2A	3707	1/1	0.91	0.13	47,47,47,47	0
56	MG	2A	3404	1/1	0.91	0.17	55,55,55,55	0
56	MG	2A	3405	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3407	1/1	0.91	0.14	69,69,69,69	0
56	MG	2A	3179	1/1	0.91	0.08	44,44,44,44	0
56	MG	2A	3409	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3436	1/1	0.91	0.21	64,64,64,64	0
56	MG	1A	3123	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3719	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3189	1/1	0.91	0.10	47,47,47,47	0
56	MG	1B	3020	1/1	0.91	0.14	57,57,57,57	0
56	MG	2A	3416	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3417	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	3978	1/1	0.91	0.14	72,72,72,72	0
56	MG	1A	3607	1/1	0.91	0.20	64,64,64,64	0
56	MG	1A	3722	1/1	0.91	0.06	32,32,32,32	0
56	MG	1A	3730	1/1	0.91	0.19	33,33,33,33	0
56	MG	1A	3609	1/1	0.91	0.24	58,58,58,58	0
56	MG	2A	3425	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3735	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3198	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3482	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	4015	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3872	1/1	0.91	0.12	55,55,55,55	0
56	MG	2A	3433	1/1	0.91	0.19	53,53,53,53	0
56	MG	1a	1680	1/1	0.91	0.18	73,73,73,73	0
56	MG	2a	1668	1/1	0.91	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3435	1/1	0.91	0.20	40,40,40,40	0
56	MG	1A	3745	1/1	0.91	0.13	37,37,37,37	0
56	MG	1E	303	1/1	0.91	0.14	39,39,39,39	0
56	MG	1A	3875	1/1	0.91	0.12	38,38,38,38	0
56	MG	2A	3441	1/1	0.91	0.30	48,48,48,48	0
56	MG	2a	1677	1/1	0.91	0.27	76,76,76,76	0
56	MG	2A	3443	1/1	0.91	0.29	58,58,58,58	0
56	MG	1A	4029	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3876	1/1	0.91	0.10	34,34,34,34	0
56	MG	1F	305	1/1	0.91	0.13	50,50,50,50	0
56	MG	2A	3448	1/1	0.91	0.30	56,56,56,56	0
56	MG	1A	3877	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3612	1/1	0.91	0.28	67,67,67,67	0
56	MG	1A	3880	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3234	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	4050	1/1	0.91	0.11	30,30,30,30	0
56	MG	1N	202	1/1	0.91	0.09	47,47,47,47	0
56	MG	2A	3240	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3747	1/1	0.91	0.14	39,39,39,39	0
56	MG	2A	3244	1/1	0.91	0.17	40,40,40,40	0
56	MG	1a	1698	1/1	0.91	0.18	61,61,61,61	0
56	MG	1t	3001	1/1	0.91	0.19	56,56,56,56	0
56	MG	2a	1704	1/1	0.91	0.29	71,71,71,71	0
56	MG	1v	3001	1/1	0.91	0.09	70,70,70,70	0
56	MG	1O	3004	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3440	1/1	0.91	0.14	58,58,58,58	0
56	MG	1A	3883	1/1	0.91	0.13	41,41,41,41	0
56	MG	1A	3754	1/1	0.91	0.10	36,36,36,36	0
56	MG	1A	3485	1/1	0.91	0.43	63,63,63,63	0
56	MG	1Q	204	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3798	1/1	0.91	0.19	56,56,56,56	0
56	MG	2A	3259	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3490	1/1	0.91	0.15	48,48,48,48	0
56	MG	2A	3483	1/1	0.91	0.21	59,59,59,59	0
56	MG	1A	4069	1/1	0.91	0.10	87,87,87,87	0
56	MG	2A	3813	1/1	0.91	0.12	68,68,68,68	0
56	MG	2A	3814	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3351	1/1	0.91	0.10	55,55,55,55	0
56	MG	1a	1711	1/1	0.91	0.09	58,58,58,58	0
56	MG	1x	107	1/1	0.91	0.23	68,68,68,68	0
56	MG	2A	3274	1/1	0.91	0.18	67,67,67,67	0
56	MG	2A	3498	1/1	0.91	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3499	1/1	0.91	0.24	59,59,59,59	0
56	MG	2A	3831	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3450	1/1	0.91	0.15	54,54,54,54	0
56	MG	2A	3835	1/1	0.91	0.10	88,88,88,88	0
56	MG	1U	203	1/1	0.91	0.13	49,49,49,49	0
56	MG	2A	3502	1/1	0.91	0.24	69,69,69,69	0
56	MG	1A	3898	1/1	0.91	0.10	72,72,72,72	0
56	MG	1A	3628	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3511	1/1	0.91	0.19	61,61,61,61	0
56	MG	2A	3520	1/1	0.91	0.07	41,41,41,41	0
56	MG	1A	3388	1/1	0.91	0.12	45,45,45,45	0
56	MG	1A	3452	1/1	0.91	0.23	52,52,52,52	0
56	MG	2A	3874	1/1	0.91	0.10	66,66,66,66	0
56	MG	2A	3876	1/1	0.91	0.17	61,61,61,61	0
56	MG	2a	1748	1/1	0.91	0.34	60,60,60,60	0
56	MG	1A	3239	1/1	0.91	0.20	58,58,58,58	0
56	MG	2a	1750	1/1	0.91	0.44	83,83,83,83	0
56	MG	2A	3288	1/1	0.91	0.10	55,55,55,55	0
56	MG	2a	1753	1/1	0.91	0.10	77,77,77,77	0
56	MG	1A	3501	1/1	0.91	0.24	58,58,58,58	0
56	MG	2a	1761	1/1	0.91	0.10	86,86,86,86	0
56	MG	12	101	1/1	0.91	0.12	56,56,56,56	0
56	MG	1a	1724	1/1	0.91	0.25	74,74,74,74	0
56	MG	2A	3900	1/1	0.91	0.30	41,41,41,41	0
56	MG	2a	1776	1/1	0.91	0.10	90,90,90,90	0
56	MG	13	102	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3903	1/1	0.91	0.11	62,62,62,62	0
56	MG	2a	1790	1/1	0.91	0.09	73,73,73,73	0
56	MG	1A	3909	1/1	0.91	0.14	32,32,32,32	0
56	MG	2a	1794	1/1	0.91	0.08	101,101,101,101	0
56	MG	2A	3907	1/1	0.91	0.17	39,39,39,39	0
56	MG	1A	3640	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3005	1/1	0.91	0.36	57,57,57,57	0
56	MG	2A	3006	1/1	0.91	0.28	56,56,56,56	0
56	MG	1A	3370	1/1	0.91	0.20	52,52,52,52	0
56	MG	2A	3305	1/1	0.91	0.23	57,57,57,57	0
56	MG	2A	3924	1/1	0.91	0.20	49,49,49,49	0
56	MG	2A	3008	1/1	0.91	0.09	48,48,48,48	0
56	MG	1A	4109	1/1	0.91	0.07	28,28,28,28	0
56	MG	2A	3030	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3643	1/1	0.91	0.20	70,70,70,70	0
56	MG	2a	1814	1/1	0.91	0.12	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	1A	4111	1/1	0.91	0.09	63,63,63,63	0
56	MG	1a	1735	1/1	0.91	0.17	50,50,50,50	0
56	MG	2A	3572	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3575	1/1	0.91	0.16	40,40,40,40	0
56	MG	2A	3316	1/1	0.91	0.42	62,62,62,62	0
56	MG	2A	3585	1/1	0.91	0.09	51,51,51,51	0
56	MG	2A	3048	1/1	0.91	0.17	31,31,31,31	0
56	MG	1A	3298	1/1	0.91	0.14	59,59,59,59	0
56	MG	2A	3322	1/1	0.91	0.20	67,67,67,67	0
56	MG	1A	4115	1/1	0.91	0.12	35,35,35,35	0
56	MG	1A	3559	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3598	1/1	0.91	0.20	64,64,64,64	0
56	MG	1A	3560	1/1	0.91	0.26	63,63,63,63	0
56	MG	2A	3057	1/1	0.91	0.15	58,58,58,58	0
56	MG	1A	3460	1/1	0.91	0.10	56,56,56,56	0
56	MG	2A	3332	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3333	1/1	0.91	0.18	60,60,60,60	0
56	MG	2D	305	1/1	0.91	0.28	47,47,47,47	0
56	MG	1a	1607	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3063	1/1	0.91	0.08	59,59,59,59	0
56	MG	1a	1608	1/1	0.91	0.28	66,66,66,66	0
56	MG	2A	3627	1/1	0.91	0.10	47,47,47,47	0
56	MG	2a	1846	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3065	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3341	1/1	0.91	0.29	59,59,59,59	0
56	MG	2F	303	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	4125	1/1	0.91	0.07	17,17,17,17	0
56	MG	1A	4130	1/1	0.91	0.17	85,85,85,85	0
56	MG	2d	303	1/1	0.91	0.10	65,65,65,65	0
56	MG	2e	3001	1/1	0.91	0.11	73,73,73,73	0
56	MG	2f	3002	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3077	1/1	0.91	0.21	32,32,32,32	0
56	MG	1A	3188	1/1	0.91	0.15	49,49,49,49	0
56	MG	2Q	3004	1/1	0.91	0.21	61,61,61,61	0
56	MG	1A	3797	1/1	0.91	0.12	42,42,42,42	0
56	MG	1a	1623	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3658	1/1	0.91	0.15	36,36,36,36	0
56	MG	1A	4143	1/1	0.91	0.08	48,48,48,48	0
56	MG	2A	3357	1/1	0.91	0.09	53,53,53,53	0
56	MG	1A	3663	1/1	0.91	0.14	21,21,21,21	0
56	MG	2A	3359	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3092	1/1	0.91	0.28	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3093	1/1	0.91	0.09	39,39,39,39	0
56	MG	1A	3336	1/1	0.91	0.19	64,64,64,64	0
56	MG	1a	1631	1/1	0.91	0.22	75,75,75,75	0
56	MG	1a	1764	1/1	0.91	0.18	67,67,67,67	0
56	MG	1A	3468	1/1	0.91	0.20	61,61,61,61	0
56	MG	1A	3674	1/1	0.91	0.22	50,50,50,50	0
56	MG	2w	106	1/1	0.91	0.17	65,65,65,65	0
56	MG	1A	3260	1/1	0.91	0.24	64,64,64,64	0
56	MG	1A	3951	1/1	0.91	0.19	38,38,38,38	0
56	MG	1A	3078	1/1	0.91	0.10	63,63,63,63	0
56	MG	2A	3674	1/1	0.91	0.11	46,46,46,46	0
56	MG	2a	1609	1/1	0.91	0.27	68,68,68,68	0
56	MG	1a	1774	1/1	0.91	0.15	56,56,56,56	0
56	MG	2A	3678	1/1	0.91	0.12	53,53,53,53	0
56	MG	1a	1779	1/1	0.91	0.15	77,77,77,77	0
56	MG	1A	3823	1/1	0.91	0.11	34,34,34,34	0
56	MG	1a	1644	1/1	0.91	0.16	48,48,48,48	0
56	MG	2a	1616	1/1	0.91	0.28	66,66,66,66	0
56	MG	1A	3585	1/1	0.91	0.16	68,68,68,68	0
56	MG	2y	3006	1/1	0.91	0.07	104,104,104,104	0
56	MG	1a	1792	1/1	0.91	0.13	57,57,57,57	0
56	MG	1A	4223	1/1	0.91	0.11	35,35,35,35	0
56	MG	1A	3590	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	4012	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3853	1/1	0.92	0.07	48,48,48,48	0
56	MG	2A	3597	1/1	0.92	0.07	49,49,49,49	0
56	MG	2A	3304	1/1	0.92	0.29	63,63,63,63	0
56	MG	25	104	1/1	0.92	0.14	49,49,49,49	0
56	MG	1E	302	1/1	0.92	0.31	65,65,65,65	0
56	MG	1A	3685	1/1	0.92	0.10	42,42,42,42	0
56	MG	1x	115	1/1	0.92	0.28	64,64,64,64	0
56	MG	2a	1601	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3687	1/1	0.92	0.09	38,38,38,38	0
56	MG	2A	3311	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3199	1/1	0.92	0.10	60,60,60,60	0
56	MG	1E	310	1/1	0.92	0.13	62,62,62,62	0
56	MG	1E	311	1/1	0.92	0.14	48,48,48,48	0
56	MG	2A	3626	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	4026	1/1	0.92	0.10	45,45,45,45	0
56	MG	1F	302	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3206	1/1	0.92	0.19	36,36,36,36	0
56	MG	2A	3004	1/1	0.92	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3633	1/1	0.92	0.12	47,47,47,47	0
56	MG	1a	1705	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	4028	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3140	1/1	0.92	0.16	47,47,47,47	0
56	MG	2A	3329	1/1	0.92	0.15	61,61,61,61	0
56	MG	1G	3002	1/1	0.92	0.15	56,56,56,56	0
56	MG	2A	3016	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3021	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3022	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3418	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3182	1/1	0.92	0.19	41,41,41,41	0
56	MG	1A	3144	1/1	0.92	0.11	64,64,64,64	0
56	MG	2A	3652	1/1	0.92	0.16	43,43,43,43	0
56	MG	1N	206	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3586	1/1	0.92	0.09	62,62,62,62	0
56	MG	2A	3044	1/1	0.92	0.13	52,52,52,52	0
56	MG	2A	3346	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	4045	1/1	0.92	0.09	27,27,27,27	0
56	MG	1A	3588	1/1	0.92	0.12	49,49,49,49	0
56	MG	2a	1638	1/1	0.92	0.10	86,86,86,86	0
56	MG	1A	4051	1/1	0.92	0.08	93,93,93,93	0
56	MG	1A	3080	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3223	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3593	1/1	0.92	0.35	58,58,58,58	0
56	MG	2A	3058	1/1	0.92	0.25	65,65,65,65	0
56	MG	1A	3268	1/1	0.92	0.20	64,64,64,64	0
56	MG	1S	3001	1/1	0.92	0.20	54,54,54,54	0
56	MG	1S	3002	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3736	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3233	1/1	0.92	0.34	55,55,55,55	0
56	MG	1A	3276	1/1	0.92	0.17	65,65,65,65	0
56	MG	1A	3110	1/1	0.92	0.13	38,38,38,38	0
56	MG	2A	3071	1/1	0.92	0.07	44,44,44,44	0
56	MG	2A	3073	1/1	0.92	0.09	57,57,57,57	0
56	MG	1U	204	1/1	0.92	0.17	38,38,38,38	0
56	MG	1V	201	1/1	0.92	0.16	59,59,59,59	0
56	MG	1a	1734	1/1	0.92	0.13	62,62,62,62	0
56	MG	1W	201	1/1	0.92	0.22	56,56,56,56	0
56	MG	1Y	201	1/1	0.92	0.11	69,69,69,69	0
56	MG	1Y	203	1/1	0.92	0.21	62,62,62,62	0
56	MG	1A	4081	1/1	0.92	0.14	84,84,84,84	0
56	MG	1Z	302	1/1	0.92	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	1A	3375	1/1	0.92	0.14	66,66,66,66	0
56	MG	2A	3709	1/1	0.92	0.09	47,47,47,47	0
56	MG	2A	3381	1/1	0.92	0.25	66,66,66,66	0
56	MG	1A	3509	1/1	0.92	0.08	60,60,60,60	0
56	MG	2a	1671	1/1	0.92	0.18	60,60,60,60	0
56	MG	1A	4088	1/1	0.92	0.08	89,89,89,89	0
56	MG	1A	3890	1/1	0.92	0.12	60,60,60,60	0
56	MG	2A	3387	1/1	0.92	0.11	54,54,54,54	0
56	MG	1A	3376	1/1	0.92	0.17	64,64,64,64	0
56	MG	2a	1678	1/1	0.92	0.22	58,58,58,58	0
56	MG	2a	1679	1/1	0.92	0.18	58,58,58,58	0
56	MG	2a	1681	1/1	0.92	0.14	54,54,54,54	0
56	MG	1a	1752	1/1	0.92	0.31	65,65,65,65	0
