



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:33 PM UTC

PDB ID : 9MTT / pdb_00009mtt
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with mRNA, A-site Q230-N5-methylated Release Factor 1, and P-site deacylated-tRNA_{cys} at 2.60Å resolution
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Deposited on : 2025-01-12
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
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

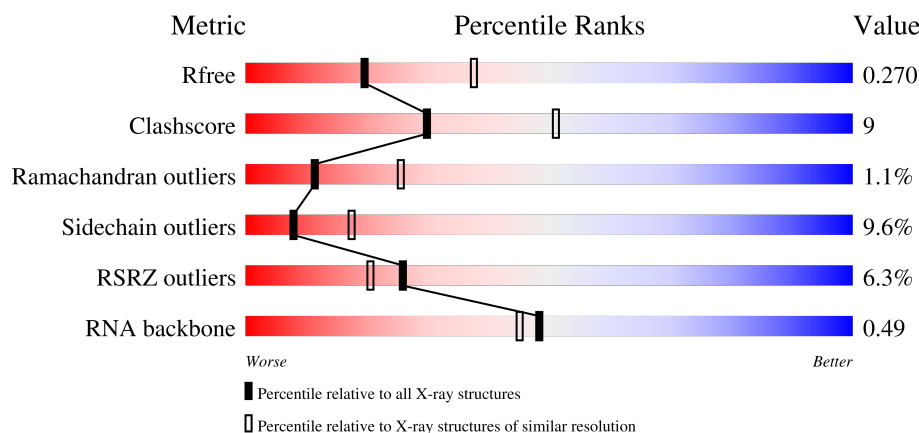
1 Overall quality at a glance

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	
1	2A	2915	
2	1B	121	

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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	354	
54	2w	354	
55	1x	74	
55	2x	74	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1733	-	-	-	X
56	MG	2a	1694	-	-	-	X
59	SF4	1d	302	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296938 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	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	118	Total	C	N	O	S	0	0	0
			919	566	190	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			907	558	188	159	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 CYS-Stop 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 protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1957	1210	361	377	9			

- Molecule 55 is a RNA chain called P-site deacylated-tRNA_{cys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	74	Total	C	N	O	P	S	0	0	0
			1577	704	280	518	74	1			
55	2x	74	Total	C	N	O	P	S	0	0	0
			1577	704	280	518	74	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1083	Total	Mg	0	0
			1083	1083		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	17	Total	Mg	0	0
			17	17		
56	1F	14	Total	Mg	0	0
			14	14		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	8	Total	Mg	0	0
			8	8		
56	1O	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	6	Total 6	Mg 6	0	0
56	1Q	7	Total 7	Mg 7	0	0
56	1R	4	Total 4	Mg 4	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1U	10	Total 10	Mg 10	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	6	Total 6	Mg 6	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	2	Total 2	Mg 2	0	0
56	10	6	Total 6	Mg 6	0	0
56	11	4	Total 4	Mg 4	0	0
56	12	3	Total 3	Mg 3	0	0
56	13	6	Total 6	Mg 6	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	8	Total 8	Mg 8	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	7	Total 7	Mg 7	0	0
56	18	4	Total 4	Mg 4	0	0
56	1a	224	Total 224	Mg 224	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1b	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	4	Total 4	Mg 4	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	4	Total 4	Mg 4	0	0
56	1w	1	Total 1	Mg 1	0	0
56	1x	13	Total 13	Mg 13	0	0
56	2A	870	Total 870	Mg 870	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2E	7	Total 7	Mg 7	0	0
56	2F	6	Total 6	Mg 6	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2P	1	Total 1	Mg 1	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	3	Total 3	Mg 3	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	4	Total 4	Mg 4	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	3	Total 3	Mg 3	0	0
56	25	5	Total 5	Mg 5	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	176	Total 176	Mg 176	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2j	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	2	Total 2	Mg 2	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0
56	2x	6	Total 6	Mg 6	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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

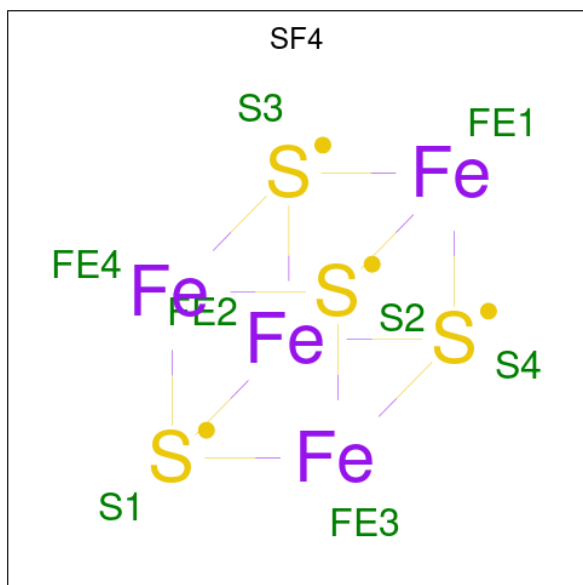
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total 1	Zn 1	0	0
58	14	1	Total 1	Zn 1	0	0
58	15	1	Total 1	Zn 1	0	0
58	16	1	Total 1	Zn 1	0	0
58	19	1	Total 1	Zn 1	0	0
58	1n	1	Total 1	Zn 1	0	0
58	2Y	1	Total 1	Zn 1	0	0
58	24	1	Total 1	Zn 1	0	0
58	25	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1841	Total	O	0	0
			1841	1841		
60	1B	66	Total	O	0	0
			66	66		
60	1D	24	Total	O	0	0
			24	24		
60	1E	27	Total	O	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1F	16	Total 16	O 16	0	0
60	1G	3	Total 3	O 3	0	0
60	1H	2	Total 2	O 2	0	0
60	1N	5	Total 5	O 5	0	0
60	1O	5	Total 5	O 5	0	0
60	1P	20	Total 20	O 20	0	0
60	1Q	5	Total 5	O 5	0	0
60	1R	15	Total 15	O 15	0	0
60	1S	4	Total 4	O 4	0	0
60	1T	5	Total 5	O 5	0	0
60	1U	15	Total 15	O 15	0	0
60	1V	7	Total 7	O 7	0	0
60	1W	12	Total 12	O 12	0	0
60	1X	7	Total 7	O 7	0	0
60	1Y	1	Total 1	O 1	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	10	Total 10	O 10	0	0
60	11	9	Total 9	O 9	0	0
60	12	4	Total 4	O 4	0	0
60	13	5	Total 5	O 5	0	0
60	15	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	16	1	Total O 1 1	0	0
60	17	8	Total O 8 8	0	0
60	18	13	Total O 13 13	0	0
60	1a	274	Total O 274 274	0	0
60	1b	1	Total O 1 1	0	0
60	1g	1	Total O 1 1	0	0
60	1l	2	Total O 2 2	0	0
60	1n	1	Total O 1 1	0	0
60	1o	1	Total O 1 1	0	0
60	1q	1	Total O 1 1	0	0
60	1u	1	Total O 1 1	0	0
60	1v	3	Total O 3 3	0	0
60	1w	2	Total O 2 2	0	0
60	1x	15	Total O 15 15	0	0
60	2A	1163	Total O 1163 1163	0	0
60	2B	25	Total O 25 25	0	0
60	2D	22	Total O 22 22	0	0
60	2E	15	Total O 15 15	0	0
60	2F	11	Total O 11 11	0	0
60	2I	1	Total O 1 1	0	0
60	2N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2O	2	Total 2	O 2	0	0
60	2P	11	Total 11	O 11	0	0
60	2Q	1	Total 1	O 1	0	0
60	2R	5	Total 5	O 5	0	0
60	2T	5	Total 5	O 5	0	0
60	2U	2	Total 2	O 2	0	0
60	2V	2	Total 2	O 2	0	0
60	2W	4	Total 4	O 4	0	0
60	2X	3	Total 3	O 3	0	0
60	2Z	1	Total 1	O 1	0	0
60	20	5	Total 5	O 5	0	0
60	21	10	Total 10	O 10	0	0
60	23	2	Total 2	O 2	0	0
60	25	2	Total 2	O 2	0	0
60	27	6	Total 6	O 6	0	0
60	28	3	Total 3	O 3	0	0
60	29	1	Total 1	O 1	0	0
60	2a	138	Total 138	O 138	0	0
60	2d	1	Total 1	O 1	0	0
60	2e	1	Total 1	O 1	0	0
60	2g	1	Total 1	O 1	0	0

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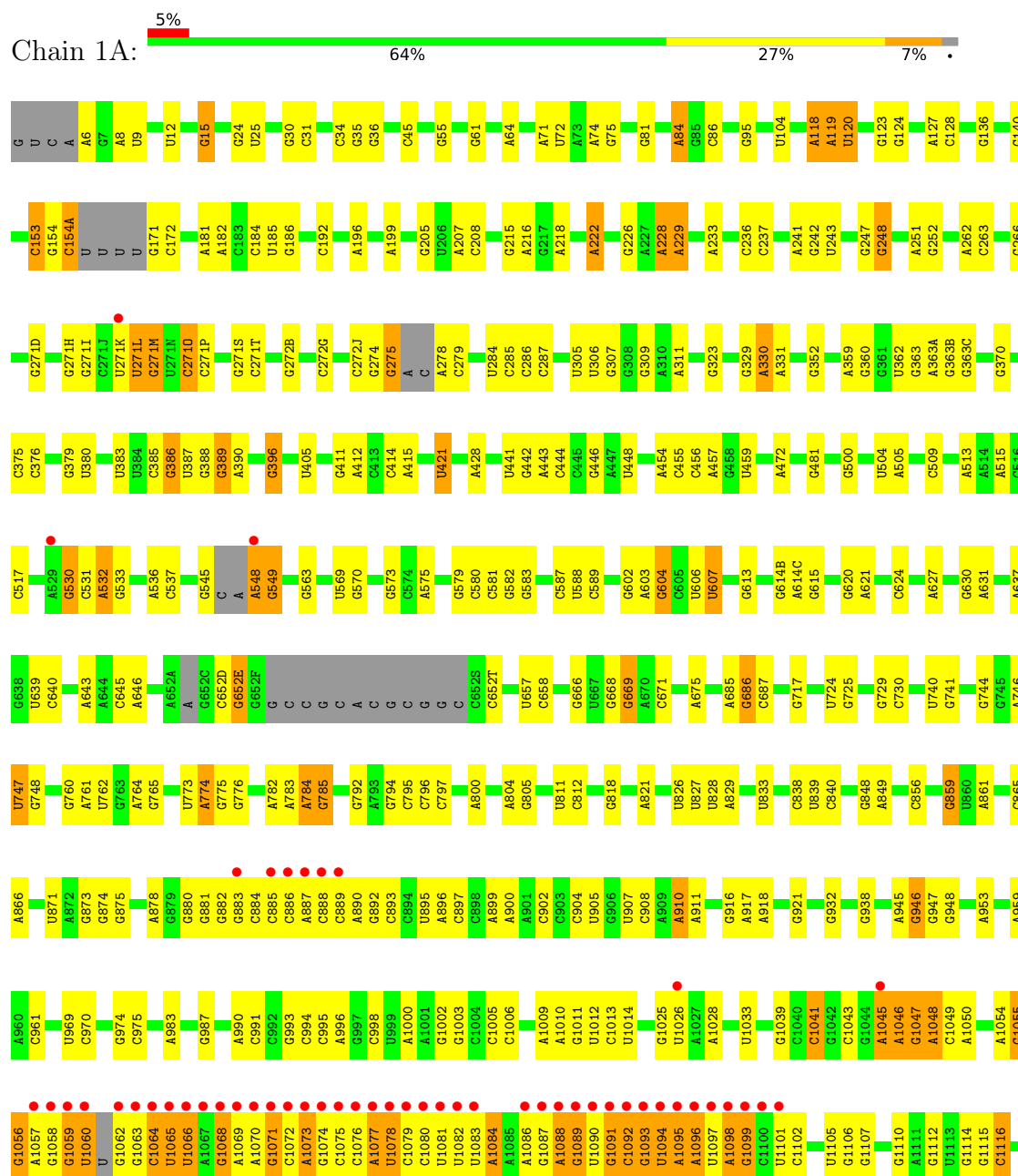
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2j	3	Total 3	O 3	0	0
60	2l	3	Total 3	O 3	0	0
60	2q	1	Total 1	O 1	0	0
60	2t	2	Total 2	O 2	0	0
60	2v	1	Total 1	O 1	0	0
60	2w	3	Total 3	O 3	0	0
60	2x	8	Total 8	O 8	0	0