56	MG	1A	3279	1/1	0.92	0.11	36,36,36,36	0
56	MG	1A	4094	1/1	0.92	0.07	79,79,79,79	0
56	MG	1A	3516	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3117	1/1	0.92	0.12	44,44,44,44	0
56	MG	15	102	1/1	0.92	0.17	44,44,44,44	0
56	MG	2A	3402	1/1	0.92	0.25	48,48,48,48	0
56	MG	1A	3439	1/1	0.92	0.12	55,55,55,55	0
56	MG	2A	3127	1/1	0.92	0.18	56,56,56,56	0
56	MG	1A	4100	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3331	1/1	0.92	0.34	69,69,69,69	0
56	MG	1a	1762	1/1	0.92	0.23	66,66,66,66	0
56	MG	2a	1696	1/1	0.92	0.19	56,56,56,56	0
56	MG	2A	3411	1/1	0.92	0.24	63,63,63,63	0
56	MG	1A	3618	1/1	0.92	0.08	49,49,49,49	0
56	MG	1A	3904	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3744	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3761	1/1	0.92	0.16	42,42,42,42	0
56	MG	2a	1705	1/1	0.92	0.17	65,65,65,65	0
56	MG	1A	3620	1/1	0.92	0.37	56,56,56,56	0
56	MG	1A	3444	1/1	0.92	0.33	58,58,58,58	0
56	MG	2A	3154	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3911	1/1	0.92	0.12	43,43,43,43	0
56	MG	1a	1770	1/1	0.92	0.35	66,66,66,66	0
56	MG	2A	3753	1/1	0.92	0.06	55,55,55,55	0
56	MG	1a	1772	1/1	0.92	0.27	68,68,68,68	0
56	MG	2A	3170	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3283	1/1	0.92	0.18	45,45,45,45	0
56	MG	1A	3526	1/1	0.92	0.32	48,48,48,48	0
56	MG	2A	3759	1/1	0.92	0.14	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	3627	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	3917	1/1	0.92	0.11	64,64,64,64	0
56	MG	2a	1722	1/1	0.92	0.10	71,71,71,71	0
56	MG	2A	3428	1/1	0.92	0.13	55,55,55,55	0
56	MG	2A	3186	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3765	1/1	0.92	0.12	67,67,67,67	0
56	MG	2a	1727	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3286	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	1789	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3190	1/1	0.92	0.08	69,69,69,69	0
56	MG	2A	3771	1/1	0.92	0.07	41,41,41,41	0
56	MG	1a	1614	1/1	0.92	0.08	76,76,76,76	0
56	MG	2A	3436	1/1	0.92	0.24	53,53,53,53	0
56	MG	1A	3290	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3024	1/1	0.92	0.17	46,46,46,46	0
56	MG	2A	3439	1/1	0.92	0.20	36,36,36,36	0
56	MG	2A	3779	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	4137	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3925	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3198	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3444	1/1	0.92	0.23	39,39,39,39	0
56	MG	2a	1744	1/1	0.92	0.16	66,66,66,66	0
56	MG	1A	3633	1/1	0.92	0.16	62,62,62,62	0
56	MG	1a	1811	1/1	0.92	0.32	66,66,66,66	0
56	MG	1a	1813	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3637	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3205	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3006	1/1	0.92	0.16	56,56,56,56	0
56	MG	2A	3452	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3340	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	4153	1/1	0.92	0.15	27,27,27,27	0
56	MG	2A	3806	1/1	0.92	0.13	67,67,67,67	0
56	MG	2a	1762	1/1	0.92	0.15	62,62,62,62	0
56	MG	1a	1633	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3811	1/1	0.92	0.14	56,56,56,56	0
56	MG	2a	1770	1/1	0.92	0.08	78,78,78,78	0
56	MG	2A	3459	1/1	0.92	0.12	49,49,49,49	0
56	MG	1A	3341	1/1	0.92	0.22	60,60,60,60	0
56	MG	2A	3461	1/1	0.92	0.35	60,60,60,60	0
56	MG	2A	3216	1/1	0.92	0.18	50,50,50,50	0
56	MG	2a	1785	1/1	0.92	0.07	89,89,89,89	0
56	MG	2a	1787	1/1	0.92	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3218	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3641	1/1	0.92	0.43	67,67,67,67	0
56	MG	1A	4168	1/1	0.92	0.14	57,57,57,57	0
56	MG	1a	1639	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3191	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3228	1/1	0.92	0.10	59,59,59,59	0
56	MG	2A	3229	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	4173	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3232	1/1	0.92	0.32	59,59,59,59	0
56	MG	2A	3475	1/1	0.92	0.12	56,56,56,56	0
56	MG	2a	1809	1/1	0.92	0.25	54,54,54,54	0
56	MG	1a	1643	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3477	1/1	0.92	0.28	60,60,60,60	0
56	MG	1A	3462	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3235	1/1	0.92	0.20	55,55,55,55	0
56	MG	1A	3947	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3802	1/1	0.92	0.10	61,61,61,61	0
56	MG	1A	4200	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3241	1/1	0.92	0.11	53,53,53,53	0
56	MG	2a	1820	1/1	0.92	0.17	73,73,73,73	0
56	MG	2A	3883	1/1	0.92	0.10	41,41,41,41	0
56	MG	2A	3490	1/1	0.92	0.14	68,68,68,68	0
56	MG	1a	1846	1/1	0.92	0.09	74,74,74,74	0
56	MG	2A	3887	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3892	1/1	0.92	0.09	39,39,39,39	0
56	MG	1a	1849	1/1	0.92	0.12	75,75,75,75	0
56	MG	2A	3494	1/1	0.92	0.12	57,57,57,57	0
56	MG	2A	3496	1/1	0.92	0.22	58,58,58,58	0
56	MG	1A	4207	1/1	0.92	0.12	24,24,24,24	0
56	MG	1A	3803	1/1	0.92	0.10	47,47,47,47	0
56	MG	1a	1860	1/1	0.92	0.08	92,92,92,92	0
56	MG	1a	1657	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	4218	1/1	0.92	0.06	32,32,32,32	0
56	MG	1A	3250	1/1	0.92	0.19	55,55,55,55	0
56	MG	2A	3503	1/1	0.92	0.09	63,63,63,63	0
56	MG	1A	3647	1/1	0.92	0.28	53,53,53,53	0
56	MG	2A	3922	1/1	0.92	0.08	38,38,38,38	0
56	MG	2A	3256	1/1	0.92	0.17	58,58,58,58	0
56	MG	2A	3508	1/1	0.92	0.23	64,64,64,64	0
56	MG	2A	3510	1/1	0.92	0.36	61,61,61,61	0
56	MG	1A	3192	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3512	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	1664	1/1	0.92	0.12	52,52,52,52	0
56	MG	1a	1884	1/1	0.92	0.16	62,62,62,62	0
56	MG	2A	3260	1/1	0.92	0.08	53,53,53,53	0
56	MG	2d	301	1/1	0.92	0.33	65,65,65,65	0
56	MG	1A	3812	1/1	0.92	0.13	60,60,60,60	0
56	MG	1B	3007	1/1	0.92	0.23	65,65,65,65	0
56	MG	2A	3525	1/1	0.92	0.09	39,39,39,39	0
56	MG	1A	3649	1/1	0.92	0.34	53,53,53,53	0
56	MG	2A	3267	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3651	1/1	0.92	0.17	61,61,61,61	0
56	MG	2A	3270	1/1	0.92	0.20	57,57,57,57	0
56	MG	2A	3271	1/1	0.92	0.19	62,62,62,62	0
56	MG	1A	3965	1/1	0.92	0.17	61,61,61,61	0
56	MG	2A	3538	1/1	0.92	0.09	62,62,62,62	0
56	MG	2A	3539	1/1	0.92	0.07	31,31,31,31	0
56	MG	2q	203	1/1	0.92	0.08	73,73,73,73	0
56	MG	2A	3540	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3821	1/1	0.92	0.15	34,34,34,34	0
56	MG	1A	3346	1/1	0.92	0.21	54,54,54,54	0
56	MG	1A	3044	1/1	0.92	0.11	42,42,42,42	0
56	MG	2D	304	1/1	0.92	0.28	45,45,45,45	0
56	MG	1A	3090	1/1	0.92	0.10	45,45,45,45	0
56	MG	1A	3471	1/1	0.92	0.13	50,50,50,50	0
56	MG	1B	3024	1/1	0.92	0.13	69,69,69,69	0
56	MG	1a	1679	1/1	0.92	0.14	58,58,58,58	0
56	MG	2w	105	1/1	0.92	0.06	74,74,74,74	0
56	MG	2A	3560	1/1	0.92	0.07	43,43,43,43	0
56	MG	2E	306	1/1	0.92	0.15	59,59,59,59	0
56	MG	2E	307	1/1	0.92	0.13	49,49,49,49	0
56	MG	2E	309	1/1	0.92	0.10	56,56,56,56	0
56	MG	1w	108	1/1	0.92	0.20	73,73,73,73	0
56	MG	1A	3404	1/1	0.92	0.28	55,55,55,55	0
56	MG	2A	3565	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	3406	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3302	1/1	0.92	0.32	59,59,59,59	0
56	MG	1B	3030	1/1	0.92	0.08	69,69,69,69	0
56	MG	2P	203	1/1	0.92	0.07	56,56,56,56	0
56	MG	2A	3576	1/1	0.92	0.15	68,68,68,68	0
56	MG	1A	3058	1/1	0.92	0.11	49,49,49,49	0
56	MG	2A	3297	1/1	0.92	0.14	67,67,67,67	0
56	MG	1a	1685	1/1	0.92	0.23	60,60,60,60	0
56	MG	1A	3562	1/1	0.92	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3306	1/1	0.92	0.16	38,38,38,38	0
56	MG	2A	3051	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3495	1/1	0.93	0.20	47,47,47,47	0
56	MG	1A	3369	1/1	0.93	0.15	63,63,63,63	0
56	MG	2A	3335	1/1	0.93	0.18	68,68,68,68	0
56	MG	1a	1736	1/1	0.93	0.20	65,65,65,65	0
56	MG	1a	1737	1/1	0.93	0.06	52,52,52,52	0
56	MG	1A	3710	1/1	0.93	0.06	44,44,44,44	0
56	MG	1A	3878	1/1	0.93	0.12	39,39,39,39	0
56	MG	2A	3343	1/1	0.93	0.15	63,63,63,63	0
56	MG	1Z	304	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3345	1/1	0.93	0.12	58,58,58,58	0
56	MG	10	102	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3711	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3066	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3350	1/1	0.93	0.19	57,57,57,57	0
56	MG	1A	3425	1/1	0.93	0.19	50,50,50,50	0
56	MG	1A	3716	1/1	0.93	0.09	26,26,26,26	0
56	MG	1A	3596	1/1	0.93	0.39	69,69,69,69	0
56	MG	2A	3072	1/1	0.93	0.06	41,41,41,41	0
56	MG	1a	1750	1/1	0.93	0.37	63,63,63,63	0
56	MG	2A	3653	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3088	1/1	0.93	0.16	50,50,50,50	0
56	MG	1A	3248	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3658	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3168	1/1	0.93	0.07	36,36,36,36	0
56	MG	1a	1754	1/1	0.93	0.35	61,61,61,61	0
56	MG	2A	3084	1/1	0.93	0.13	46,46,46,46	0
56	MG	2A	3664	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3886	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3088	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3723	1/1	0.93	0.09	27,27,27,27	0
56	MG	1A	3729	1/1	0.93	0.07	27,27,27,27	0
56	MG	2A	3369	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3602	1/1	0.93	0.40	70,70,70,70	0
56	MG	2a	1635	1/1	0.93	0.34	62,62,62,62	0
56	MG	2a	1637	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3332	1/1	0.93	0.41	66,66,66,66	0
56	MG	17	104	1/1	0.93	0.13	60,60,60,60	0
56	MG	1A	3893	1/1	0.93	0.14	64,64,64,64	0
56	MG	2A	3685	1/1	0.93	0.13	66,66,66,66	0
56	MG	2A	3688	1/1	0.93	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3897	1/1	0.93	0.08	71,71,71,71	0
56	MG	2A	3102	1/1	0.93	0.14	32,32,32,32	0
56	MG	1A	3170	1/1	0.93	0.18	58,58,58,58	0
56	MG	2A	3104	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	3608	1/1	0.93	0.27	60,60,60,60	0
56	MG	2a	1652	1/1	0.93	0.17	61,61,61,61	0
56	MG	2A	3380	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3109	1/1	0.93	0.29	59,59,59,59	0
56	MG	1A	3742	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	4120	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3114	1/1	0.93	0.38	61,61,61,61	0
56	MG	1A	3253	1/1	0.93	0.11	53,53,53,53	0
56	MG	2A	3388	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3389	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3390	1/1	0.93	0.25	46,46,46,46	0
56	MG	1A	3902	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3744	1/1	0.93	0.14	28,28,28,28	0
56	MG	2A	3394	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3905	1/1	0.93	0.09	21,21,21,21	0
56	MG	2a	1666	1/1	0.93	0.42	69,69,69,69	0
56	MG	2A	3124	1/1	0.93	0.14	58,58,58,58	0
56	MG	2A	3397	1/1	0.93	0.16	40,40,40,40	0
56	MG	1A	3906	1/1	0.93	0.24	56,56,56,56	0
56	MG	1a	1775	1/1	0.93	0.29	65,65,65,65	0
56	MG	1A	3510	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3721	1/1	0.93	0.12	73,73,73,73	0
56	MG	1A	3127	1/1	0.93	0.24	41,41,41,41	0
56	MG	1A	3029	1/1	0.93	0.19	35,35,35,35	0
56	MG	1A	3750	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3515	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3151	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3615	1/1	0.93	0.24	59,59,59,59	0
56	MG	2A	3410	1/1	0.93	0.09	65,65,65,65	0
56	MG	1A	3011	1/1	0.93	0.12	42,42,42,42	0
56	MG	1a	1796	1/1	0.93	0.15	65,65,65,65	0
56	MG	1a	1800	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3442	1/1	0.93	0.08	53,53,53,53	0
56	MG	1a	1803	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3739	1/1	0.93	0.07	56,56,56,56	0
56	MG	1A	3918	1/1	0.93	0.20	72,72,72,72	0
56	MG	1A	3619	1/1	0.93	0.34	63,63,63,63	0
56	MG	2A	3172	1/1	0.93	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3173	1/1	0.93	0.11	53,53,53,53	0
56	MG	2A	3747	1/1	0.93	0.12	50,50,50,50	0
56	MG	1a	1810	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3176	1/1	0.93	0.13	53,53,53,53	0
56	MG	2a	1698	1/1	0.93	0.11	60,60,60,60	0
56	MG	2a	1699	1/1	0.93	0.17	57,57,57,57	0
56	MG	1A	3339	1/1	0.93	0.23	54,54,54,54	0
56	MG	1A	3521	1/1	0.93	0.19	59,59,59,59	0
56	MG	2A	3181	1/1	0.93	0.21	53,53,53,53	0
56	MG	1A	3624	1/1	0.93	0.30	61,61,61,61	0
56	MG	1A	4183	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3299	1/1	0.93	0.18	61,61,61,61	0
56	MG	2A	3430	1/1	0.93	0.17	62,62,62,62	0
56	MG	1a	1641	1/1	0.93	0.17	61,61,61,61	0
56	MG	1A	3930	1/1	0.93	0.12	45,45,45,45	0
56	MG	1a	1823	1/1	0.93	0.15	57,57,57,57	0
56	MG	1a	1825	1/1	0.93	0.08	68,68,68,68	0
56	MG	1A	3768	1/1	0.93	0.08	20,20,20,20	0
56	MG	2A	3196	1/1	0.93	0.09	41,41,41,41	0
56	MG	2a	1714	1/1	0.93	0.07	76,76,76,76	0
56	MG	1A	3769	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	4209	1/1	0.93	0.08	84,84,84,84	0
56	MG	1A	3210	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3143	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3040	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	4226	1/1	0.93	0.12	42,42,42,42	0
56	MG	1a	1655	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3207	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3304	1/1	0.93	0.24	58,58,58,58	0
56	MG	2A	3210	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3456	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	3783	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3631	1/1	0.93	0.34	66,66,66,66	0
56	MG	1a	1661	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3455	1/1	0.93	0.30	62,62,62,62	0
56	MG	1A	3632	1/1	0.93	0.11	65,65,65,65	0
56	MG	2a	1734	1/1	0.93	0.30	68,68,68,68	0
56	MG	1A	3533	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3790	1/1	0.93	0.09	55,55,55,55	0
56	MG	1a	1859	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3393	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3794	1/1	0.93	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3224	1/1	0.93	0.21	64,64,64,64	0
56	MG	2A	3225	1/1	0.93	0.23	58,58,58,58	0
56	MG	1a	1868	1/1	0.93	0.09	83,83,83,83	0
56	MG	1a	1666	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3792	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3216	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3104	1/1	0.93	0.16	45,45,45,45	0
56	MG	1A	3796	1/1	0.93	0.10	23,23,23,23	0
56	MG	1A	3311	1/1	0.93	0.19	58,58,58,58	0
56	MG	1A	3966	1/1	0.93	0.14	44,44,44,44	0
56	MG	2a	1751	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3820	1/1	0.93	0.10	70,70,70,70	0
56	MG	1A	3352	1/1	0.93	0.34	42,42,42,42	0
56	MG	2A	3474	1/1	0.93	0.35	61,61,61,61	0
56	MG	2A	3824	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3353	1/1	0.93	0.08	46,46,46,46	0
56	MG	1b	3002	1/1	0.93	0.16	69,69,69,69	0
56	MG	1A	3467	1/1	0.93	0.20	56,56,56,56	0
56	MG	1n	101	1/1	0.93	0.20	52,52,52,52	0
56	MG	2A	3479	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3187	1/1	0.93	0.15	49,49,49,49	0
56	MG	1n	104	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3405	1/1	0.93	0.18	42,42,42,42	0
56	MG	1A	3227	1/1	0.93	0.17	53,53,53,53	0
56	MG	1D	301	1/1	0.93	0.17	29,29,29,29	0
56	MG	2A	3489	1/1	0.93	0.08	56,56,56,56	0
56	MG	2a	1791	1/1	0.93	0.10	84,84,84,84	0
56	MG	1A	3979	1/1	0.93	0.16	56,56,56,56	0
56	MG	2A	3857	1/1	0.93	0.10	37,37,37,37	0
56	MG	2A	3859	1/1	0.93	0.08	49,49,49,49	0
56	MG	1D	303	1/1	0.93	0.11	51,51,51,51	0
56	MG	1D	305	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3228	1/1	0.93	0.19	53,53,53,53	0
56	MG	1A	3985	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3813	1/1	0.93	0.10	16,16,16,16	0
56	MG	2A	3879	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3016	1/1	0.93	0.23	61,61,61,61	0
56	MG	1A	3557	1/1	0.93	0.27	61,61,61,61	0
56	MG	1A	3275	1/1	0.93	0.17	35,35,35,35	0
56	MG	1A	4003	1/1	0.93	0.10	67,67,67,67	0
56	MG	1A	4009	1/1	0.93	0.08	62,62,62,62	0
56	MG	2A	3888	1/1	0.93	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1815	1/1	0.93	0.16	63,63,63,63	0
56	MG	1a	1695	1/1	0.93	0.21	54,54,54,54	0
56	MG	1A	4010	1/1	0.93	0.13	43,43,43,43	0
56	MG	1A	3413	1/1	0.93	0.10	56,56,56,56	0
56	MG	2A	3269	1/1	0.93	0.16	69,69,69,69	0
56	MG	1A	3317	1/1	0.93	0.30	63,63,63,63	0
56	MG	1A	3662	1/1	0.93	0.18	59,59,59,59	0
56	MG	1A	3060	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3515	1/1	0.93	0.11	50,50,50,50	0
56	MG	2a	1825	1/1	0.93	0.16	76,76,76,76	0
56	MG	2A	3517	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3086	1/1	0.93	0.21	41,41,41,41	0
56	MG	2A	3275	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3241	1/1	0.93	0.15	42,42,42,42	0
56	MG	1x	116	1/1	0.93	0.13	73,73,73,73	0
56	MG	2A	3280	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3844	1/1	0.93	0.15	40,40,40,40	0
56	MG	2A	3925	1/1	0.93	0.22	43,43,43,43	0
56	MG	2A	3526	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3574	1/1	0.93	0.22	43,43,43,43	0
56	MG	2A	3930	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3676	1/1	0.93	0.11	37,37,37,37	0
56	MG	2a	1842	1/1	0.93	0.12	75,75,75,75	0
56	MG	1A	4031	1/1	0.93	0.10	76,76,76,76	0
56	MG	1O	3002	1/1	0.93	0.23	55,55,55,55	0
56	MG	1A	3677	1/1	0.93	0.18	51,51,51,51	0
56	MG	1A	3419	1/1	0.93	0.13	43,43,43,43	0
56	MG	1A	3852	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3292	1/1	0.93	0.24	58,58,58,58	0
56	MG	2A	3293	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3680	1/1	0.93	0.15	57,57,57,57	0
56	MG	2B	3009	1/1	0.93	0.14	65,65,65,65	0
56	MG	1A	3486	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	4046	1/1	0.93	0.11	31,31,31,31	0
56	MG	1A	3365	1/1	0.93	0.24	59,59,59,59	0
56	MG	1A	3491	1/1	0.93	0.11	64,64,64,64	0
56	MG	1A	4053	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3689	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3559	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	4056	1/1	0.93	0.08	44,44,44,44	0
56	MG	2B	3019	1/1	0.93	0.23	79,79,79,79	0
56	MG	2n	101	1/1	0.93	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3024	1/1	0.93	0.48	53,53,53,53	0
56	MG	2A	3025	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3026	1/1	0.93	0.14	37,37,37,37	0
56	MG	2A	3027	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3571	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3692	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3323	1/1	0.93	0.22	41,41,41,41	0
56	MG	2E	304	1/1	0.93	0.16	72,72,72,72	0
56	MG	2v	103	1/1	0.93	0.22	60,60,60,60	0
56	MG	2A	3037	1/1	0.93	0.16	36,36,36,36	0
56	MG	1A	3868	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3583	1/1	0.93	0.07	38,38,38,38	0
56	MG	2E	308	1/1	0.93	0.10	45,45,45,45	0
56	MG	2A	3039	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3017	1/1	0.93	0.24	41,41,41,41	0
56	MG	2A	3317	1/1	0.93	0.17	64,64,64,64	0
56	MG	2A	3041	1/1	0.93	0.18	41,41,41,41	0
56	MG	2A	3042	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3321	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3043	1/1	0.93	0.09	46,46,46,46	0
56	MG	2A	3324	1/1	0.93	0.19	51,51,51,51	0
56	MG	2A	3603	1/1	0.93	0.18	51,51,51,51	0
56	MG	1V	202	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3046	1/1	0.93	0.15	45,45,45,45	0
56	MG	2A	3047	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3613	1/1	0.93	0.09	48,48,48,48	0
56	MG	2A	3615	1/1	0.93	0.13	49,49,49,49	0
56	MG	1A	3587	1/1	0.93	0.19	67,67,67,67	0
56	MG	2A	3618	1/1	0.93	0.11	56,56,56,56	0
56	MG	23	101	1/1	0.93	0.22	57,57,57,57	0
57	K	2A	3939	1/1	0.93	0.14	75,75,75,75	0
56	MG	1a	1732	1/1	0.93	0.10	66,66,66,66	0
58	CPT	1A	4181	3/5	0.93	0.15	61,61,64,93	3
56	MG	1A	3494	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3306	1/1	0.94	0.08	51,51,51,51	0
56	MG	2O	8001	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3809	1/1	0.94	0.07	44,44,44,44	0
56	MG	2Q	3001	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3109	1/1	0.94	0.06	51,51,51,51	0
56	MG	2A	3309	1/1	0.94	0.26	59,59,59,59	0
56	MG	2R	202	1/1	0.94	0.13	57,57,57,57	0
56	MG	1A	3972	1/1	0.94	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3596	1/1	0.94	0.10	22,22,22,22	0
56	MG	1B	3032	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3032	1/1	0.94	0.08	47,47,47,47	0
56	MG	2V	201	1/1	0.94	0.12	62,62,62,62	0
56	MG	2X	102	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3599	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3973	1/1	0.94	0.18	56,56,56,56	0
56	MG	20	102	1/1	0.94	0.14	58,58,58,58	0
56	MG	1A	3218	1/1	0.94	0.23	49,49,49,49	0
56	MG	1A	3976	1/1	0.94	0.08	75,75,75,75	0
56	MG	1A	3219	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3047	1/1	0.94	0.10	27,27,27,27	0
56	MG	2A	3319	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3661	1/1	0.94	0.15	32,32,32,32	0
56	MG	2A	3617	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3980	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3818	1/1	0.94	0.10	34,34,34,34	0
56	MG	2A	3323	1/1	0.94	0.21	60,60,60,60	0
56	MG	1A	3476	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3288	1/1	0.94	0.22	52,52,52,52	0
56	MG	1E	304	1/1	0.94	0.18	29,29,29,29	0
56	MG	2A	3327	1/1	0.94	0.15	54,54,54,54	0
56	MG	1E	305	1/1	0.94	0.17	59,59,59,59	0
56	MG	1A	3222	1/1	0.94	0.15	51,51,51,51	0
56	MG	1A	3564	1/1	0.94	0.08	56,56,56,56	0
56	MG	2A	3631	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3632	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3824	1/1	0.94	0.08	40,40,40,40	0
56	MG	2a	1614	1/1	0.94	0.29	65,65,65,65	0
56	MG	2A	3052	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3668	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	4004	1/1	0.94	0.09	61,61,61,61	0
56	MG	1A	3827	1/1	0.94	0.11	21,21,21,21	0
56	MG	2a	1619	1/1	0.94	0.20	62,62,62,62	0
56	MG	2A	3336	1/1	0.94	0.08	47,47,47,47	0
56	MG	1F	303	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3338	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3059	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3828	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3672	1/1	0.94	0.07	11,11,11,11	0
56	MG	1A	3344	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	4014	1/1	0.94	0.08	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	1G	3003	1/1	0.94	0.10	67,67,67,67	0
56	MG	1A	3840	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3571	1/1	0.94	0.23	46,46,46,46	0
56	MG	2a	1632	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3111	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3349	1/1	0.94	0.21	64,64,64,64	0
56	MG	2A	3070	1/1	0.94	0.13	41,41,41,41	0
56	MG	2a	1636	1/1	0.94	0.08	81,81,81,81	0
56	MG	1N	205	1/1	0.94	0.13	61,61,61,61	0
56	MG	1A	4021	1/1	0.94	0.21	58,58,58,58	0
56	MG	1A	4022	1/1	0.94	0.07	68,68,68,68	0
56	MG	2A	3076	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	4025	1/1	0.94	0.10	23,23,23,23	0
56	MG	2A	3078	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3226	1/1	0.94	0.07	51,51,51,51	0
56	MG	2A	3675	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3846	1/1	0.94	0.18	65,65,65,65	0
56	MG	1A	3483	1/1	0.94	0.12	58,58,58,58	0
56	MG	2A	3082	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3682	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3362	1/1	0.94	0.09	59,59,59,59	0
56	MG	1a	1745	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	3293	1/1	0.94	0.13	67,67,67,67	0
56	MG	2A	3366	1/1	0.94	0.19	59,59,59,59	0
56	MG	1Q	202	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	4030	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3684	1/1	0.94	0.06	33,33,33,33	0
56	MG	1R	201	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	4032	1/1	0.94	0.08	78,78,78,78	0
56	MG	2A	3095	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3579	1/1	0.94	0.18	54,54,54,54	0
56	MG	1A	4034	1/1	0.94	0.11	42,42,42,42	0
56	MG	1S	3003	1/1	0.94	0.09	74,74,74,74	0
56	MG	1A	3085	1/1	0.94	0.29	41,41,41,41	0
56	MG	1a	1757	1/1	0.94	0.10	69,69,69,69	0