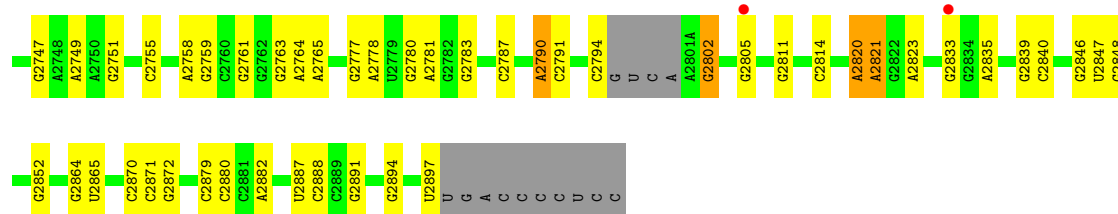
3 Residue-property plots

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

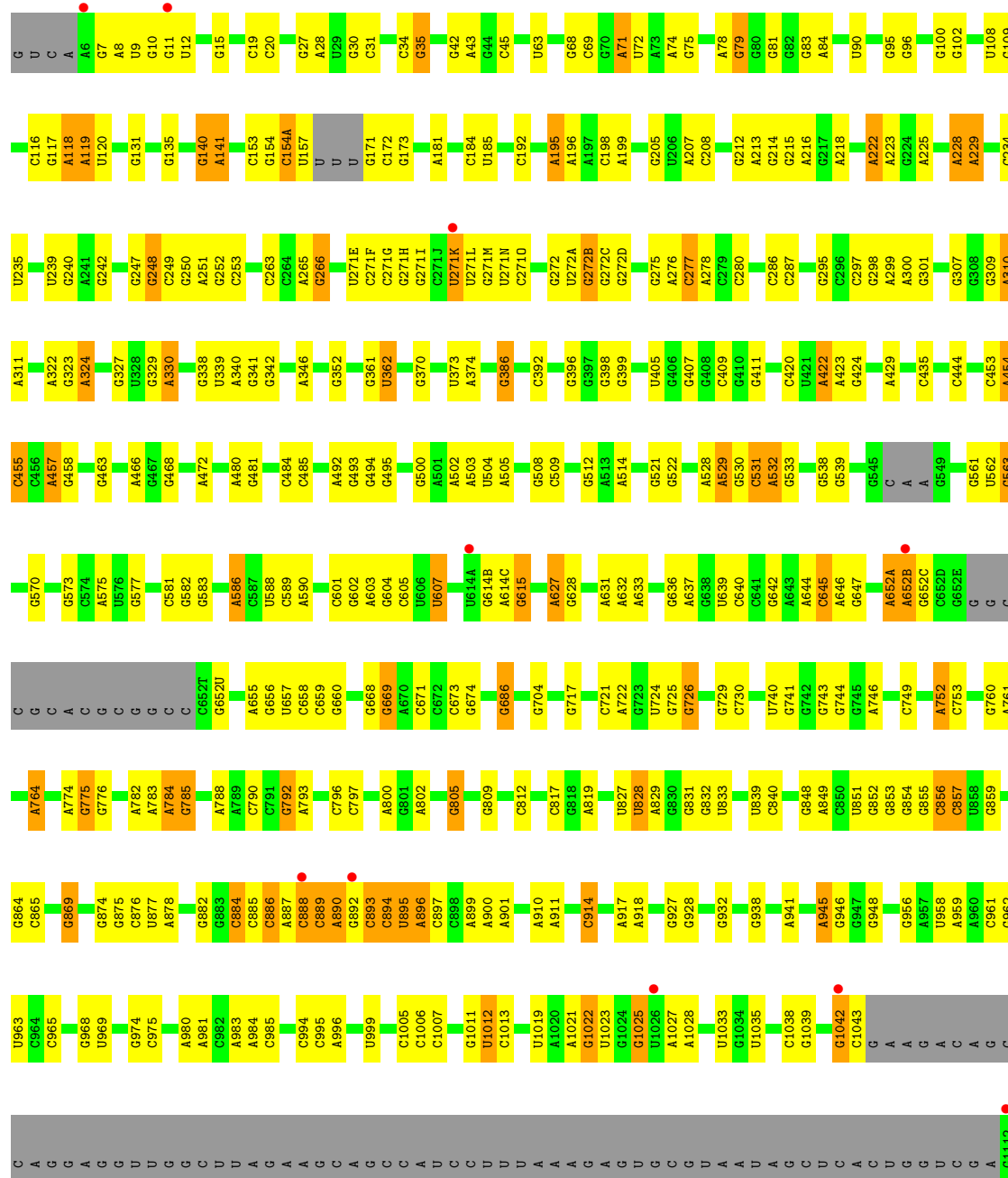
• Molecule 1: 23S Ribosomal RNA



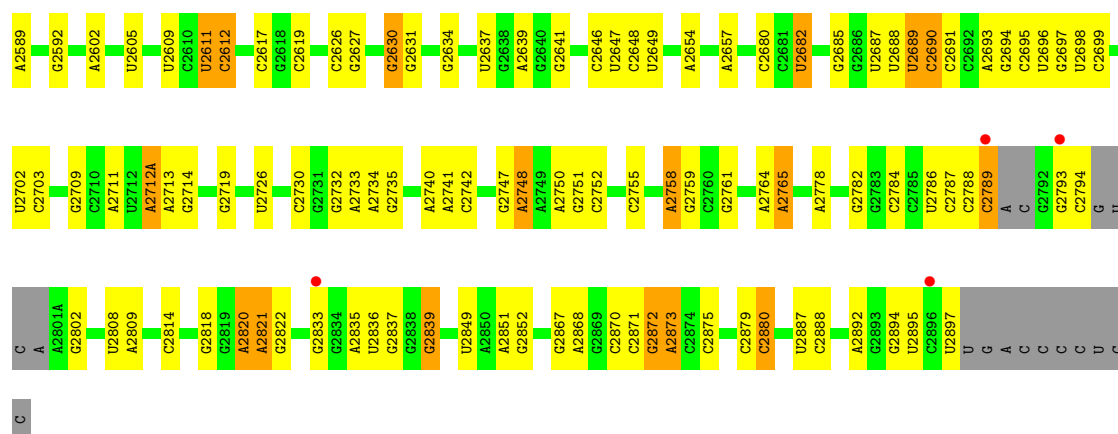
G2618	U2506	G2377	C2168	C2108	C1996	C1881	G1763	C1607	G1459	A1359	A1241	G1125
C2619	C2507	A2278	A2169	U2109	G1997	C1882	G1764	A1608	G1460	A1360	G1252	A1128
C2626	G2508	G2279	A2170	C2110	A2001	G1883	G1769	A1609	G1461	G1364	A1253	G1133
G2627	G2512	G2280	A2171	C2111	G2002	A1889	A1773	A1610		A1365	G1256	U1132
G2628	G2513	C2283	A2172	U2112	A2013	A1890		A1637	C1467	C1370		C1135
A2618		C2284	C2174	A2114	A2014	G1891	U1778	A1641	C1468	U1283		G1136
A2623		C2285	C2175	G2115		C1892	U1779	G1642	G1473	G1371	U1263	G1137
G2630		A2286	A2176	G2116	A2020		U1780			A1373	U1284	G1138
A2631	G2521	A2287	C2177	A2117	G2021	G1899	C1781	G1647	G1482	A1376	U1267	
A2632	U2522	A2288	C2178	U2118	U2022	A1901	C1782	C1648	G1484	U1274	A1268	
		G2289	C2179	G2119	U2023	C1902	A1783		G1485			A1142A
		G2290	U2180	G2120					G1486	A1379		C1152
		U2291	G2181	G2121	G2029	G1906	A1784	G1651	A1486	G1380	G1271	
		C2292	C2182	U2122	A2030	A1652	A1785	A1652	G1487	A1272	A1155	
		C2293	C2183	G2123	A2031	G1853	A1786	G1653	G1488	U1273		
		C2294	G2184	G2124	A2032	A1654		A1654	U1489	G1384	C1158	
			C2185	G2125	G2032		C1790		A1490	G1385		
		A2298		A2126	A2033	C1914	A1791	A1665		A1275	A1276	
		G2299	U2189	C2127		U1915			C1493			G1164
			C2190	G2128	G2038	U1916	U1794	A1668		G1400		U1165
		G2303	C2191	C2129	C2039	U1917	C1795	A1669	A1508	G1401	G1281	C1166
		G2304	G2192	U2130			U1796	C1670	C1509			
		A2305	G2193	U2131	C2043	G1929	C1797	U1671	A1509A	U1405	A1284	G1173
		C2306		U2132		G1930	U1798	C1672	A1509B	U1406		A1174
		G2307	A2198	G2133	U2047	U1931	C1799	U1673		C1407	U1292	U1175
				A2134	G2048		C1800	G1674	U1512		C1293	G1176
		U2312	U2203	A2135	G2049	A1936	C1801	C1675	C1513	A1412		A1177
		G2313	C2205	C2136	A2050	A1937	A1802	A1676	G1525	G1413	U1300	C1178
		C2314	C2206	C2137	A2051	A1938	A1803	A1677			A1301	
		G2315	G2207	C2138	G2052	U1939	C1804		G1528A	G1415	A1302	C1179
			A2208	C2139	A2054		U1805	U1692		C1417	G1303	
		G2319	C2224	C2140	G2055	C1942	A1812	U1693	C1532	U1420		C1185
		A2320	A2225	G2141	G2056	G1949	G1813	G1696	G	G1309	G1310	G1186
		G2321	C2226	C2142		G1950	A1814		U	G1311	U1312	G1187
		G2325	A2227	C2143	A2059	U1951	A1815	A1700	A	G1424	U1313	U1188
		C2326	G2228	C2145	A2060		A1816	G1703	C	G1425	C1315	A1194
		A2327		G2146	A2061	U1955	G1817		G1537	A1427		U1198
		G2328	C2238	C2147	A2062	U1956	U1818	C1712	C1547	C1428	U1199	C1200
		C2329	G2239	G2148		C1957		U1713	C1548	G1429	C1201	G1201
				C2149	G2069	C1958	G1824	G1714		C1430	A1322	C1202
		U2243	U2243	U2150			G1828		A1558	U1431		G1203
		U2245	U2245	G2151	U2074	C1962	A1829	G1721	G1559	G1332	G1333	
		G2246	G2246	G2152	U2075	U1963		A1722	G1560	U1438	G1334	A1210
		A2247	A2247	G2153	G2093	G1964	U1833	G1739	A1569	U1439	U1335	U1211
		C2248	C2248	G2155		A1965		G1740		A1439	A1336	U1217
				G2156	U2096	C1967	G1839		U1578	G1442	G1337	
		G2251	G2251	G2157	C2097	G1968		C1743	A1579			G1223
			G2255	A2158	U2098	A1969	A1847		A1580	A1445	A1342	
		C2256		G2159	U2099	A1970		C1745A				G1226
		A2268	A2268	G2160	G2100	A1971	G1858	G1746	C1584	G1448	G1343	A1226
				C2161	G2101	A1972			A1586	G1449	C1345	G1227
		G2271	G2271	G2162	U2102	A1986	G1866	G1753		G1450		
				C2163			C1866	C1754			U1352	G1235
				C2164	G2104		A1876	A1755	G1593			
			A2274	G2165	C2105	G1992	A1877	G1756	G1594	A1452		G1239
			C2275	G2166	U1993	U1992	G1878		U1453		G1356	
			G2276	U2167	C2107			A1762	G1595	G1455		U1240