56	MG	2A	3705	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3378	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3688	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3106	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	4039	1/1	0.94	0.08	80,80,80,80	0
56	MG	1A	3584	1/1	0.94	0.13	35,35,35,35	0
56	MG	1A	3009	1/1	0.94	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1U	205	1/1	0.94	0.17	33,33,33,33	0
56	MG	1U	208	1/1	0.94	0.15	44,44,44,44	0
56	MG	1A	3693	1/1	0.94	0.12	41,41,41,41	0
56	MG	1A	4047	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	4048	1/1	0.94	0.10	25,25,25,25	0
56	MG	2A	3120	1/1	0.94	0.10	45,45,45,45	0
56	MG	1X	104	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3049	1/1	0.94	0.19	41,41,41,41	0
56	MG	2A	3125	1/1	0.94	0.06	51,51,51,51	0
56	MG	1a	1769	1/1	0.94	0.27	60,60,60,60	0
56	MG	1A	3417	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3174	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3132	1/1	0.94	0.12	66,66,66,66	0
56	MG	2A	3133	1/1	0.94	0.13	48,48,48,48	0
56	MG	2A	3136	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3869	1/1	0.94	0.14	27,27,27,27	0
56	MG	2A	3140	1/1	0.94	0.19	41,41,41,41	0
56	MG	2A	3737	1/1	0.94	0.07	51,51,51,51	0
56	MG	2A	3141	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3589	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3145	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3235	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3147	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3050	1/1	0.94	0.18	38,38,38,38	0
56	MG	10	103	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	3183	1/1	0.94	0.12	59,59,59,59	0
56	MG	1A	3594	1/1	0.94	0.20	32,32,32,32	0
56	MG	1A	3712	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	4066	1/1	0.94	0.11	19,19,19,19	0
56	MG	2A	3418	1/1	0.94	0.08	67,67,67,67	0
56	MG	2A	3419	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3595	1/1	0.94	0.28	59,59,59,59	0
56	MG	1A	3243	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3167	1/1	0.94	0.09	49,49,49,49	0
56	MG	1a	1797	1/1	0.94	0.16	57,57,57,57	0
56	MG	1A	3360	1/1	0.94	0.14	64,64,64,64	0
56	MG	1A	4082	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3124	1/1	0.94	0.22	46,46,46,46	0
56	MG	1A	4085	1/1	0.94	0.06	81,81,81,81	0
56	MG	1A	3719	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3028	1/1	0.94	0.08	44,44,44,44	0
56	MG	2a	1724	1/1	0.94	0.19	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	3307	1/1	0.94	0.25	47,47,47,47	0
56	MG	1A	3603	1/1	0.94	0.15	60,60,60,60	0
56	MG	2A	3432	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3185	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3772	1/1	0.94	0.11	73,73,73,73	0
56	MG	18	103	1/1	0.94	0.16	48,48,48,48	0
56	MG	2A	3187	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3604	1/1	0.94	0.29	66,66,66,66	0
56	MG	1A	3432	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3734	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	4096	1/1	0.94	0.07	75,75,75,75	0
56	MG	1A	3506	1/1	0.94	0.19	52,52,52,52	0
56	MG	1a	1824	1/1	0.94	0.07	75,75,75,75	0
56	MG	2A	3442	1/1	0.94	0.33	60,60,60,60	0
56	MG	1A	3308	1/1	0.94	0.28	55,55,55,55	0
56	MG	1A	3130	1/1	0.94	0.13	76,76,76,76	0
56	MG	2A	3787	1/1	0.94	0.07	36,36,36,36	0
56	MG	2A	3788	1/1	0.94	0.09	36,36,36,36	0
56	MG	1A	3894	1/1	0.94	0.06	37,37,37,37	0
56	MG	1a	1828	1/1	0.94	0.06	68,68,68,68	0
56	MG	1A	3895	1/1	0.94	0.26	53,53,53,53	0
56	MG	2A	3792	1/1	0.94	0.08	70,70,70,70	0
56	MG	2A	3200	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3435	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3093	1/1	0.94	0.07	50,50,50,50	0
56	MG	1a	1617	1/1	0.94	0.08	46,46,46,46	0
56	MG	1a	1620	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3454	1/1	0.94	0.23	53,53,53,53	0
56	MG	1A	3135	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	4112	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3457	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3209	1/1	0.94	0.10	49,49,49,49	0
56	MG	1a	1624	1/1	0.94	0.19	60,60,60,60	0
56	MG	2A	3211	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3094	1/1	0.94	0.23	50,50,50,50	0
56	MG	2A	3821	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3614	1/1	0.94	0.10	44,44,44,44	0
56	MG	2a	1779	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3097	1/1	0.94	0.10	54,54,54,54	0
56	MG	1a	1855	1/1	0.94	0.12	83,83,83,83	0
56	MG	2A	3825	1/1	0.94	0.09	43,43,43,43	0
56	MG	2A	3465	1/1	0.94	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3466	1/1	0.94	0.18	51,51,51,51	0
56	MG	2A	3828	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3749	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3217	1/1	0.94	0.14	69,69,69,69	0
56	MG	2a	1797	1/1	0.94	0.13	70,70,70,70	0
56	MG	2a	1799	1/1	0.94	0.17	65,65,65,65	0
56	MG	1a	1857	1/1	0.94	0.07	66,66,66,66	0
56	MG	1A	3052	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3752	1/1	0.94	0.15	33,33,33,33	0
56	MG	1A	3519	1/1	0.94	0.11	42,42,42,42	0
56	MG	1a	1865	1/1	0.94	0.09	55,55,55,55	0
56	MG	1a	1634	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	4129	1/1	0.94	0.15	76,76,76,76	0
56	MG	1A	3099	1/1	0.94	0.10	52,52,52,52	0
56	MG	2A	3855	1/1	0.94	0.19	56,56,56,56	0
56	MG	2A	3856	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3257	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3756	1/1	0.94	0.08	24,24,24,24	0
56	MG	1a	1876	1/1	0.94	0.06	74,74,74,74	0
56	MG	1A	3196	1/1	0.94	0.35	36,36,36,36	0
56	MG	1A	4140	1/1	0.94	0.10	57,57,57,57	0
56	MG	2a	1818	1/1	0.94	0.25	64,64,64,64	0
56	MG	1A	3447	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3875	1/1	0.94	0.07	68,68,68,68	0
56	MG	2A	3486	1/1	0.94	0.21	64,64,64,64	0
56	MG	1A	3525	1/1	0.94	0.18	39,39,39,39	0
56	MG	1A	3916	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3239	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3884	1/1	0.94	0.07	51,51,51,51	0
56	MG	1A	3448	1/1	0.94	0.16	47,47,47,47	0
56	MG	1e	3001	1/1	0.94	0.14	72,72,72,72	0
56	MG	1A	3002	1/1	0.94	0.10	52,52,52,52	0
56	MG	2A	3243	1/1	0.94	0.20	55,55,55,55	0
56	MG	2a	1832	1/1	0.94	0.17	61,61,61,61	0
56	MG	2A	3891	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	4156	1/1	0.94	0.13	71,71,71,71	0
56	MG	1a	1648	1/1	0.94	0.16	53,53,53,53	0
56	MG	1a	1651	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3899	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	4161	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3101	1/1	0.94	0.07	30,30,30,30	0
56	MG	2A	3251	1/1	0.94	0.19	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	1A	3057	1/1	0.94	0.15	65,65,65,65	0
56	MG	1A	3324	1/1	0.94	0.10	64,64,64,64	0
56	MG	2A	3254	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	4171	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3924	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3912	1/1	0.94	0.10	88,88,88,88	0
56	MG	2A	3509	1/1	0.94	0.18	62,62,62,62	0
56	MG	2A	3921	1/1	0.94	0.18	38,38,38,38	0
56	MG	2a	1853	1/1	0.94	0.12	52,52,52,52	0
56	MG	1w	104	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3455	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3774	1/1	0.94	0.07	44,44,44,44	0
56	MG	1w	107	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	4176	1/1	0.94	0.06	54,54,54,54	0
56	MG	2A	3928	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3262	1/1	0.94	0.10	54,54,54,54	0
56	MG	1a	1663	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3205	1/1	0.94	0.07	46,46,46,46	0
56	MG	2A	3266	1/1	0.94	0.25	64,64,64,64	0
56	MG	1A	3931	1/1	0.94	0.18	46,46,46,46	0
56	MG	1A	3153	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3634	1/1	0.94	0.27	41,41,41,41	0
56	MG	1A	4206	1/1	0.94	0.07	44,44,44,44	0
56	MG	2A	3531	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3934	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3636	1/1	0.94	0.11	35,35,35,35	0
56	MG	2A	3273	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3155	1/1	0.94	0.24	45,45,45,45	0
56	MG	1A	4216	1/1	0.94	0.23	40,40,40,40	0
56	MG	1A	4217	1/1	0.94	0.24	47,47,47,47	0
56	MG	1A	3156	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3941	1/1	0.94	0.16	52,52,52,52	0
56	MG	2A	3541	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3539	1/1	0.94	0.20	56,56,56,56	0
56	MG	1A	4227	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3461	1/1	0.94	0.10	58,58,58,58	0
56	MG	1y	101	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3790	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3949	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3544	1/1	0.94	0.18	50,50,50,50	0
56	MG	1A	3158	1/1	0.94	0.09	41,41,41,41	0
56	MG	1B	3009	1/1	0.94	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	1A	3271	1/1	0.94	0.29	57,57,57,57	0
56	MG	1A	3273	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3550	1/1	0.94	0.26	45,45,45,45	0
56	MG	1A	3213	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3798	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3554	1/1	0.94	0.10	27,27,27,27	0
56	MG	2A	3017	1/1	0.94	0.08	49,49,49,49	0
56	MG	1B	3022	1/1	0.94	0.07	58,58,58,58	0
56	MG	1A	3161	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3582	1/1	0.94	0.07	48,48,48,48	0
56	MG	1A	3652	1/1	0.94	0.18	42,42,42,42	0
56	MG	2F	306	1/1	0.94	0.06	51,51,51,51	0
56	MG	1A	3653	1/1	0.94	0.20	62,62,62,62	0
58	CPT	2A	3919	4/5	0.94	0.15	68,86,92,111	4
56	MG	1A	4213	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3045	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3547	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3128	1/1	0.95	0.21	53,53,53,53	0
56	MG	2A	3263	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	4036	1/1	0.95	0.15	84,84,84,84	0
56	MG	1A	3129	1/1	0.95	0.07	34,34,34,34	0
56	MG	2a	1628	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3025	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	4040	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	3384	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3487	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3055	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3713	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3817	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3714	1/1	0.95	0.07	35,35,35,35	0
56	MG	1a	1771	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3489	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3276	1/1	0.95	0.08	66,66,66,66	0
56	MG	2A	3277	1/1	0.95	0.09	64,64,64,64	0
56	MG	1B	3010	1/1	0.95	0.15	40,40,40,40	0
56	MG	2A	3062	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3113	1/1	0.95	0.07	42,42,42,42	0
56	MG	1B	3012	1/1	0.95	0.06	55,55,55,55	0
56	MG	1A	3133	1/1	0.95	0.24	34,34,34,34	0
56	MG	1a	1782	1/1	0.95	0.09	67,67,67,67	0
56	MG	2A	3285	1/1	0.95	0.07	40,40,40,40	0
56	MG	1B	3014	1/1	0.95	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1787	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3114	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3289	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3389	1/1	0.95	0.06	53,53,53,53	0
56	MG	1A	3231	1/1	0.95	0.13	45,45,45,45	0
56	MG	2A	3767	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3826	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	4059	1/1	0.95	0.08	45,45,45,45	0
56	MG	2A	3294	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3391	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	4061	1/1	0.95	0.08	72,72,72,72	0
56	MG	1a	1799	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3167	1/1	0.95	0.20	41,41,41,41	0
56	MG	1a	1638	1/1	0.95	0.25	56,56,56,56	0
56	MG	1A	4064	1/1	0.95	0.07	9,9,9,9	0
56	MG	2A	3083	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	1804	1/1	0.95	0.26	38,38,38,38	0
56	MG	2A	3085	1/1	0.95	0.09	56,56,56,56	0
56	MG	1a	1805	1/1	0.95	0.06	65,65,65,65	0
56	MG	1A	3830	1/1	0.95	0.07	57,57,57,57	0