• Molecule 1: 23S Ribosomal RNA



U2493	G2405	C2317	G2186	A2126	C2040	A1927	A1786	G1647	U	G1429	G1315	U1211	U1113
G2494	U2406	G2318	G2187	G2127	U2041	A1928	A1789	C1648	A	C1430	U1316	A1220	G1114
G2495	C2319	C2128	C2188	C2128	C2042	G1929	G1789	G1651	C1536	U1431	C1318	A1221	G1115
C2496	A2320	U2189	U2189	U2189	A2043	G1930	A1791	G1652	G1537	G1434	G1319	G1223	C1116
A2497	G2321	G2130	G2191	U2130	G2049	A1937	U1794	G1653	G1538	C1437	C1320	A1226	C1123
C2498	A2322	U2132	G2191	U2132	C2050	A1938	C1795	A1654	U1540	C1437	C1333	A1226	C1124
C2499	G2325	G2133	C2196	G2133	A2051	U1938	U1796	C1657	C1547	A1445	C1333	A1226	G1125
G2502	C2326	U2197	U2197	A2134	G2052	U1939	C1797	C1658	C1547	A1445	C1333	A1226	A1129
A2503	A2327	A2198	A2198	A2135	G2055	U1940	U1798	C1658	A1554	C1446	C1337	A1241	U1130
U2504	A2328	C2136	G2207	C2136	C2055	C1941	U1798	C1658	A1554	C1446	C1337	A1241	U1131
G2505	G2329	C2137	G2207	C2137	G2056	U1942	U1799	A1664	A1558	G1447	C1338	G1248	G1132
U2506	G2330	C2138	G2207	C2138	A2060	U1943	C1800	G1666	G1559	G1448	C1341	A1248	U1141
C2507	A2422	C2139	A2208	C2139	G2061	U1943	G1801	G1667	C1559	A1449	U1341	A1248	U1142
G2513	A2425	U2218	G2218	C2140	A2062	U1955	C1802	A1668	A1566	G1450	A1342	A1253	U1133
U2514	A2426	G2141	G2219	C2141	A2062	U1955	A1803	A1668	A1566	G1450	A1342	A1253	C1135
C2515	A2427	C2142	G2220	C2142	C2063	C1958	G1814	C1670	A1567	U1452	C1345	A1254	G1136
A2518	A2428	U2144	G2221	C2144	C2064	C1958	G1815	C1671	A1567	U1452	C1345	A1254	G1139
G2524	A2429	C2145	G2222	C2145	C2065	C1962	G1816	C1672	A1568	G1455	U1352	U1255	C1140
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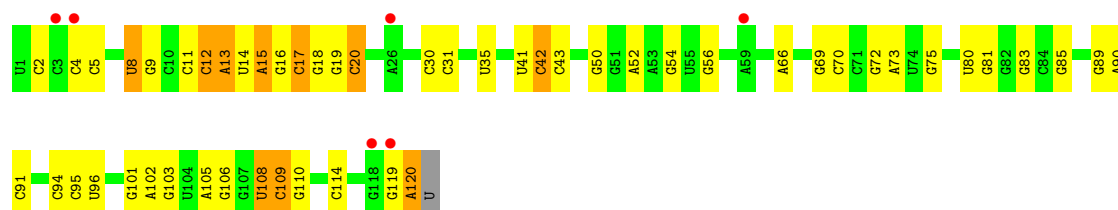
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 69% 28% .



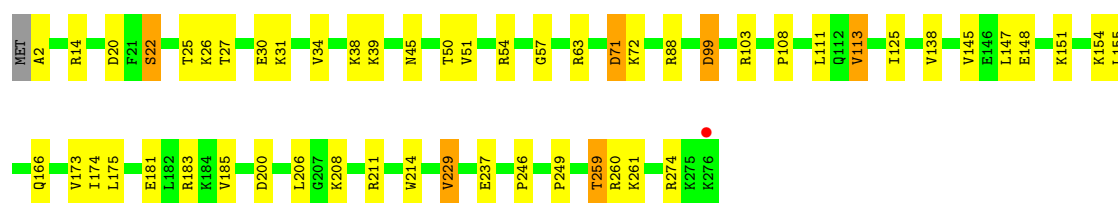
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 5% 56% 35% 8% .



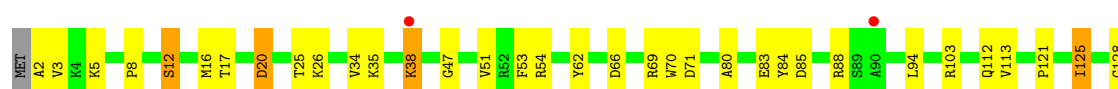
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 80% 17% .



• Molecule 3: 50S ribosomal protein L2

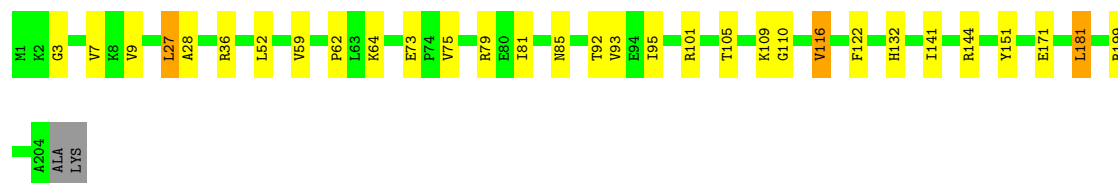
Chain 2D: % 78% 19% .





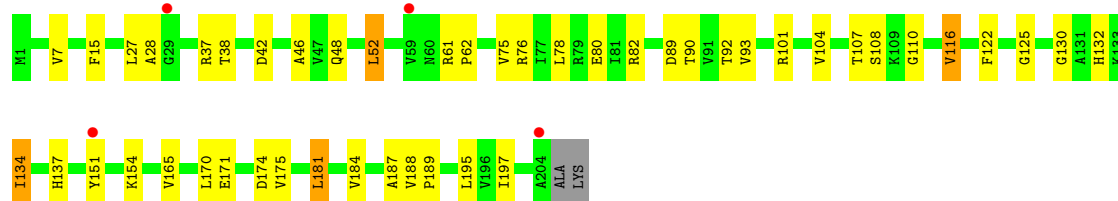
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 84% 14% ..



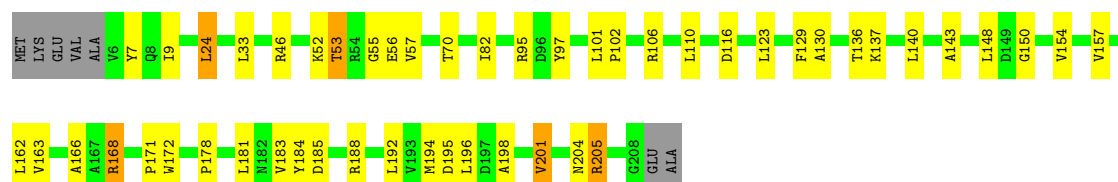
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 2% 76% 21% ..



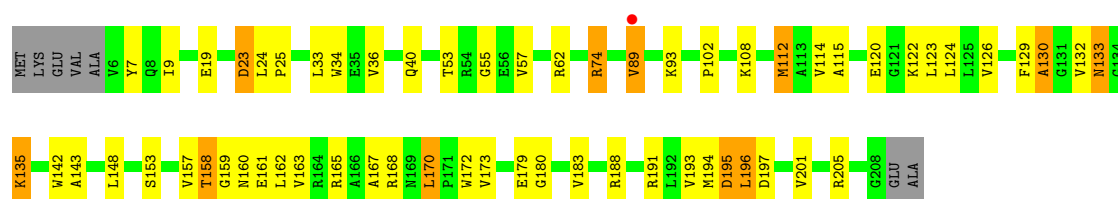
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 73% 21% ..



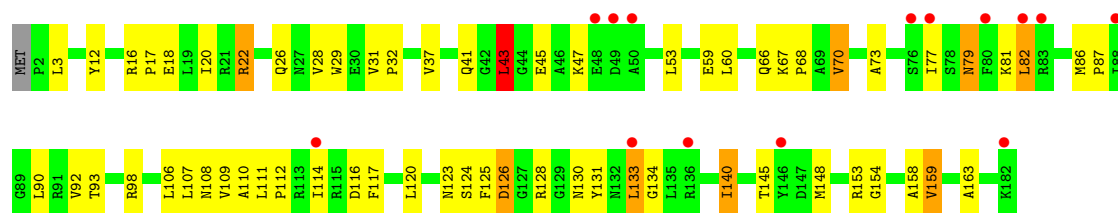
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 68% 24% 5% .

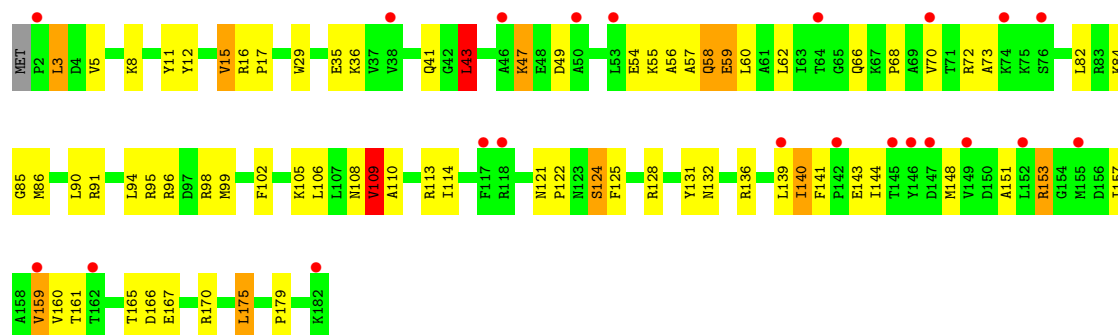


• Molecule 6: 50S ribosomal protein L5

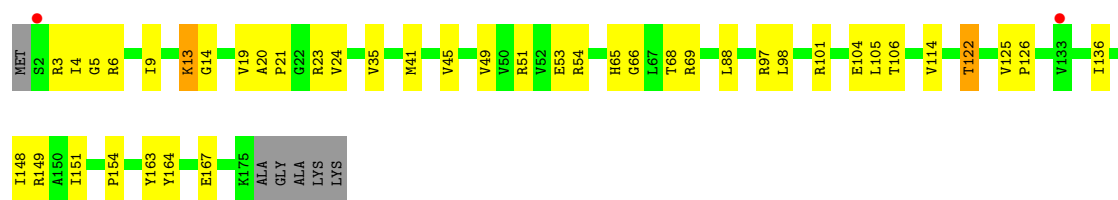
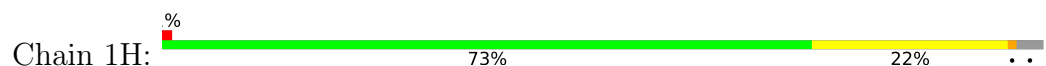
Chain 1G: 8% 65% 30% ..