56	MG	2A	3784	1/1	0.95	0.12	55,55,55,55	0
56	MG	2a	1674	1/1	0.95	0.13	43,43,43,43	0
56	MG	1B	3029	1/1	0.95	0.12	64,64,64,64	0
56	MG	2a	1676	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3786	1/1	0.95	0.07	57,57,57,57	0
56	MG	2A	3505	1/1	0.95	0.23	59,59,59,59	0
56	MG	1A	3635	1/1	0.95	0.11	51,51,51,51	0
56	MG	2a	1680	1/1	0.95	0.14	48,48,48,48	0
56	MG	1B	3031	1/1	0.95	0.10	54,54,54,54	0
56	MG	1a	1812	1/1	0.95	0.12	72,72,72,72	0
56	MG	1A	3938	1/1	0.95	0.11	38,38,38,38	0
56	MG	2a	1685	1/1	0.95	0.26	66,66,66,66	0
56	MG	1a	1814	1/1	0.95	0.10	58,58,58,58	0
56	MG	2A	3098	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3836	1/1	0.95	0.12	70,70,70,70	0
56	MG	2A	3100	1/1	0.95	0.18	59,59,59,59	0
56	MG	1A	4076	1/1	0.95	0.05	29,29,29,29	0
56	MG	2A	3799	1/1	0.95	0.06	51,51,51,51	0
56	MG	1B	3035	1/1	0.95	0.08	66,66,66,66	0
56	MG	1B	3036	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	4079	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3105	1/1	0.95	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1822	1/1	0.95	0.11	64,64,64,64	0
56	MG	2A	3809	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3810	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3441	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3567	1/1	0.95	0.17	31,31,31,31	0
56	MG	1A	3138	1/1	0.95	0.31	40,40,40,40	0
56	MG	2A	3818	1/1	0.95	0.08	51,51,51,51	0
56	MG	1a	1656	1/1	0.95	0.11	66,66,66,66	0
56	MG	1D	309	1/1	0.95	0.05	43,43,43,43	0
56	MG	1A	3443	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	4086	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3503	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3395	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3445	1/1	0.95	0.14	62,62,62,62	0
56	MG	2A	3122	1/1	0.95	0.17	52,52,52,52	0
56	MG	1A	3396	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3544	1/1	0.95	0.10	50,50,50,50	0
56	MG	1E	306	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	4091	1/1	0.95	0.09	71,71,71,71	0
56	MG	2A	3833	1/1	0.95	0.08	68,68,68,68	0
56	MG	1A	3055	1/1	0.95	0.20	53,53,53,53	0
56	MG	1a	1667	1/1	0.95	0.28	71,71,71,71	0
56	MG	1a	1842	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3843	1/1	0.95	0.08	53,53,53,53	0
56	MG	2A	3844	1/1	0.95	0.08	53,53,53,53	0
56	MG	2A	3552	1/1	0.95	0.08	52,52,52,52	0
56	MG	1a	1843	1/1	0.95	0.06	81,81,81,81	0
56	MG	1a	1844	1/1	0.95	0.07	59,59,59,59	0
56	MG	2A	3342	1/1	0.95	0.23	54,54,54,54	0
56	MG	2A	3853	1/1	0.95	0.06	30,30,30,30	0
56	MG	1A	4093	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3139	1/1	0.95	0.07	48,48,48,48	0
56	MG	1a	1847	1/1	0.95	0.07	79,79,79,79	0
56	MG	2A	3563	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3564	1/1	0.95	0.10	37,37,37,37	0
56	MG	1a	1669	1/1	0.95	0.11	60,60,60,60	0
56	MG	2A	3869	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3645	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3570	1/1	0.95	0.08	43,43,43,43	0
56	MG	2a	1738	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	3583	1/1	0.95	0.42	63,63,63,63	0
56	MG	1A	3237	1/1	0.95	0.37	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3574	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	4097	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3351	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3578	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3118	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3512	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3277	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	4106	1/1	0.95	0.07	50,50,50,50	0
56	MG	2A	3889	1/1	0.95	0.07	62,62,62,62	0
56	MG	2A	3586	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3201	1/1	0.95	0.11	45,45,45,45	0
56	MG	2A	3591	1/1	0.95	0.09	36,36,36,36	0
56	MG	2A	3157	1/1	0.95	0.15	56,56,56,56	0
56	MG	2A	3898	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3160	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3654	1/1	0.95	0.22	46,46,46,46	0
56	MG	2A	3163	1/1	0.95	0.08	49,49,49,49	0
56	MG	1I	3001	1/1	0.95	0.07	66,66,66,66	0
56	MG	2a	1767	1/1	0.95	0.06	99,99,99,99	0
56	MG	2a	1769	1/1	0.95	0.07	76,76,76,76	0
56	MG	1A	3403	1/1	0.95	0.20	55,55,55,55	0
56	MG	1A	3084	1/1	0.95	0.14	44,44,44,44	0
56	MG	2a	1773	1/1	0.95	0.07	52,52,52,52	0
56	MG	2A	3169	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3282	1/1	0.95	0.30	46,46,46,46	0
56	MG	1A	3760	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3518	1/1	0.95	0.09	59,59,59,59	0
56	MG	2a	1783	1/1	0.95	0.07	87,87,87,87	0
56	MG	1A	3244	1/1	0.95	0.07	57,57,57,57	0
56	MG	2A	3920	1/1	0.95	0.10	39,39,39,39	0
56	MG	2a	1789	1/1	0.95	0.12	76,76,76,76	0
56	MG	1O	3003	1/1	0.95	0.15	53,53,53,53	0
56	MG	2A	3175	1/1	0.95	0.17	48,48,48,48	0
56	MG	1A	3763	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3764	1/1	0.95	0.09	48,48,48,48	0
56	MG	1f	3001	1/1	0.95	0.09	39,39,39,39	0
56	MG	2a	1796	1/1	0.95	0.06	71,71,71,71	0
56	MG	1A	4121	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3620	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3183	1/1	0.95	0.10	43,43,43,43	0
56	MG	1P	201	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3409	1/1	0.95	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3932	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3981	1/1	0.95	0.06	53,53,53,53	0
56	MG	2A	3935	1/1	0.95	0.07	53,53,53,53	0
56	MG	2a	1807	1/1	0.95	0.10	66,66,66,66	0
56	MG	1A	3284	1/1	0.95	0.24	46,46,46,46	0
56	MG	1A	3664	1/1	0.95	0.06	59,59,59,59	0
56	MG	1Q	205	1/1	0.95	0.07	44,44,44,44	0
56	MG	1a	1701	1/1	0.95	0.24	62,62,62,62	0
56	MG	2B	3004	1/1	0.95	0.13	68,68,68,68	0
56	MG	1A	3033	1/1	0.95	0.22	39,39,39,39	0
56	MG	2A	3386	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	4131	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3598	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3772	1/1	0.95	0.17	52,52,52,52	0
56	MG	1A	3999	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	4001	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3667	1/1	0.95	0.10	52,52,52,52	0
56	MG	1U	201	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3642	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3326	1/1	0.95	0.09	60,60,60,60	0
56	MG	1A	4145	1/1	0.95	0.07	80,80,80,80	0
56	MG	1A	3671	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3207	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3649	1/1	0.95	0.10	36,36,36,36	0
56	MG	2a	1829	1/1	0.95	0.09	74,74,74,74	0
56	MG	2a	1830	1/1	0.95	0.13	60,60,60,60	0
56	MG	2A	3206	1/1	0.95	0.06	48,48,48,48	0
56	MG	2A	3651	1/1	0.95	0.17	45,45,45,45	0
56	MG	1U	207	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	3177	1/1	0.95	0.20	42,42,42,42	0
56	MG	2A	3403	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	4154	1/1	0.95	0.25	49,49,49,49	0
56	MG	2A	3657	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	4155	1/1	0.95	0.21	48,48,48,48	0
56	MG	2a	1839	1/1	0.95	0.19	59,59,59,59	0
56	MG	2A	3659	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3780	1/1	0.95	0.06	44,44,44,44	0
56	MG	1a	1720	1/1	0.95	0.08	60,60,60,60	0
56	MG	2A	3662	1/1	0.95	0.06	43,43,43,43	0
56	MG	1W	202	1/1	0.95	0.13	50,50,50,50	0
56	MG	1a	1722	1/1	0.95	0.22	58,58,58,58	0
56	MG	1X	103	1/1	0.95	0.10	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	2F	305	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3178	1/1	0.95	0.08	32,32,32,32	0
56	MG	2F	307	1/1	0.95	0.28	53,53,53,53	0
56	MG	1A	3251	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3671	1/1	0.95	0.06	30,30,30,30	0
56	MG	2a	1855	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3605	1/1	0.95	0.18	55,55,55,55	0
56	MG	2P	202	1/1	0.95	0.17	51,51,51,51	0
56	MG	2A	3219	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3220	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3180	1/1	0.95	0.11	27,27,27,27	0
56	MG	1Z	301	1/1	0.95	0.19	46,46,46,46	0
56	MG	2A	3680	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	4018	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3148	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3001	1/1	0.95	0.38	61,61,61,61	0
56	MG	2U	3002	1/1	0.95	0.23	54,54,54,54	0
56	MG	1A	3107	1/1	0.95	0.19	40,40,40,40	0
56	MG	2A	3687	1/1	0.95	0.09	49,49,49,49	0
56	MG	10	101	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3034	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3473	1/1	0.95	0.20	44,44,44,44	0
56	MG	2A	3692	1/1	0.95	0.07	59,59,59,59	0
56	MG	1A	3217	1/1	0.95	0.07	58,58,58,58	0
56	MG	2v	101	1/1	0.95	0.19	68,68,68,68	0
56	MG	23	102	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3477	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3010	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	4191	1/1	0.95	0.10	45,45,45,45	0
56	MG	11	102	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3020	1/1	0.95	0.12	34,34,34,34	0
56	MG	27	101	1/1	0.95	0.08	43,43,43,43	0
56	MG	11	103	1/1	0.95	0.06	40,40,40,40	0
56	MG	1a	1742	1/1	0.95	0.32	59,59,59,59	0
56	MG	1A	4195	1/1	0.95	0.09	29,29,29,29	0
56	MG	11	105	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3337	1/1	0.95	0.28	64,64,64,64	0
56	MG	13	101	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	4197	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3246	1/1	0.95	0.22	40,40,40,40	0
56	MG	2A	3029	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3126	1/1	0.95	0.34	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	3249	1/1	0.95	0.18	59,59,59,59	0
56	MG	1A	4201	1/1	0.95	0.30	43,43,43,43	0
56	MG	1A	4204	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3018	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3426	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	4208	1/1	0.95	0.19	50,50,50,50	0
56	MG	1A	3427	1/1	0.95	0.16	56,56,56,56	0
58	CPT	1A	4178	4/5	0.95	0.19	54,68,71,73	4
56	MG	1A	4210	1/1	0.95	0.21	45,45,45,45	0
56	MG	2A	3450	1/1	0.95	0.22	49,49,49,49	0
58	CPT	2A	3915	4/5	0.95	0.13	54,71,73,90	4
56	MG	1A	4211	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3804	1/1	0.95	0.10	43,43,43,43	0
58	CPT	2I	201	4/5	0.95	0.19	38,50,68,87	4
59	ZN	2n	102	1/1	0.95	0.07	97,97,97,97	0
56	MG	1a	1612	1/1	0.96	0.08	23,23,23,23	0
56	MG	1a	1613	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3402	1/1	0.96	0.07	65,65,65,65	0
56	MG	1A	4049	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	1776	1/1	0.96	0.09	50,50,50,50	0
56	MG	1a	1777	1/1	0.96	0.18	63,63,63,63	0
56	MG	1a	1616	1/1	0.96	0.14	55,55,55,55	0
56	MG	1a	1781	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3799	1/1	0.96	0.07	19,19,19,19	0
56	MG	1A	3091	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3801	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3480	1/1	0.96	0.09	58,58,58,58	0
56	MG	2A	3281	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3549	1/1	0.96	0.20	49,49,49,49	0
56	MG	1A	3066	1/1	0.96	0.23	58,58,58,58	0
56	MG	2A	3484	1/1	0.96	0.19	55,55,55,55	0
56	MG	2A	3485	1/1	0.96	0.07	59,59,59,59	0
56	MG	1a	1790	1/1	0.96	0.06	52,52,52,52	0
56	MG	1a	1625	1/1	0.96	0.18	50,50,50,50	0
56	MG	2a	1640	1/1	0.96	0.21	49,49,49,49	0
56	MG	2a	1641	1/1	0.96	0.25	52,52,52,52	0
56	MG	1A	3621	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3758	1/1	0.96	0.07	78,78,78,78	0
56	MG	1a	1627	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3919	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3267	1/1	0.96	0.09	50,50,50,50	0
56	MG	1B	3016	1/1	0.96	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	3018	1/1	0.96	0.20	30,30,30,30	0
56	MG	2A	3495	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3921	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3706	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	4062	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3707	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3708	1/1	0.96	0.07	58,58,58,58	0
56	MG	1A	3709	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3298	1/1	0.96	0.09	68,68,68,68	0
56	MG	1A	3926	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3553	1/1	0.96	0.41	58,58,58,58	0
56	MG	1A	4073	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	4074	1/1	0.96	0.05	31,31,31,31	0
56	MG	2A	3507	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3045	1/1	0.96	0.13	38,38,38,38	0
56	MG	2A	3094	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3407	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	4078	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3097	1/1	0.96	0.05	37,37,37,37	0
56	MG	2A	3514	1/1	0.96	0.07	54,54,54,54	0
56	MG	1A	3408	1/1	0.96	0.14	55,55,55,55	0
56	MG	1A	3449	1/1	0.96	0.13	63,63,63,63	0
56	MG	2A	3518	1/1	0.96	0.05	36,36,36,36	0
56	MG	1a	1820	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	3368	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	4083	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3500	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	3137	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3561	1/1	0.96	0.07	43,43,43,43	0
56	MG	1D	304	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	3502	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3112	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3272	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3802	1/1	0.96	0.07	62,62,62,62	0
56	MG	2A	3112	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3102	1/1	0.96	0.22	41,41,41,41	0
56	MG	1E	301	1/1	0.96	0.10	25,25,25,25	0
56	MG	1A	3727	1/1	0.96	0.06	25,25,25,25	0
56	MG	2A	3116	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3948	1/1	0.96	0.06	19,19,19,19	0
56	MG	1A	3832	1/1	0.96	0.06	33,33,33,33	0
56	MG	2A	3812	1/1	0.96	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3274	1/1	0.96	0.13	55,55,55,55	0
56	MG	1A	3568	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3815	1/1	0.96	0.05	64,64,64,64	0
56	MG	2A	3816	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3953	1/1	0.96	0.11	38,38,38,38	0
56	MG	2A	3123	1/1	0.96	0.24	64,64,64,64	0
56	MG	2A	3547	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3732	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3549	1/1	0.96	0.06	54,54,54,54	0
56	MG	1E	309	1/1	0.96	0.23	40,40,40,40	0
56	MG	2A	3126	1/1	0.96	0.05	55,55,55,55	0
56	MG	1A	3570	1/1	0.96	0.25	41,41,41,41	0
56	MG	1A	3842	1/1	0.96	0.05	59,59,59,59	0
56	MG	2A	3555	1/1	0.96	0.15	61,61,61,61	0
56	MG	2A	3556	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3129	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3959	1/1	0.96	0.24	29,29,29,29	0
56	MG	1A	3247	1/1	0.96	0.12	63,63,63,63	0
56	MG	1A	3572	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3135	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3837	1/1	0.96	0.17	75,75,75,75	0
56	MG	2A	3838	1/1	0.96	0.07	78,78,78,78	0
56	MG	1A	3508	1/1	0.96	0.19	34,34,34,34	0
56	MG	2A	3841	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3964	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3138	1/1	0.96	0.26	42,42,42,42	0
56	MG	2a	1721	1/1	0.96	0.13	69,69,69,69	0
56	MG	1A	3181	1/1	0.96	0.09	38,38,38,38	0
56	MG	1G	3001	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3310	1/1	0.96	0.06	35,35,35,35	0
56	MG	2A	3850	1/1	0.96	0.06	28,28,28,28	0
56	MG	2A	3142	1/1	0.96	0.20	41,41,41,41	0
56	MG	2A	3852	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3143	1/1	0.96	0.06	31,31,31,31	0
56	MG	2A	3854	1/1	0.96	0.07	44,44,44,44	0
56	MG	1a	1861	1/1	0.96	0.07	55,55,55,55	0
56	MG	1a	1862	1/1	0.96	0.06	59,59,59,59	0
56	MG	2A	3577	1/1	0.96	0.08	55,55,55,55	0
56	MG	1a	1863	1/1	0.96	0.05	63,63,63,63	0
56	MG	2A	3862	1/1	0.96	0.05	65,65,65,65	0
56	MG	2A	3866	1/1	0.96	0.06	62,62,62,62	0
56	MG	1A	3848	1/1	0.96	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3148	1/1	0.96	0.19	33,33,33,33	0
56	MG	1G	3004	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	4113	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3511	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3646	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3590	1/1	0.96	0.04	36,36,36,36	0
56	MG	2A	3877	1/1	0.96	0.10	57,57,57,57	0
56	MG	1A	3159	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3155	1/1	0.96	0.07	47,47,47,47	0
56	MG	1N	203	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	4118	1/1	0.96	0.06	42,42,42,42	0
56	MG	1a	1878	1/1	0.96	0.34	64,64,64,64	0
56	MG	1A	3224	1/1	0.96	0.11	60,60,60,60	0
56	MG	2A	3164	1/1	0.96	0.09	54,54,54,54	0
56	MG	1a	1880	1/1	0.96	0.21	39,39,39,39	0
56	MG	1a	1881	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3601	1/1	0.96	0.15	58,58,58,58	0
56	MG	1a	1688	1/1	0.96	0.05	69,69,69,69	0
56	MG	2a	1759	1/1	0.96	0.11	91,91,91,91	0
56	MG	2a	1760	1/1	0.96	0.14	80,80,80,80	0
56	MG	2A	3894	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3895	1/1	0.96	0.11	52,52,52,52	0
56	MG	2A	3604	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3168	1/1	0.96	0.08	36,36,36,36	0
56	MG	2a	1766	1/1	0.96	0.09	69,69,69,69	0
56	MG	2A	3606	1/1	0.96	0.05	56,56,56,56	0
56	MG	1A	3581	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3610	1/1	0.96	0.07	54,54,54,54	0
56	MG	2A	3611	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	4122	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3650	1/1	0.96	0.24	52,52,52,52	0
56	MG	2A	3906	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3614	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3751	1/1	0.96	0.14	47,47,47,47	0
56	MG	2a	1782	1/1	0.96	0.07	86,86,86,86	0
56	MG	1A	3204	1/1	0.96	0.08	32,32,32,32	0
56	MG	1l	202	1/1	0.96	0.09	82,82,82,82	0
56	MG	2A	3911	1/1	0.96	0.15	70,70,70,70	0
56	MG	1A	4126	1/1	0.96	0.07	69,69,69,69	0
56	MG	1a	1696	1/1	0.96	0.24	58,58,58,58	0
56	MG	1A	4128	1/1	0.96	0.07	52,52,52,52	0
56	MG	2a	1792	1/1	0.96	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3421	1/1	0.96	0.10	51,51,51,51	0
56	MG	1a	1699	1/1	0.96	0.41	68,68,68,68	0
56	MG	2A	3182	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3383	1/1	0.96	0.10	64,64,64,64	0
56	MG	1A	3465	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3466	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3983	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	4135	1/1	0.96	0.10	64,64,64,64	0
56	MG	1A	3382	1/1	0.96	0.09	51,51,51,51	0
56	MG	2a	1803	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3383	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3089	1/1	0.96	0.11	49,49,49,49	0
56	MG	1A	4141	1/1	0.96	0.11	17,17,17,17	0
56	MG	1A	3106	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3994	1/1	0.96	0.04	39,39,39,39	0
56	MG	2A	3938	1/1	0.96	0.11	81,81,81,81	0
56	MG	2A	3943	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3874	1/1	0.96	0.08	33,33,33,33	0
56	MG	2B	3001	1/1	0.96	0.16	65,65,65,65	0
56	MG	1A	3659	1/1	0.96	0.11	34,34,34,34	0
56	MG	1x	102	1/1	0.96	0.19	58,58,58,58	0
56	MG	1A	3348	1/1	0.96	0.15	60,60,60,60	0
56	MG	1A	3350	1/1	0.96	0.14	48,48,48,48	0
56	MG	1a	1714	1/1	0.96	0.13	42,42,42,42	0
56	MG	2B	3007	1/1	0.96	0.08	57,57,57,57	0
56	MG	2A	3401	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3524	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3648	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3765	1/1	0.96	0.12	50,50,50,50	0
56	MG	1x	109	1/1	0.96	0.10	57,57,57,57	0
56	MG	1A	4005	1/1	0.96	0.06	54,54,54,54	0
56	MG	2A	3406	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	4008	1/1	0.96	0.07	59,59,59,59	0
56	MG	1A	3428	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3655	1/1	0.96	0.13	50,50,50,50	0
56	MG	2B	3018	1/1	0.96	0.10	61,61,61,61	0
56	MG	1A	3475	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	4167	1/1	0.96	0.09	46,46,46,46	0
56	MG	2D	301	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3527	1/1	0.96	0.14	34,34,34,34	0
56	MG	1W	204	1/1	0.96	0.11	41,41,41,41	0
56	MG	1X	102	1/1	0.96	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4170	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3229	1/1	0.96	0.25	56,56,56,56	0
56	MG	1A	3770	1/1	0.96	0.14	36,36,36,36	0
56	MG	1A	3530	1/1	0.96	0.13	53,53,53,53	0
56	MG	2A	3665	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	4174	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3667	1/1	0.96	0.19	53,53,53,53	0
56	MG	1A	3669	1/1	0.96	0.07	45,45,45,45	0
56	MG	1a	1731	1/1	0.96	0.18	68,68,68,68	0
56	MG	1A	3773	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3221	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3003	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3888	1/1	0.96	0.08	42,42,42,42	0
56	MG	2a	1850	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	4184	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3285	1/1	0.96	0.26	40,40,40,40	0
56	MG	1A	4186	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	4189	1/1	0.96	0.10	46,46,46,46	0
56	MG	10	104	1/1	0.96	0.10	57,57,57,57	0
56	MG	2A	3683	1/1	0.96	0.05	37,37,37,37	0
56	MG	2A	3011	1/1	0.96	0.07	46,46,46,46	0
56	MG	2f	3001	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3015	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3431	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	4023	1/1	0.96	0.07	44,44,44,44	0
56	MG	1a	1741	1/1	0.96	0.27	61,61,61,61	0
56	MG	2R	201	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	4024	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3230	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3693	1/1	0.96	0.10	68,68,68,68	0
56	MG	2T	201	1/1	0.96	0.08	64,64,64,64	0
56	MG	2T	202	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3116	1/1	0.96	0.19	38,38,38,38	0
56	MG	1A	3289	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	4202	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3322	1/1	0.96	0.11	46,46,46,46	0
56	MG	1a	1748	1/1	0.96	0.39	69,69,69,69	0
56	MG	2A	3028	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3896	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3781	1/1	0.96	0.15	55,55,55,55	0
56	MG	2A	3702	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3031	1/1	0.96	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	3258	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3034	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3147	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3031	1/1	0.96	0.20	32,32,32,32	0
56	MG	1A	3540	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3686	1/1	0.96	0.09	20,20,20,20	0
56	MG	1A	3903	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3712	1/1	0.96	0.05	51,51,51,51	0
56	MG	1A	3169	1/1	0.96	0.19	43,43,43,43	0
56	MG	1A	3542	1/1	0.96	0.10	47,47,47,47	0
56	MG	18	102	1/1	0.96	0.11	54,54,54,54	0
56	MG	2A	3716	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3236	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	4041	1/1	0.96	0.05	70,70,70,70	0
56	MG	1a	1601	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	4224	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	4225	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3691	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3488	1/1	0.96	0.15	58,58,58,58	0
56	MG	1B	3001	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3131	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3727	1/1	0.96	0.10	53,53,53,53	0
58	CPT	1A	4182	4/5	0.96	0.13	64,84,85,87	4
58	CPT	2A	3914	4/5	0.96	0.18	44,54,55,67	4
56	MG	1a	1609	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3730	1/1	0.96	0.06	31,31,31,31	0
56	MG	2A	3054	1/1	0.96	0.16	55,55,55,55	0
56	MG	1B	3003	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3910	1/1	0.96	0.13	29,29,29,29	0