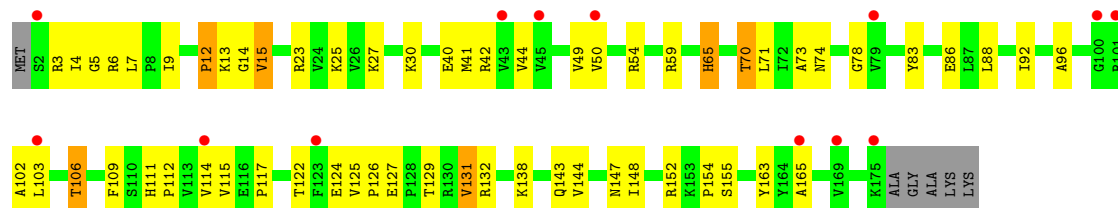
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

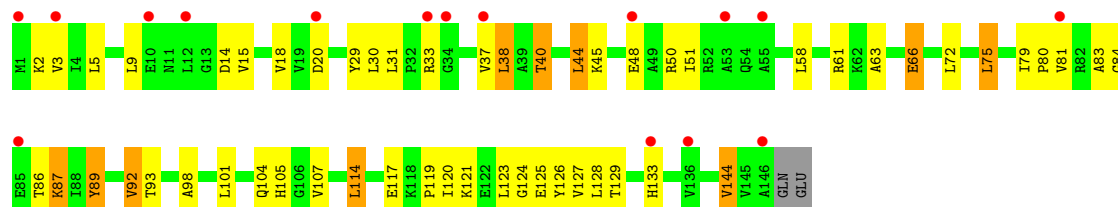


• Molecule 7: 50S ribosomal protein L6

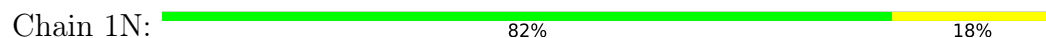




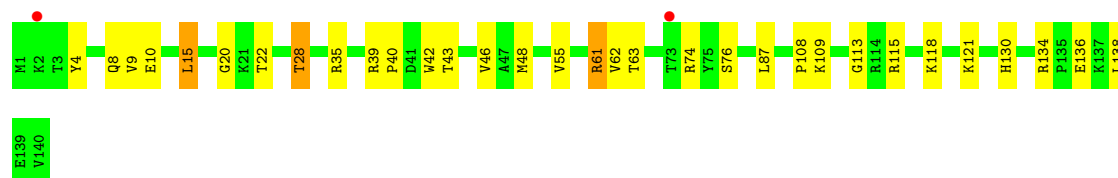
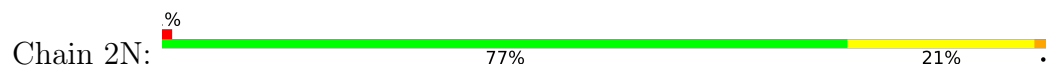
• Molecule 8: 50S ribosomal protein L9



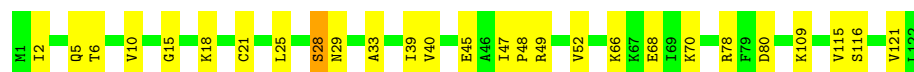
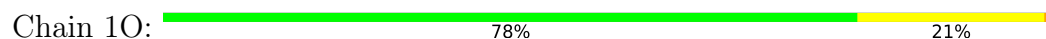
• Molecule 9: 50S ribosomal protein L13



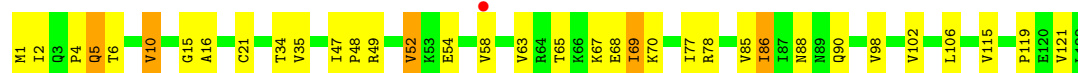
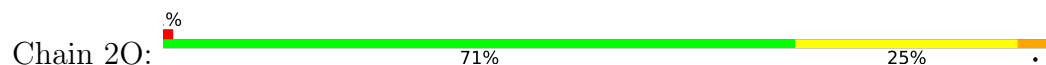
• Molecule 9: 50S ribosomal protein L13



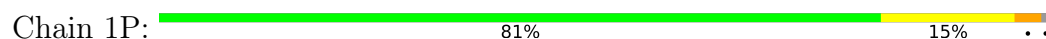
• Molecule 10: 50S ribosomal protein L14

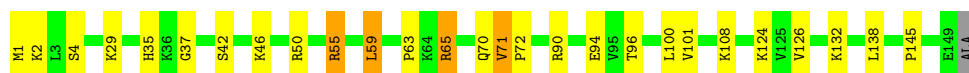


• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15

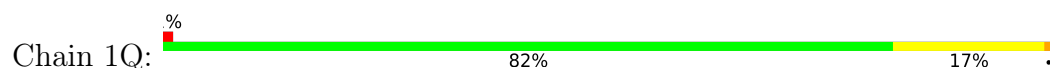




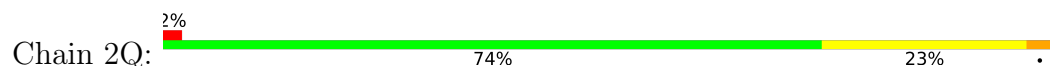
- Molecule 11: 50S ribosomal protein L15



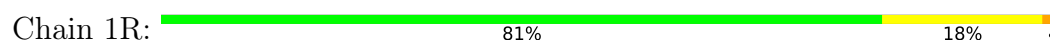
- Molecule 12: 50S ribosomal protein L16



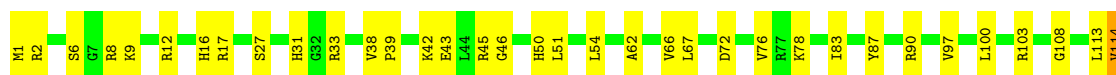
- Molecule 12: 50S ribosomal protein L16



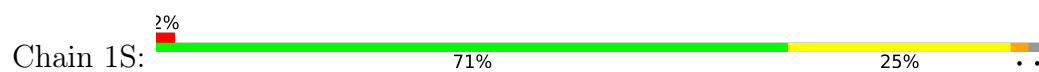
- Molecule 13: 50S ribosomal protein L17



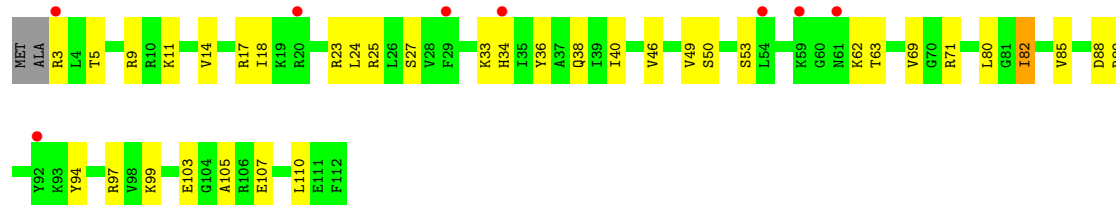
- Molecule 13: 50S ribosomal protein L17



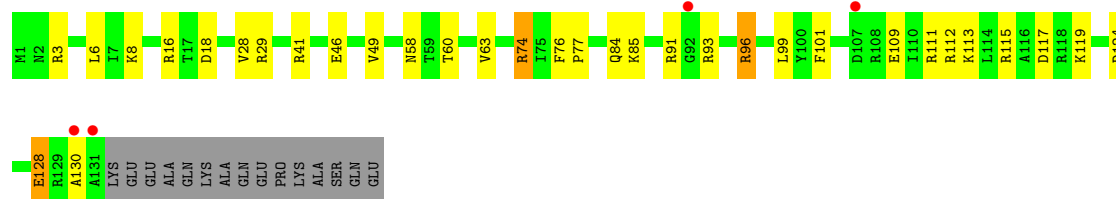
- Molecule 14: 50S ribosomal protein L18



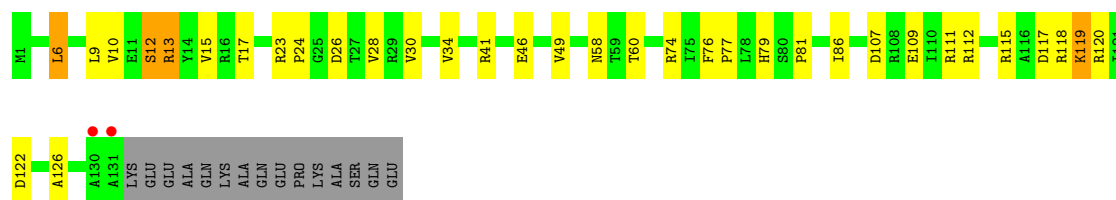
- Molecule 14: 50S ribosomal protein L18



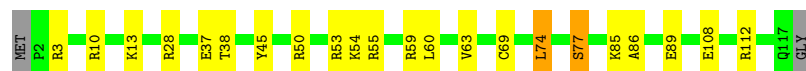
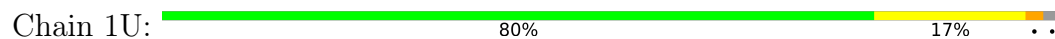
- Molecule 15: 50S ribosomal protein L19



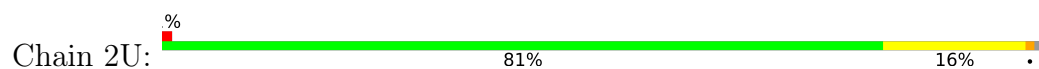
- Molecule 15: 50S ribosomal protein L19

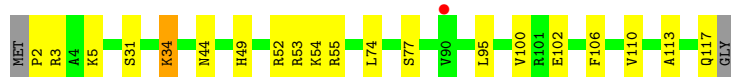


- Molecule 16: 50S ribosomal protein L20

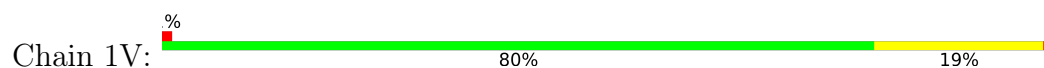


- Molecule 16: 50S ribosomal protein L20





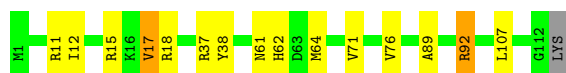
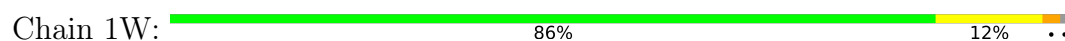
- Molecule 17: 50S ribosomal protein L21



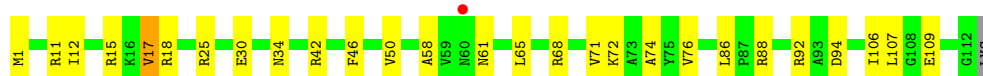
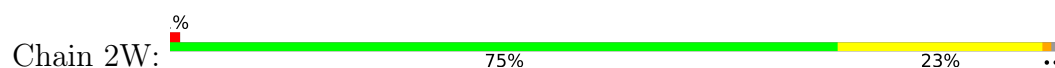
- Molecule 17: 50S ribosomal protein L21



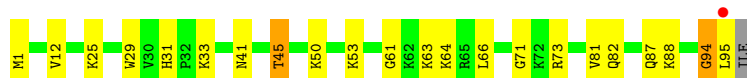
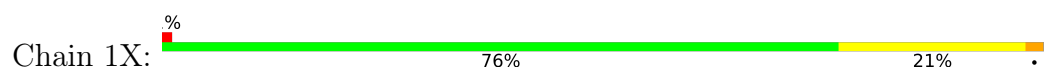
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