56	MG	1a	1780	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3330	1/1	0.97	0.30	65,65,65,65	0
56	MG	1A	3077	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	3582	1/1	0.97	0.19	43,43,43,43	0
56	MG	1a	1785	1/1	0.97	0.14	41,41,41,41	0
56	MG	1a	1786	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3836	1/1	0.97	0.06	74,74,74,74	0
56	MG	1A	3748	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3042	1/1	0.97	0.11	32,32,32,32	0
56	MG	1A	3175	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	3855	1/1	0.97	0.05	57,57,57,57	0
56	MG	2A	3842	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3453	1/1	0.97	0.17	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	1D	306	1/1	0.97	0.13	34,34,34,34	0
56	MG	1D	308	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3623	1/1	0.97	0.04	49,49,49,49	0
56	MG	2A	3848	1/1	0.97	0.09	69,69,69,69	0
56	MG	2A	3624	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3857	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3237	1/1	0.97	0.11	46,46,46,46	0
56	MG	1D	310	1/1	0.97	0.22	34,34,34,34	0
56	MG	1a	1798	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3858	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3860	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3975	1/1	0.97	0.05	90,90,90,90	0
56	MG	1A	3861	1/1	0.97	0.26	37,37,37,37	0
56	MG	1A	3176	1/1	0.97	0.33	42,42,42,42	0
56	MG	2A	3860	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3225	1/1	0.97	0.20	44,44,44,44	0
56	MG	1a	1650	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3079	1/1	0.97	0.10	44,44,44,44	0
56	MG	1a	1809	1/1	0.97	0.05	56,56,56,56	0
56	MG	2A	3638	1/1	0.97	0.13	52,52,52,52	0
56	MG	2A	3639	1/1	0.97	0.07	39,39,39,39	0
56	MG	2A	3873	1/1	0.97	0.05	66,66,66,66	0
56	MG	1a	1652	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3134	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3660	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	4119	1/1	0.97	0.08	53,53,53,53	0
56	MG	2A	3878	1/1	0.97	0.06	68,68,68,68	0
56	MG	1A	3281	1/1	0.97	0.17	39,39,39,39	0
56	MG	2a	1703	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3758	1/1	0.97	0.10	31,31,31,31	0
56	MG	2A	3646	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3459	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3069	1/1	0.97	0.04	31,31,31,31	0
56	MG	1A	3986	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3592	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3990	1/1	0.97	0.05	9,9,9,9	0
56	MG	1A	3105	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3890	1/1	0.97	0.17	31,31,31,31	0
56	MG	2A	3074	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3136	1/1	0.97	0.06	48,48,48,48	0
56	MG	2a	1715	1/1	0.97	0.07	60,60,60,60	0
56	MG	2A	3893	1/1	0.97	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3995	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3054	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3026	1/1	0.97	0.14	51,51,51,51	0
56	MG	1A	3032	1/1	0.97	0.34	37,37,37,37	0
56	MG	1A	3287	1/1	0.97	0.12	52,52,52,52	0
56	MG	1A	3670	1/1	0.97	0.06	19,19,19,19	0
56	MG	1A	3083	1/1	0.97	0.10	34,34,34,34	0
56	MG	1a	1830	1/1	0.97	0.05	79,79,79,79	0
56	MG	2A	3902	1/1	0.97	0.14	51,51,51,51	0
56	MG	1A	3600	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	4007	1/1	0.97	0.07	67,67,67,67	0
56	MG	2A	3905	1/1	0.97	0.05	68,68,68,68	0
56	MG	1A	3027	1/1	0.97	0.23	33,33,33,33	0
56	MG	1a	1835	1/1	0.97	0.06	64,64,64,64	0
56	MG	1N	204	1/1	0.97	0.16	55,55,55,55	0
56	MG	1A	3021	1/1	0.97	0.04	35,35,35,35	0
56	MG	1A	3146	1/1	0.97	0.14	35,35,35,35	0
56	MG	2A	3670	1/1	0.97	0.13	50,50,50,50	0
56	MG	1A	4147	1/1	0.97	0.09	10,10,10,10	0
56	MG	2A	3672	1/1	0.97	0.06	61,61,61,61	0
56	MG	1A	4148	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	4149	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	4011	1/1	0.97	0.06	57,57,57,57	0
56	MG	2A	3676	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3678	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3238	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3679	1/1	0.97	0.07	50,50,50,50	0
56	MG	2A	3927	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3189	1/1	0.97	0.21	51,51,51,51	0
56	MG	1a	1848	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3889	1/1	0.97	0.06	42,42,42,42	0
56	MG	1a	1854	1/1	0.97	0.05	86,86,86,86	0
56	MG	1A	4016	1/1	0.97	0.05	62,62,62,62	0
56	MG	2A	3933	1/1	0.97	0.13	47,47,47,47	0
56	MG	1A	4158	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3240	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3683	1/1	0.97	0.07	54,54,54,54	0
56	MG	2a	1755	1/1	0.97	0.05	65,65,65,65	0
56	MG	2A	3937	1/1	0.97	0.21	41,41,41,41	0
56	MG	2a	1757	1/1	0.97	0.10	68,68,68,68	0
56	MG	2a	1758	1/1	0.97	0.04	83,83,83,83	0
56	MG	1a	1689	1/1	0.97	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3940	1/1	0.97	0.14	50,50,50,50	0
56	MG	2A	3941	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3690	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3110	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	4163	1/1	0.97	0.24	35,35,35,35	0
56	MG	1R	202	1/1	0.97	0.27	40,40,40,40	0
56	MG	1A	4019	1/1	0.97	0.05	67,67,67,67	0
56	MG	1A	3295	1/1	0.97	0.15	31,31,31,31	0
56	MG	1a	1864	1/1	0.97	0.05	61,61,61,61	0
56	MG	1A	3474	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	4169	1/1	0.97	0.13	49,49,49,49	0
56	MG	2a	1774	1/1	0.97	0.16	52,52,52,52	0
56	MG	1a	1870	1/1	0.97	0.08	30,30,30,30	0
56	MG	2A	3119	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3354	1/1	0.97	0.24	39,39,39,39	0
56	MG	1A	3035	1/1	0.97	0.08	33,33,33,33	0
56	MG	2a	1781	1/1	0.97	0.05	82,82,82,82	0
56	MG	1A	3061	1/1	0.97	0.28	53,53,53,53	0
56	MG	1A	3036	1/1	0.97	0.17	24,24,24,24	0
56	MG	2a	1784	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3690	1/1	0.97	0.14	31,31,31,31	0
56	MG	1A	3193	1/1	0.97	0.17	36,36,36,36	0
56	MG	2a	1788	1/1	0.97	0.06	73,73,73,73	0
56	MG	1A	3543	1/1	0.97	0.23	36,36,36,36	0
56	MG	1U	206	1/1	0.97	0.15	29,29,29,29	0
56	MG	2A	3493	1/1	0.97	0.06	55,55,55,55	0
56	MG	2A	3710	1/1	0.97	0.04	27,27,27,27	0
56	MG	1A	3064	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	3616	1/1	0.97	0.10	51,51,51,51	0
56	MG	2A	3130	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3117	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3065	1/1	0.97	0.09	35,35,35,35	0
56	MG	2a	1798	1/1	0.97	0.06	85,85,85,85	0
56	MG	1A	3249	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3700	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	4193	1/1	0.97	0.10	41,41,41,41	0
56	MG	1X	101	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	4194	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3154	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3007	1/1	0.97	0.09	45,45,45,45	0
56	MG	1A	4037	1/1	0.97	0.07	74,74,74,74	0
56	MG	1A	4199	1/1	0.97	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1808	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	3705	1/1	0.97	0.07	42,42,42,42	0
56	MG	1Y	205	1/1	0.97	0.17	49,49,49,49	0
56	MG	1A	3200	1/1	0.97	0.22	46,46,46,46	0
56	MG	1A	3623	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	4203	1/1	0.97	0.24	31,31,31,31	0
56	MG	1A	3120	1/1	0.97	0.30	49,49,49,49	0
56	MG	2A	3149	1/1	0.97	0.12	36,36,36,36	0
56	MG	2A	3516	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3552	1/1	0.97	0.20	32,32,32,32	0
56	MG	2A	3736	1/1	0.97	0.04	52,52,52,52	0
56	MG	1A	4044	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3806	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3915	1/1	0.97	0.10	48,48,48,48	0
56	MG	2A	3740	1/1	0.97	0.07	50,50,50,50	0
56	MG	2Q	3003	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3203	1/1	0.97	0.11	45,45,45,45	0
56	MG	1w	109	1/1	0.97	0.06	68,68,68,68	0
56	MG	2A	3156	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3121	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3158	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3159	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3092	1/1	0.97	0.15	22,22,22,22	0
56	MG	2A	3161	1/1	0.97	0.12	53,53,53,53	0
56	MG	1x	101	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3160	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3535	1/1	0.97	0.05	33,33,33,33	0
56	MG	2X	101	1/1	0.97	0.10	52,52,52,52	0
56	MG	1x	103	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3069	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3814	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	4054	1/1	0.97	0.19	56,56,56,56	0
56	MG	1A	4221	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	4222	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3542	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3372	1/1	0.97	0.18	51,51,51,51	0
56	MG	1A	3164	1/1	0.97	0.25	49,49,49,49	0
56	MG	1A	3209	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3071	1/1	0.97	0.08	16,16,16,16	0
56	MG	1A	3125	1/1	0.97	0.27	48,48,48,48	0
56	MG	1A	3212	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3499	1/1	0.97	0.23	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	3177	1/1	0.97	0.16	53,53,53,53	0
56	MG	2A	3770	1/1	0.97	0.08	48,48,48,48	0
56	MG	17	103	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3320	1/1	0.97	0.17	52,52,52,52	0
56	MG	1A	3724	1/1	0.97	0.12	38,38,38,38	0
56	MG	1B	3005	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3725	1/1	0.97	0.08	35,35,35,35	0
56	MG	2A	3558	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3184	1/1	0.97	0.09	43,43,43,43	0
56	MG	19	101	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3726	1/1	0.97	0.04	42,42,42,42	0
56	MG	1A	3935	1/1	0.97	0.08	42,42,42,42	0
56	MG	1a	1602	1/1	0.97	0.30	62,62,62,62	0
56	MG	1A	4068	1/1	0.97	0.15	80,80,80,80	0
56	MG	1A	3096	1/1	0.97	0.17	27,27,27,27	0
56	MG	2A	3568	1/1	0.97	0.12	62,62,62,62	0
56	MG	1A	4071	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3829	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3030	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3831	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3573	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3074	1/1	0.97	0.06	28,28,28,28	0
56	MG	1A	3942	1/1	0.97	0.09	52,52,52,52	0
56	MG	1B	3017	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3013	1/1	0.97	0.04	37,37,37,37	0
56	MG	2A	3795	1/1	0.97	0.05	48,48,48,48	0
56	MG	2A	3014	1/1	0.97	0.07	38,38,38,38	0
56	MG	2A	3580	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3833	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3075	1/1	0.97	0.26	48,48,48,48	0
56	MG	2A	3203	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3946	1/1	0.97	0.15	36,36,36,36	0
56	MG	2A	3804	1/1	0.97	0.05	53,53,53,53	0
56	MG	2A	3018	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3587	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3807	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3733	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3325	1/1	0.97	0.16	51,51,51,51	0
56	MG	1A	3838	1/1	0.97	0.04	70,70,70,70	0
56	MG	1a	1618	1/1	0.97	0.04	40,40,40,40	0
56	MG	2a	1642	1/1	0.97	0.35	41,41,41,41	0
56	MG	1A	3735	1/1	0.97	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3393	1/1	0.97	0.07	47,47,47,47	0
56	MG	1a	1621	1/1	0.97	0.05	36,36,36,36	0
56	MG	1B	3025	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3841	1/1	0.97	0.05	55,55,55,55	0
56	MG	2A	3817	1/1	0.97	0.07	53,53,53,53	0
57	K	1A	3577	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3952	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3819	1/1	0.97	0.05	78,78,78,78	0
56	MG	1A	3573	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3600	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3269	1/1	0.97	0.07	47,47,47,47	0
58	CPT	1I	3002	4/5	0.97	0.14	40,48,69,81	4
58	CPT	1a	1883	4/5	0.97	0.08	75,75,78,117	4