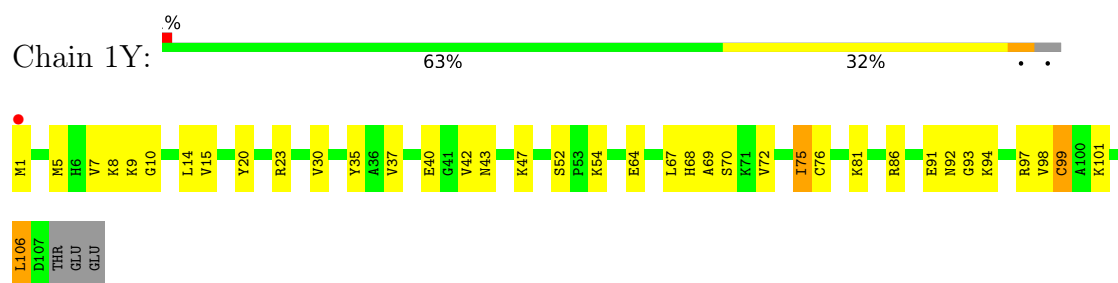
- Molecule 19: 50S ribosomal protein L23



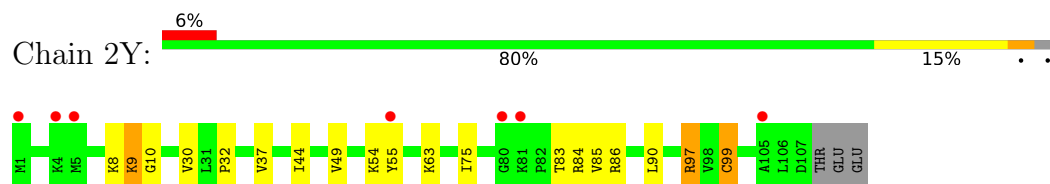
- Molecule 19: 50S ribosomal protein L23



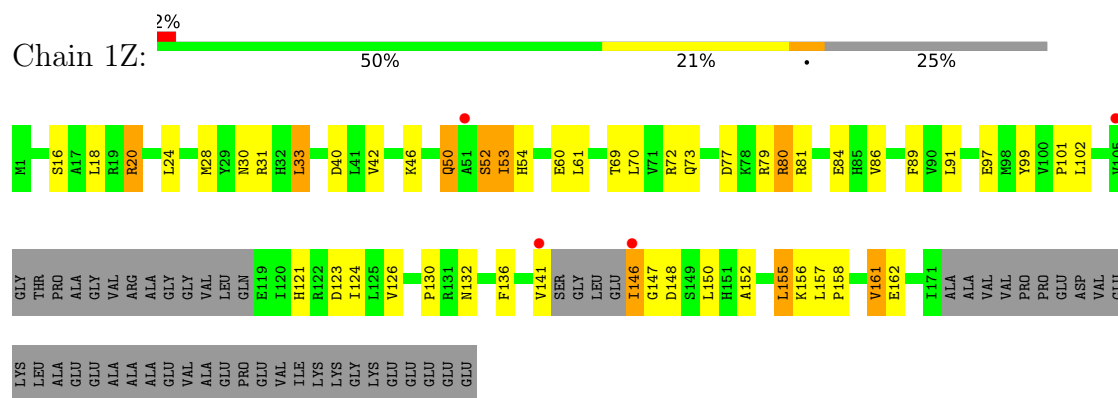
- Molecule 20: 50S ribosomal protein L24



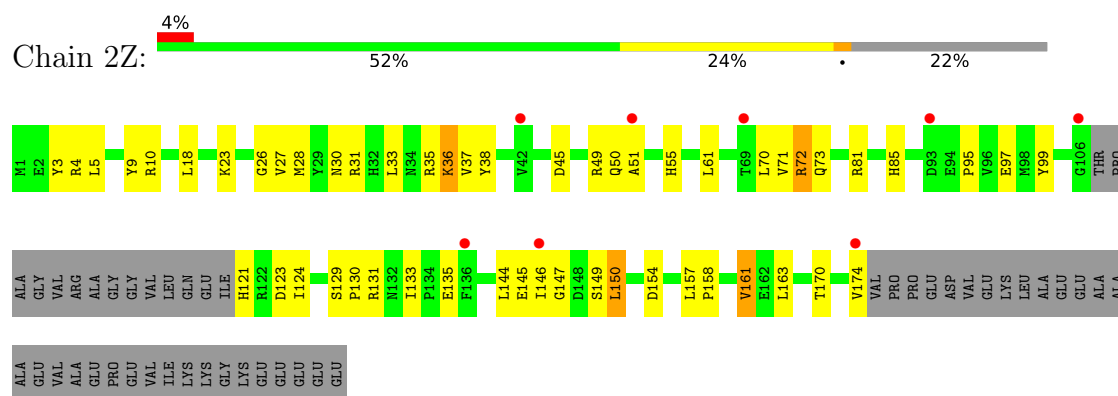
- Molecule 20: 50S ribosomal protein L24



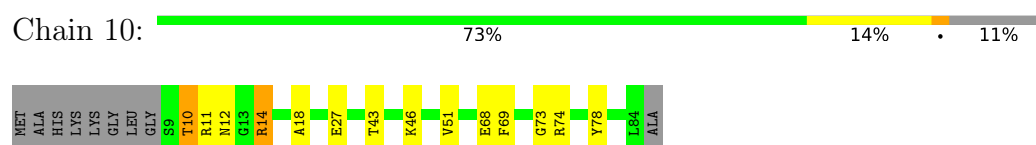
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



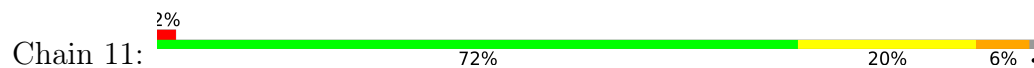
- Molecule 22: 50S ribosomal protein L27



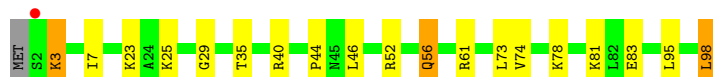
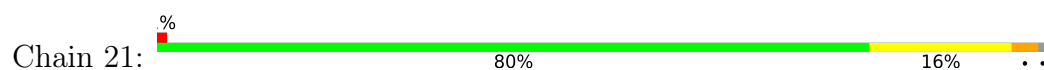
- Molecule 22: 50S ribosomal protein L27



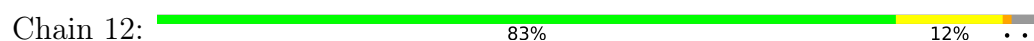
- Molecule 23: 50S ribosomal protein L28



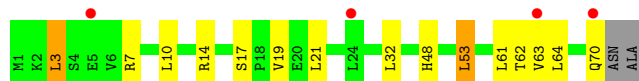
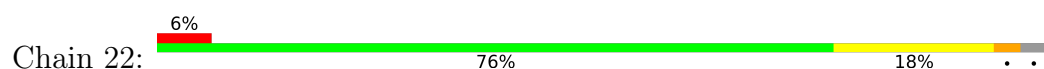
- Molecule 23: 50S ribosomal protein L28



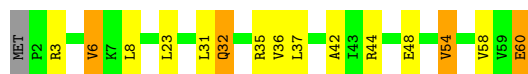
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



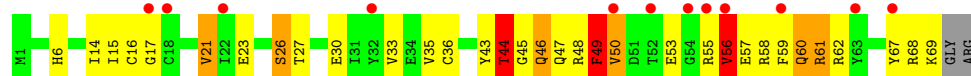
- Molecule 25: 50S ribosomal protein L30



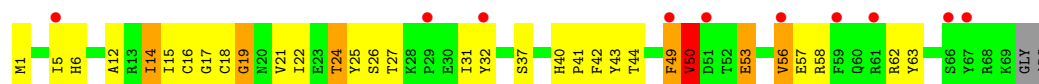
- Molecule 25: 50S ribosomal protein L30



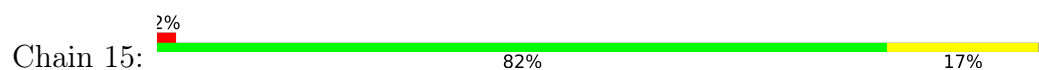
- Molecule 26: 50S ribosomal protein L31



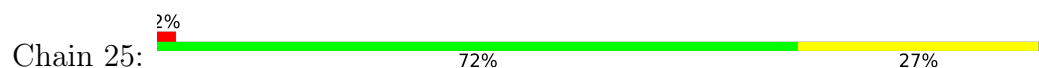
- Molecule 26: 50S ribosomal protein L31



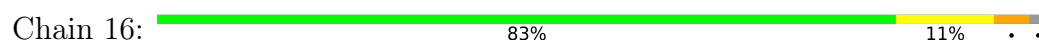
- Molecule 27: 50S ribosomal protein L32



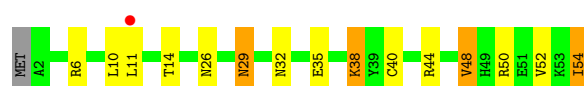
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



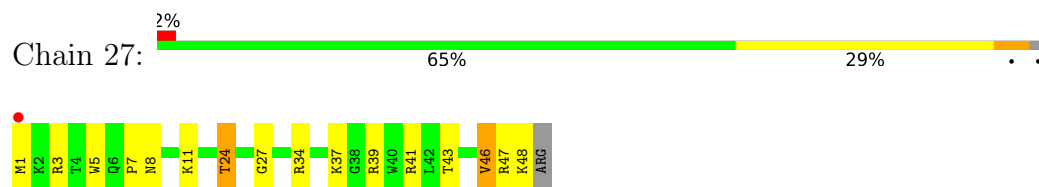
- Molecule 28: 50S ribosomal protein L33



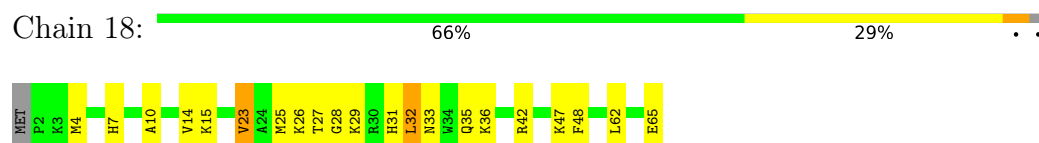
- Molecule 29: 50S ribosomal protein L34



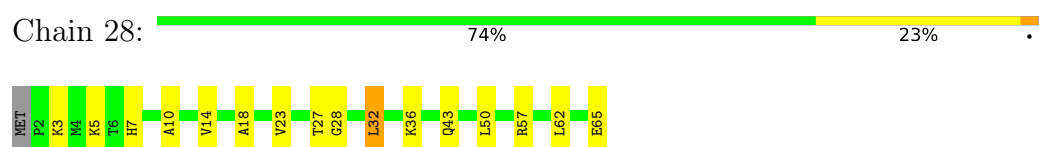
- Molecule 29: 50S ribosomal protein L34



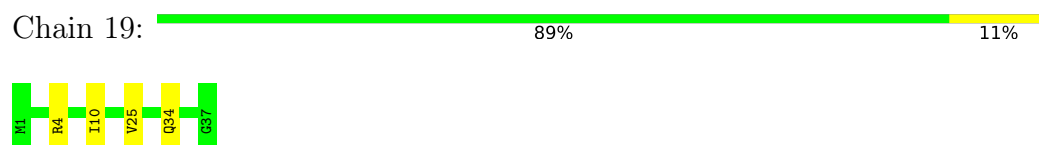
- Molecule 30: 50S ribosomal protein L35



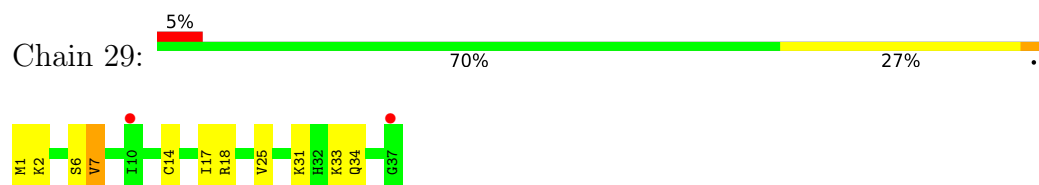
- Molecule 30: 50S ribosomal protein L35



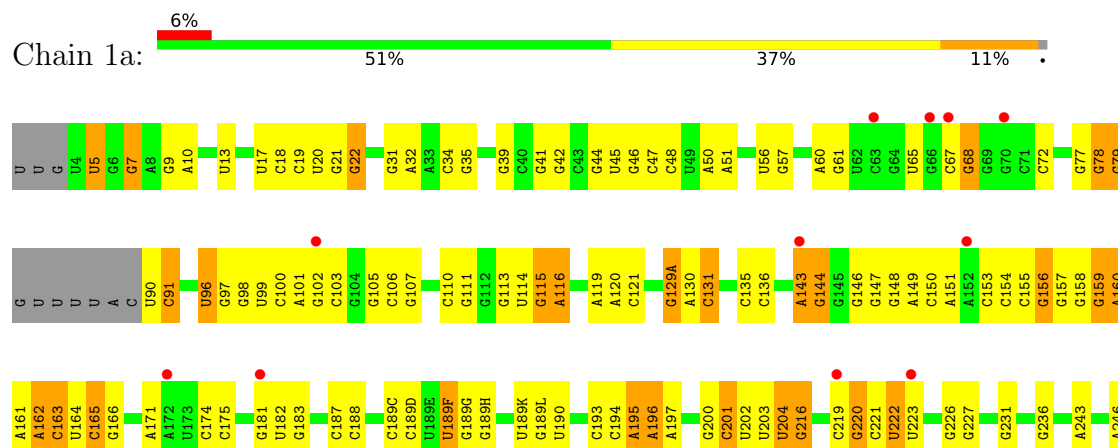
- Molecule 31: 50S ribosomal protein L36