56	MG	1A	3171	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3387	1/1	0.97	0.05	32,32,32,32	0
58	CPT	2A	3917	4/5	0.97	0.11	59,63,68,93	4
56	MG	1A	3076	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3220	1/1	0.97	0.13	58,58,58,58	0
56	MG	2A	3036	1/1	0.97	0.14	40,40,40,40	0
59	ZN	24	501	1/1	0.97	0.05	95,95,95,95	0
56	MG	2A	3609	1/1	0.97	0.04	36,36,36,36	0
56	MG	1a	1839	1/1	0.98	0.04	88,88,88,88	0
56	MG	1a	1649	1/1	0.98	0.10	40,40,40,40	0
56	MG	2A	3364	1/1	0.98	0.20	57,57,57,57	0
56	MG	2a	1768	1/1	0.98	0.06	72,72,72,72	0
56	MG	2A	3019	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3529	1/1	0.98	0.14	34,34,34,34	0
56	MG	1W	203	1/1	0.98	0.21	34,34,34,34	0
56	MG	2a	1772	1/1	0.98	0.05	75,75,75,75	0
56	MG	2A	3134	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	4157	1/1	0.98	0.07	44,44,44,44	0
56	MG	2a	1775	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3262	1/1	0.98	0.09	56,56,56,56	0
56	MG	2a	1777	1/1	0.98	0.04	75,75,75,75	0
56	MG	1a	1845	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	4159	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	4160	1/1	0.98	0.27	34,34,34,34	0
56	MG	1A	3566	1/1	0.98	0.16	34,34,34,34	0
56	MG	1A	3010	1/1	0.98	0.12	37,37,37,37	0
56	MG	1a	1850	1/1	0.98	0.03	62,62,62,62	0
56	MG	1a	1852	1/1	0.98	0.05	65,65,65,65	0
56	MG	1A	3067	1/1	0.98	0.13	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	2a	1786	1/1	0.98	0.09	66,66,66,66	0
56	MG	2A	3762	1/1	0.98	0.19	30,30,30,30	0
56	MG	1A	4164	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3033	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	4165	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	3179	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3682	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3943	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3068	1/1	0.98	0.08	17,17,17,17	0
56	MG	1A	3056	1/1	0.98	0.13	33,33,33,33	0
56	MG	1A	3728	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3157	1/1	0.98	0.25	43,43,43,43	0
56	MG	1A	3070	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	3301	1/1	0.98	0.06	41,41,41,41	0
56	MG	2a	1650	1/1	0.98	0.14	60,60,60,60	0
56	MG	2A	3775	1/1	0.98	0.07	54,54,54,54	0
56	MG	1a	1866	1/1	0.98	0.08	65,65,65,65	0
56	MG	1a	1867	1/1	0.98	0.05	59,59,59,59	0
56	MG	1A	3835	1/1	0.98	0.07	60,60,60,60	0
56	MG	1a	1869	1/1	0.98	0.04	66,66,66,66	0
56	MG	2A	3513	1/1	0.98	0.04	70,70,70,70	0
56	MG	1A	3005	1/1	0.98	0.10	50,50,50,50	0
56	MG	1D	307	1/1	0.98	0.13	41,41,41,41	0
56	MG	1a	1872	1/1	0.98	0.06	47,47,47,47	0
56	MG	1A	3103	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3242	1/1	0.98	0.18	34,34,34,34	0
56	MG	2A	3519	1/1	0.98	0.10	60,60,60,60	0
56	MG	1A	3839	1/1	0.98	0.07	48,48,48,48	0
56	MG	1A	3784	1/1	0.98	0.07	31,31,31,31	0
56	MG	2A	3942	1/1	0.98	0.07	54,54,54,54	0
56	MG	1A	4187	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3785	1/1	0.98	0.06	23,23,23,23	0
56	MG	1A	4190	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3305	1/1	0.98	0.23	35,35,35,35	0
56	MG	1A	4192	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3737	1/1	0.98	0.13	30,30,30,30	0
56	MG	2A	3529	1/1	0.98	0.07	29,29,29,29	0
56	MG	1a	1885	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	4101	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	4103	1/1	0.98	0.03	52,52,52,52	0
56	MG	1A	3139	1/1	0.98	0.05	36,36,36,36	0
56	MG	2A	3178	1/1	0.98	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3789	1/1	0.98	0.07	44,44,44,44	0
56	MG	1a	1778	1/1	0.98	0.08	47,47,47,47	0
56	MG	1l	201	1/1	0.98	0.16	39,39,39,39	0
56	MG	1A	4198	1/1	0.98	0.20	34,34,34,34	0
56	MG	1A	3739	1/1	0.98	0.06	31,31,31,31	0
56	MG	2a	1683	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3214	1/1	0.98	0.25	39,39,39,39	0
56	MG	1A	3741	1/1	0.98	0.10	33,33,33,33	0
56	MG	2A	3543	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3162	1/1	0.98	0.15	35,35,35,35	0
56	MG	1a	1784	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3374	1/1	0.98	0.09	48,48,48,48	0
56	MG	2A	3075	1/1	0.98	0.14	29,29,29,29	0
56	MG	2D	303	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3696	1/1	0.98	0.07	10,10,10,10	0
56	MG	1A	4205	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3163	1/1	0.98	0.28	34,34,34,34	0
56	MG	1A	3037	1/1	0.98	0.21	35,35,35,35	0
56	MG	1A	3699	1/1	0.98	0.16	28,28,28,28	0
56	MG	2A	3195	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3554	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3141	1/1	0.98	0.14	35,35,35,35	0
56	MG	2A	3686	1/1	0.98	0.09	32,32,32,32	0
56	MG	2a	1851	1/1	0.98	0.04	71,71,71,71	0
56	MG	2a	1852	1/1	0.98	0.12	64,64,64,64	0
56	MG	1A	4117	1/1	0.98	0.04	69,69,69,69	0
56	MG	2A	3314	1/1	0.98	0.05	59,59,59,59	0
56	MG	1a	1793	1/1	0.98	0.06	47,47,47,47	0
56	MG	1A	4043	1/1	0.98	0.11	66,66,66,66	0
56	MG	1A	3701	1/1	0.98	0.05	31,31,31,31	0
56	MG	2A	3086	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3142	1/1	0.98	0.08	13,13,13,13	0
56	MG	1A	4214	1/1	0.98	0.05	44,44,44,44	0
56	MG	1A	4215	1/1	0.98	0.27	33,33,33,33	0
56	MG	1A	3859	1/1	0.98	0.08	45,45,45,45	0
56	MG	2A	3566	1/1	0.98	0.13	37,37,37,37	0
56	MG	2A	3567	1/1	0.98	0.10	40,40,40,40	0
56	MG	2P	201	1/1	0.98	0.04	45,45,45,45	0
56	MG	2A	3091	1/1	0.98	0.08	42,42,42,42	0
56	MG	1A	3703	1/1	0.98	0.04	36,36,36,36	0
56	MG	1a	1802	1/1	0.98	0.18	53,53,53,53	0
56	MG	1A	3073	1/1	0.98	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4219	1/1	0.98	0.09	35,35,35,35	0
56	MG	1A	4220	1/1	0.98	0.21	42,42,42,42	0
56	MG	1a	1619	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3038	1/1	0.98	0.29	39,39,39,39	0
56	MG	1A	3982	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3012	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	4127	1/1	0.98	0.04	71,71,71,71	0
56	MG	2A	3579	1/1	0.98	0.05	30,30,30,30	0
56	MG	1P	202	1/1	0.98	0.18	29,29,29,29	0
56	MG	1A	4052	1/1	0.98	0.08	58,58,58,58	0
56	MG	1A	3195	1/1	0.98	0.21	49,49,49,49	0
56	MG	1A	3865	1/1	0.98	0.06	51,51,51,51	0
56	MG	2A	3584	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3866	1/1	0.98	0.05	67,67,67,67	0
56	MG	2A	3107	1/1	0.98	0.12	36,36,36,36	0
56	MG	2A	3858	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3987	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	4134	1/1	0.98	0.03	20,20,20,20	0
56	MG	2A	3589	1/1	0.98	0.07	41,41,41,41	0
56	MG	2A	3863	1/1	0.98	0.05	54,54,54,54	0
56	MG	2A	3865	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3349	1/1	0.98	0.25	50,50,50,50	0
56	MG	1A	4136	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3013	1/1	0.98	0.17	33,33,33,33	0
56	MG	1A	3062	1/1	0.98	0.14	38,38,38,38	0
56	MG	2A	3870	1/1	0.98	0.04	56,56,56,56	0
56	MG	1A	3992	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3230	1/1	0.98	0.28	44,44,44,44	0
56	MG	1A	3041	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3871	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3927	1/1	0.98	0.17	30,30,30,30	0
58	CPT	1A	4177	4/5	0.98	0.10	33,49,52,60	4
56	MG	1A	3928	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	4146	1/1	0.98	0.06	60,60,60,60	0
58	CPT	1A	4180	4/5	0.98	0.09	60,66,67,81	4
56	MG	1A	3015	1/1	0.98	0.04	39,39,39,39	0
56	MG	2A	3880	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3095	1/1	0.98	0.06	36,36,36,36	0
56	MG	2A	3882	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3151	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3202	1/1	0.98	0.23	28,28,28,28	0
58	CPT	2A	3916	4/5	0.98	0.14	62,65,84,86	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3012	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3022	1/1	0.98	0.09	27,27,27,27	0
56	MG	1A	4072	1/1	0.98	0.05	26,26,26,26	0
56	MG	1A	4006	1/1	0.98	0.08	57,57,57,57	0
59	ZN	14	501	1/1	0.98	0.06	84,84,84,84	0
59	ZN	2Y	501	1/1	0.98	0.05	80,80,80,80	0
56	MG	2A	3742	1/1	0.98	0.06	34,34,34,34	0
59	ZN	29	501	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3675	1/1	0.98	0.07	59,59,59,59	0
60	SF4	2d	302	8/8	0.98	0.04	61,66,79,85	0
56	MG	1A	3731	1/1	0.99	0.08	34,34,34,34	0
56	MG	17	101	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3807	1/1	0.99	0.05	45,45,45,45	0
56	MG	1A	4080	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3808	1/1	0.99	0.11	33,33,33,33	0
56	MG	1F	304	1/1	0.99	0.16	36,36,36,36	0
56	MG	1A	3955	1/1	0.99	0.08	44,44,44,44	0
56	MG	1A	3849	1/1	0.99	0.09	23,23,23,23	0
56	MG	1A	3957	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3232	1/1	0.99	0.14	47,47,47,47	0
56	MG	2I	202	1/1	0.99	0.04	64,64,64,64	0
56	MG	1A	3775	1/1	0.99	0.06	24,24,24,24	0
56	MG	2A	3602	1/1	0.99	0.07	37,37,37,37	0
56	MG	1A	3046	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3720	1/1	0.99	0.04	36,36,36,36	0
56	MG	1A	3989	1/1	0.99	0.03	58,58,58,58	0
56	MG	1A	3962	1/1	0.99	0.06	34,34,34,34	0
56	MG	1A	3014	1/1	0.99	0.04	31,31,31,31	0
56	MG	2A	3832	1/1	0.99	0.05	55,55,55,55	0
56	MG	2A	3608	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3939	1/1	0.99	0.08	40,40,40,40	0
56	MG	1A	3993	1/1	0.99	0.05	33,33,33,33	0
56	MG	1X	105	1/1	0.99	0.09	35,35,35,35	0
56	MG	2A	3720	1/1	0.99	0.08	55,55,55,55	0
56	MG	1A	3673	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	4133	1/1	0.99	0.07	31,31,31,31	0
56	MG	2A	3840	1/1	0.99	0.06	64,64,64,64	0
56	MG	1A	3815	1/1	0.99	0.08	56,56,56,56	0
56	MG	2A	3009	1/1	0.99	0.09	34,34,34,34	0
56	MG	1A	3108	1/1	0.99	0.07	39,39,39,39	0
56	MG	1A	3997	1/1	0.99	0.05	41,41,41,41	0
56	MG	2a	1754	1/1	0.99	0.07	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4098	1/1	0.99	0.02	38,38,38,38	0
56	MG	2A	3728	1/1	0.99	0.02	27,27,27,27	0
56	MG	2A	3847	1/1	0.99	0.11	35,35,35,35	0
56	MG	1A	4138	1/1	0.99	0.03	59,59,59,59	0
56	MG	1A	3998	1/1	0.99	0.04	57,57,57,57	0
56	MG	1A	3968	1/1	0.99	0.06	32,32,32,32	0
56	MG	1A	4188	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	4000	1/1	0.99	0.02	42,42,42,42	0
56	MG	1A	3969	1/1	0.99	0.07	44,44,44,44	0
56	MG	1a	1851	1/1	0.99	0.05	45,45,45,45	0
56	MG	2a	1765	1/1	0.99	0.02	69,69,69,69	0
56	MG	1Q	201	1/1	0.99	0.10	36,36,36,36	0
56	MG	1a	1853	1/1	0.99	0.02	59,59,59,59	0
56	MG	1A	3008	1/1	0.99	0.15	31,31,31,31	0
56	MG	1A	4144	1/1	0.99	0.04	53,53,53,53	0
56	MG	2A	3797	1/1	0.99	0.02	56,56,56,56	0
56	MG	1A	4105	1/1	0.99	0.05	41,41,41,41	0
56	MG	2A	3861	1/1	0.99	0.03	34,34,34,34	0
56	MG	1A	3782	1/1	0.99	0.07	40,40,40,40	0
56	MG	2A	3800	1/1	0.99	0.04	60,60,60,60	0
56	MG	2A	3864	1/1	0.99	0.03	58,58,58,58	0
56	MG	1a	1808	1/1	0.99	0.10	59,59,59,59	0
56	MG	1A	3819	1/1	0.99	0.09	46,46,46,46	0
56	MG	2A	3528	1/1	0.99	0.03	54,54,54,54	0
56	MG	2A	3745	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	4070	1/1	0.99	0.04	74,74,74,74	0
56	MG	2A	3530	1/1	0.99	0.03	34,34,34,34	0
56	MG	1A	3394	1/1	0.99	0.19	35,35,35,35	0
56	MG	1A	3043	1/1	0.99	0.04	38,38,38,38	0
59	ZN	1Y	202	1/1	0.99	0.02	64,64,64,64	0
56	MG	1A	3003	1/1	0.99	0.12	29,29,29,29	0
59	ZN	15	101	1/1	0.99	0.12	61,61,61,61	0
59	ZN	1n	103	1/1	0.99	0.03	63,63,63,63	0
56	MG	1A	3020	1/1	0.99	0.04	26,26,26,26	0
56	MG	1A	3280	1/1	0.99	0.08	31,31,31,31	0
59	ZN	25	103	1/1	0.99	0.03	53,53,53,53	0
59	ZN	26	102	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3569	1/1	0.99	0.10	27,27,27,27	0
56	MG	1a	1817	1/1	0.99	0.02	43,43,43,43	0
60	SF4	1d	501	8/8	0.99	0.04	57,62,70,72	0
56	MG	1A	4077	1/1	0.99	0.03	38,38,38,38	0
59	ZN	19	102	1/1	1.00	0.01	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	1834	1/1	1.00	0.04	53,53,53,53	0
56	MG	1a	1794	1/1	1.00	0.03	35,35,35,35	0
56	MG	1A	4150	1/1	1.00	0.09	30,30,30,30	0
56	MG	2A	3872	1/1	1.00	0.09	34,34,34,34	0
58	CPT	1a	1882	4/5	1.00	0.07	60,68,79,89	0
56	MG	1A	4102	1/1	1.00	0.03	20,20,20,20	0
56	MG	1A	3794	1/1	1.00	0.05	44,44,44,44	0
56	MG	1A	4067	1/1	1.00	0.05	29,29,29,29	0
59	ZN	16	102	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.