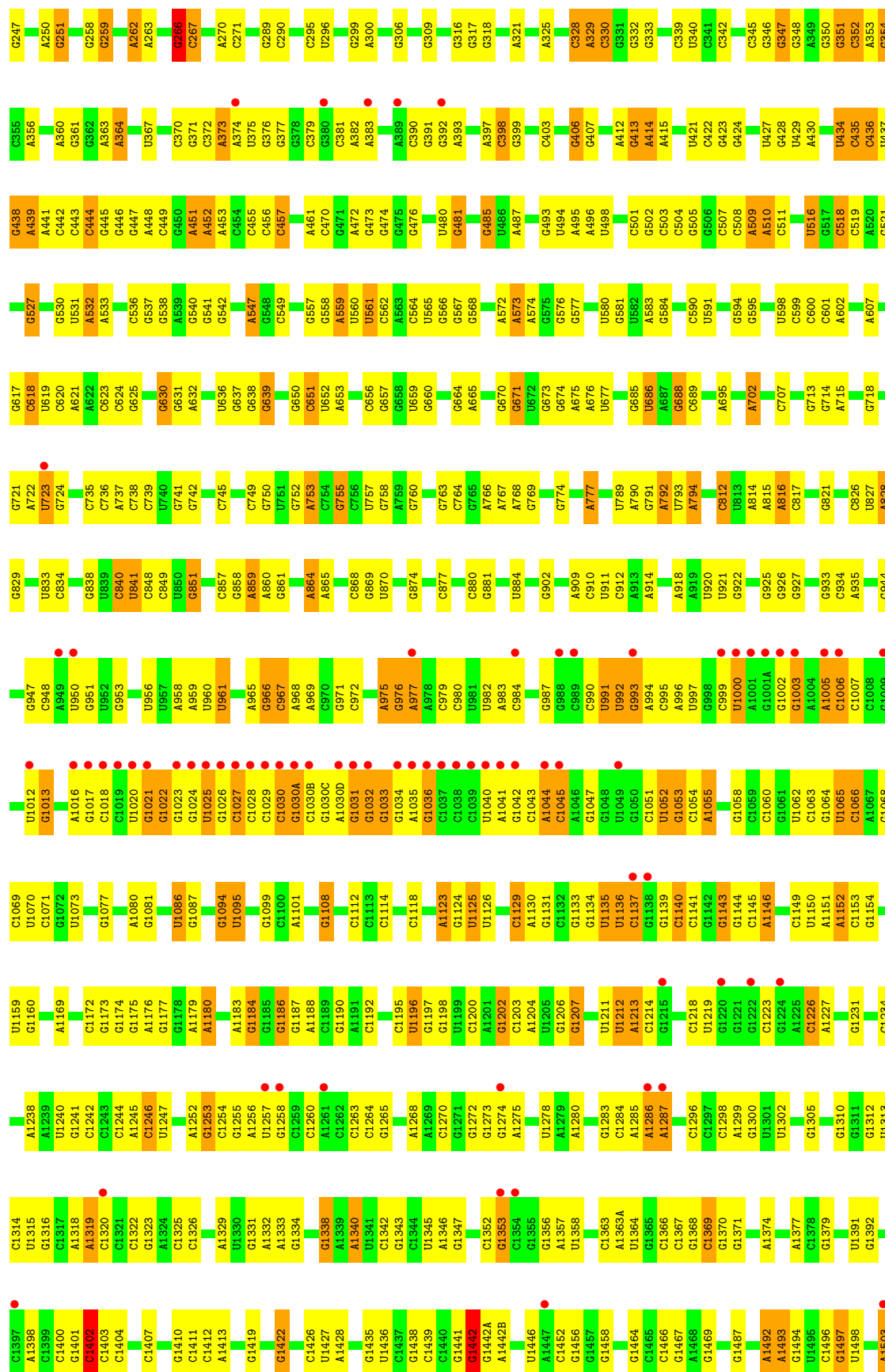


- Molecule 31: 50S ribosomal protein L36



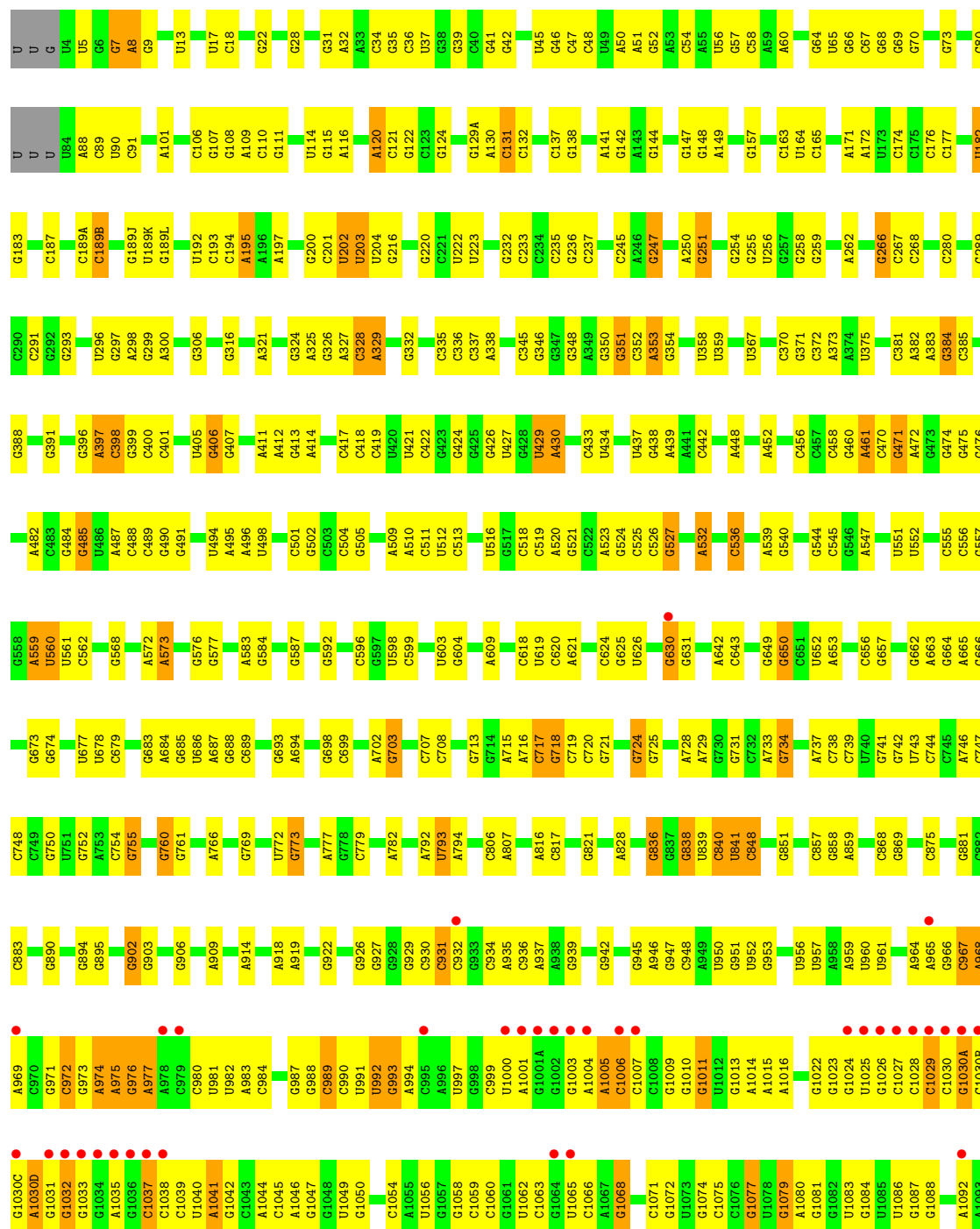
- Molecule 32: 16S Ribosomal RNA

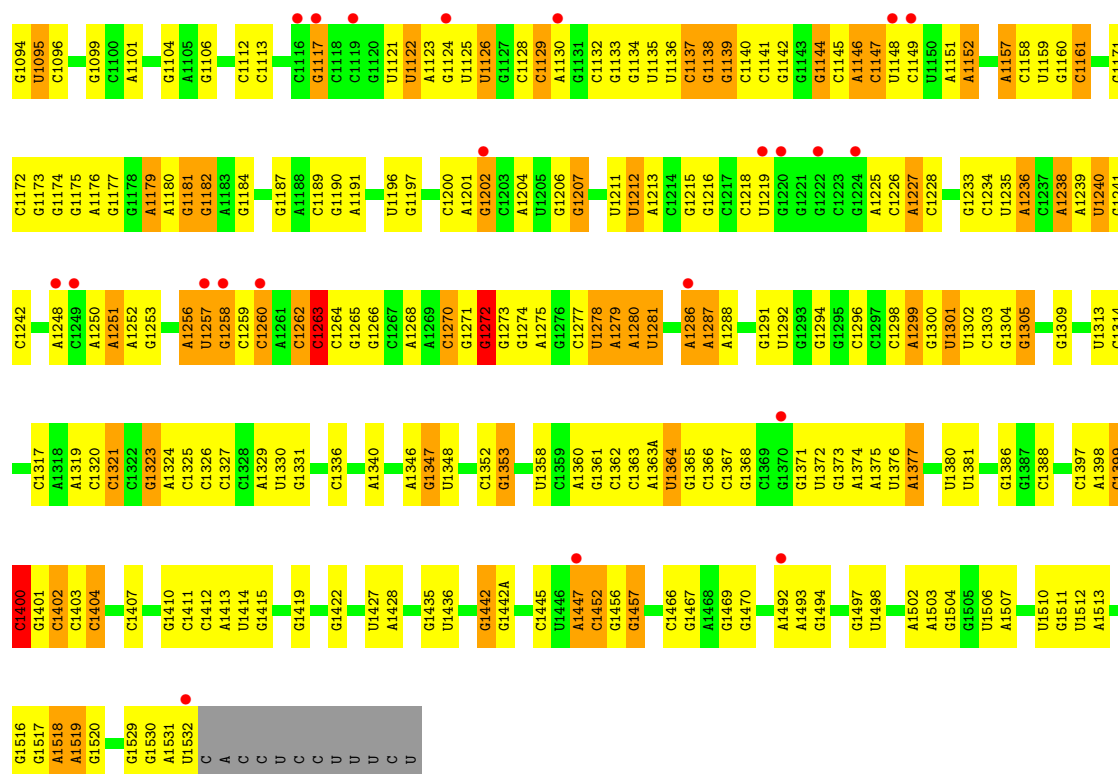




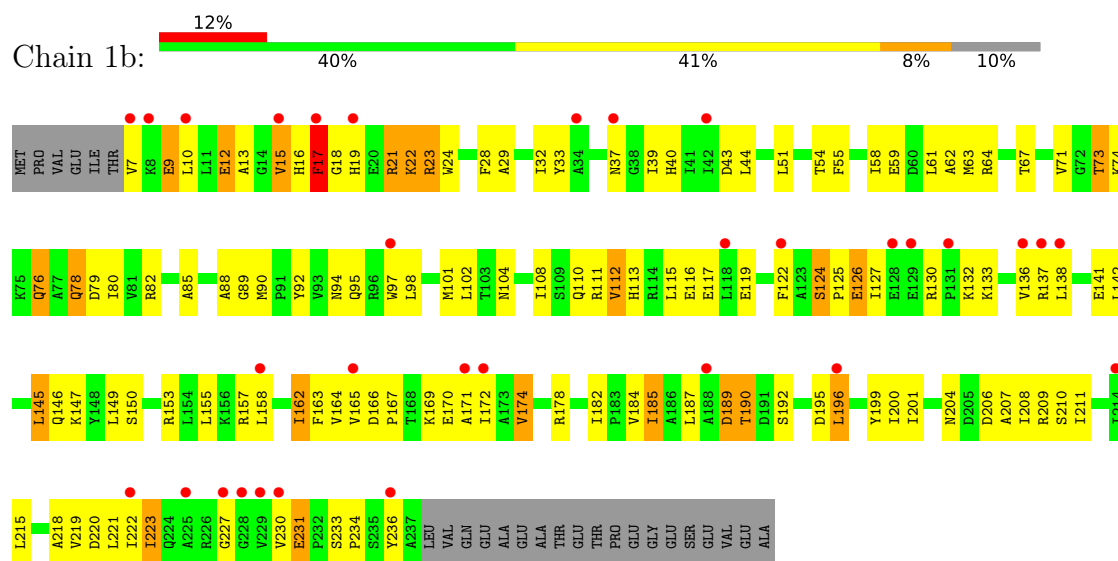


- Molecule 32: 16S Ribosomal RNA

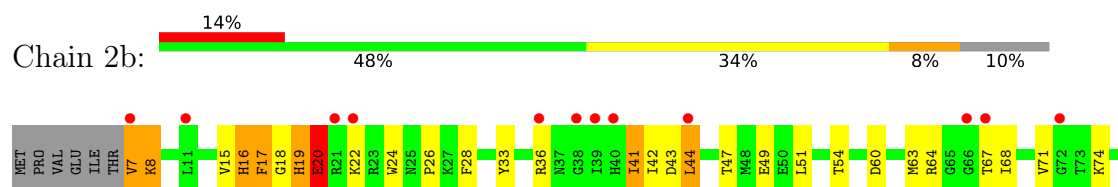


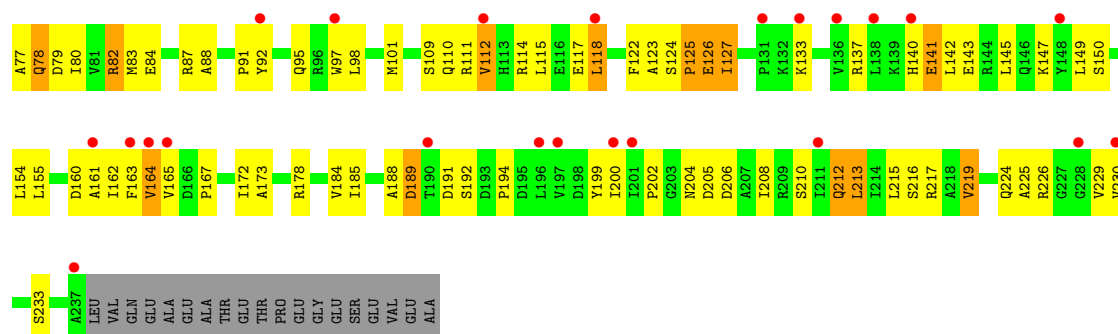


• Molecule 33: 30S ribosomal protein S2

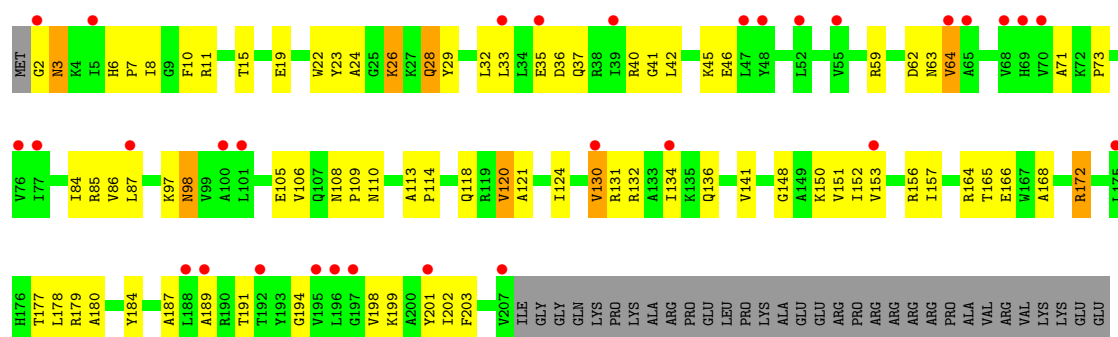


• Molecule 33: 30S ribosomal protein S2

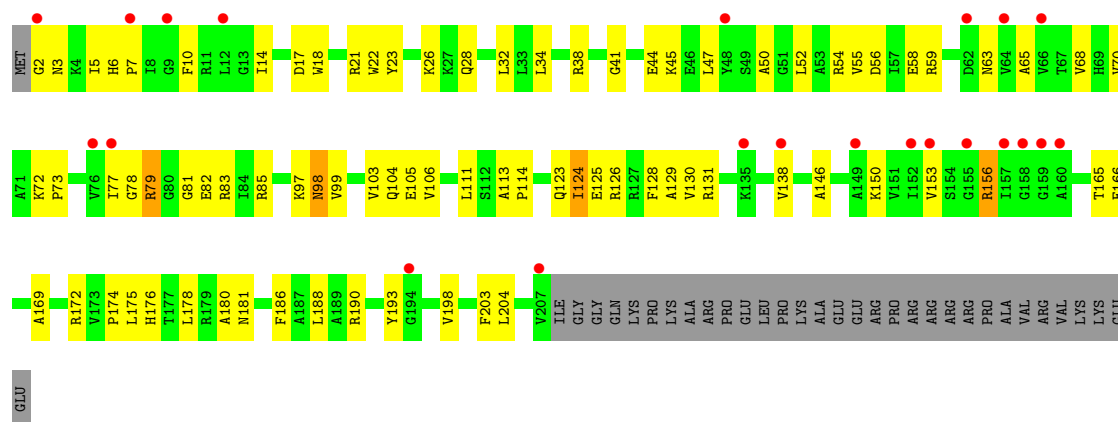




• Molecule 34: 30S ribosomal protein S3

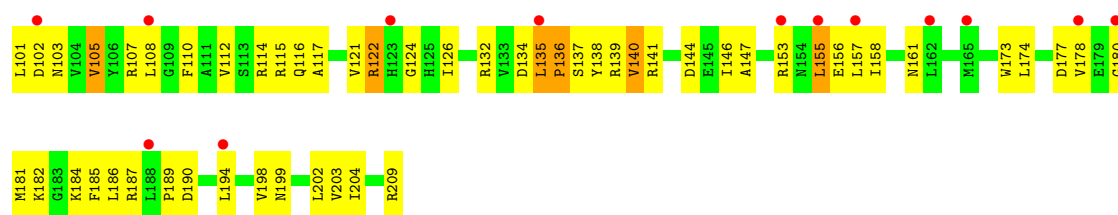


• Molecule 34: 30S ribosomal protein S3

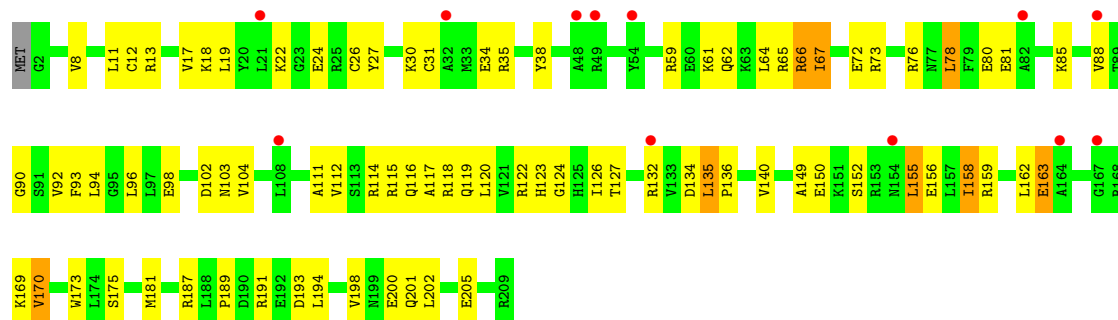


• Molecule 35: 30S ribosomal protein S4

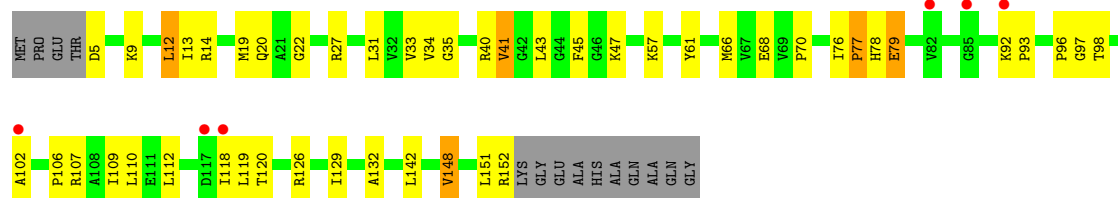




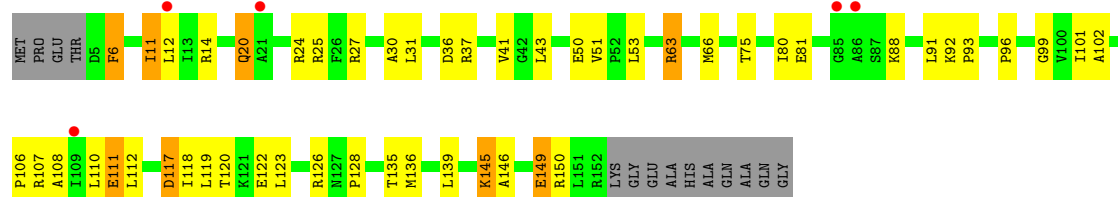
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



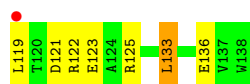
• Molecule 36: 30S ribosomal protein S5



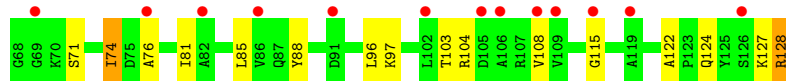
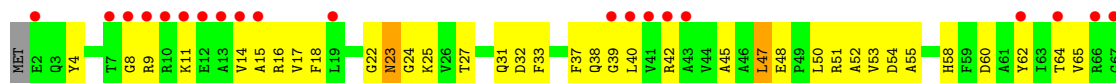
• Molecule 37: 30S ribosomal protein S6



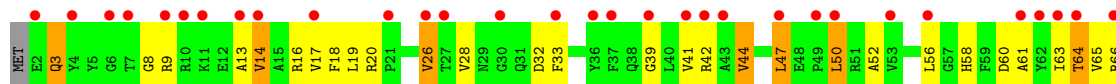
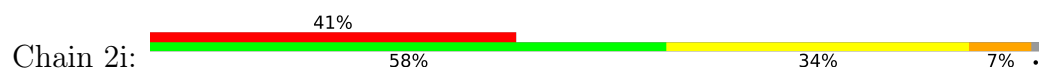
- Chain 2h:
-



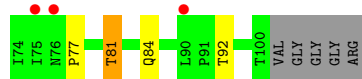
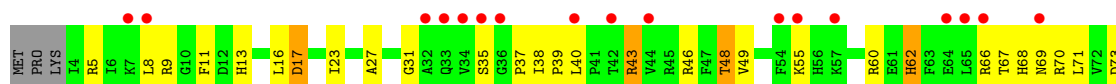
• Molecule 40: 30S ribosomal protein S9



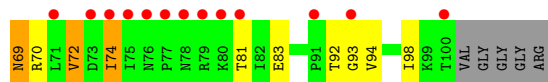
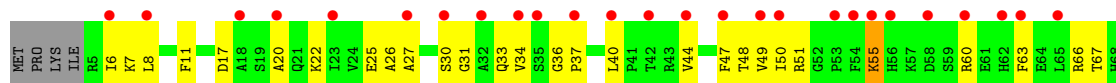
• Molecule 40: 30S ribosomal protein S9



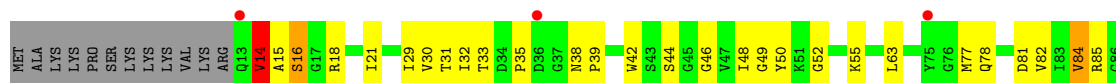
• Molecule 41: 30S ribosomal protein S10



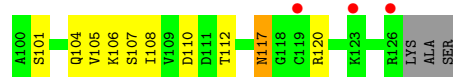
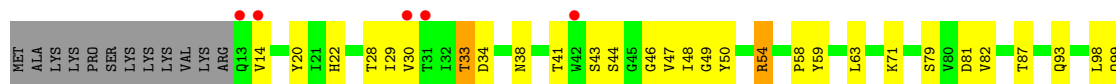
• Molecule 41: 30S ribosomal protein S10



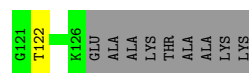
• Molecule 42: 30S ribosomal protein S11



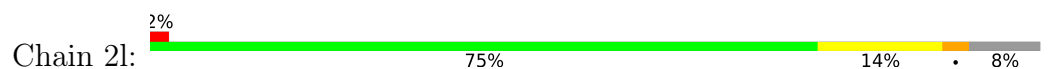
- Molecule 42: 30S ribosomal protein S11



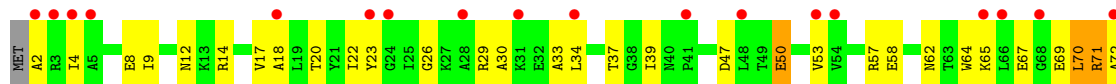
- Molecule 43: 30S ribosomal protein S12



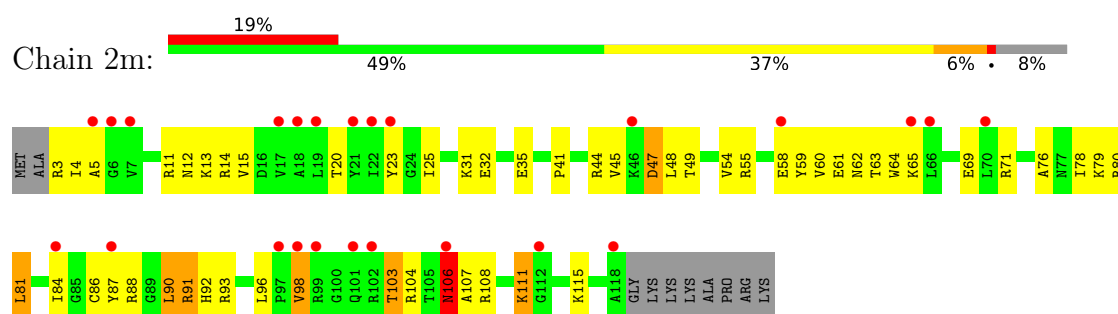
- Molecule 43: 30S ribosomal protein S12



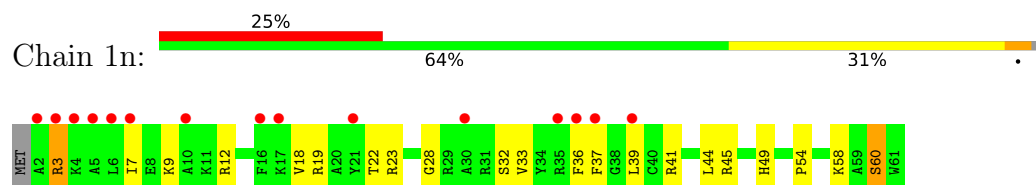
- Molecule 44: 30S ribosomal protein S13



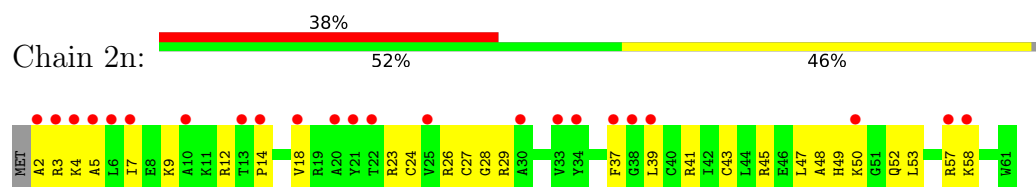
- Molecule 44: 30S ribosomal protein S13



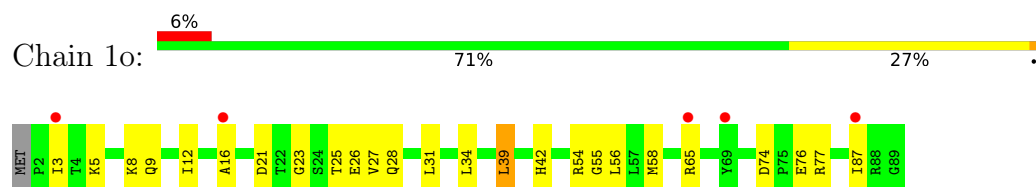
- Molecule 45: 30S ribosomal protein S14 type Z



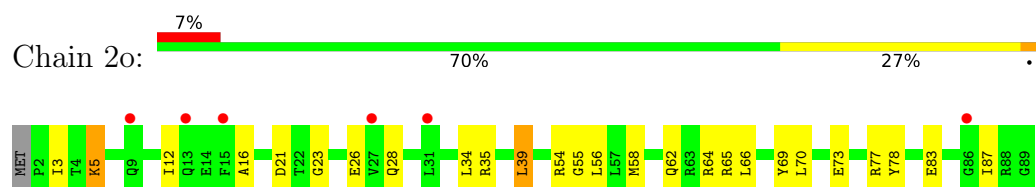
- Molecule 45: 30S ribosomal protein S14 type Z



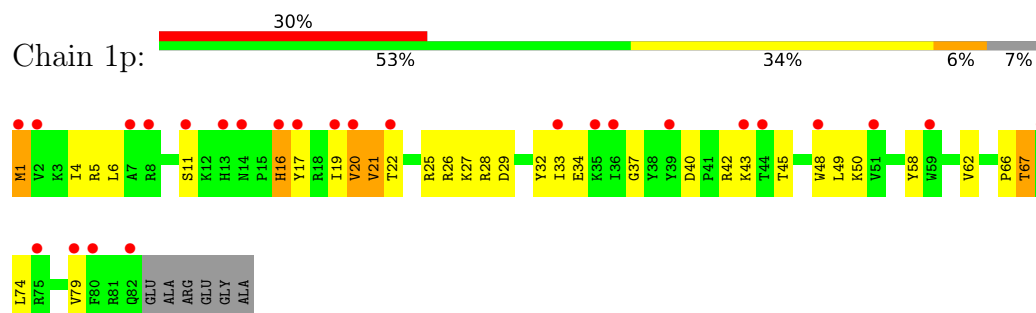
- Molecule 46: 30S ribosomal protein S15



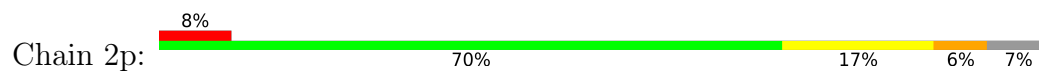
- Molecule 46: 30S ribosomal protein S15



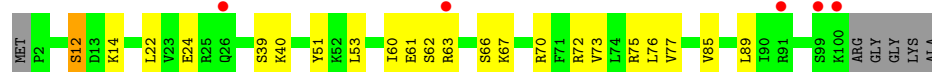
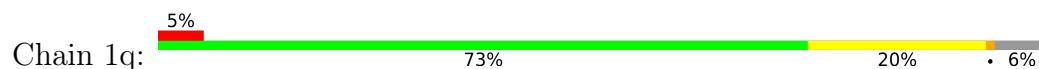
- Molecule 47: 30S ribosomal protein S16



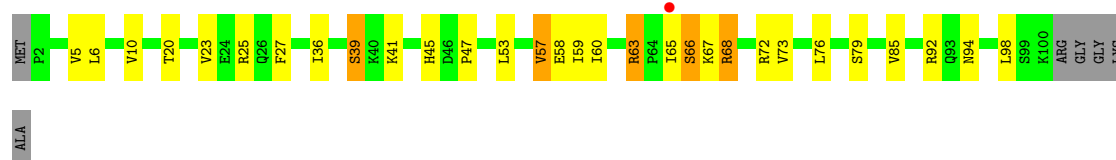
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



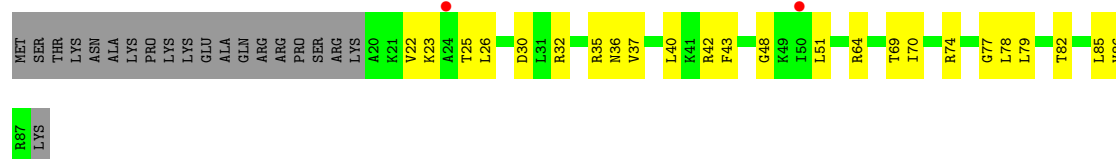
- Molecule 48: 30S ribosomal protein S17



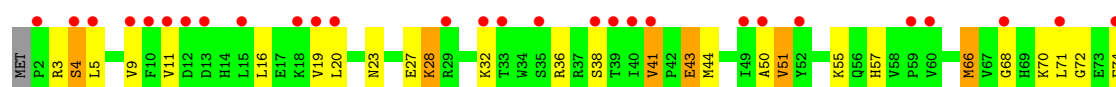
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19



Chain 1v:

Category	Percentage
Red	17%
Green	21%
Yellow	25%
Orange	8%
Grey	46%

Legend:

Category	Percentage
G	17%
C	21%
C	25%
A	8%
A	46%
G	17%
G	21%
G	25%
G	8%
G	46%
G10	17%
U11	21%
A12	25%
A13	8%
U19	46%
A20	17%
A21	21%
U22	25%
A	8%
A	46%

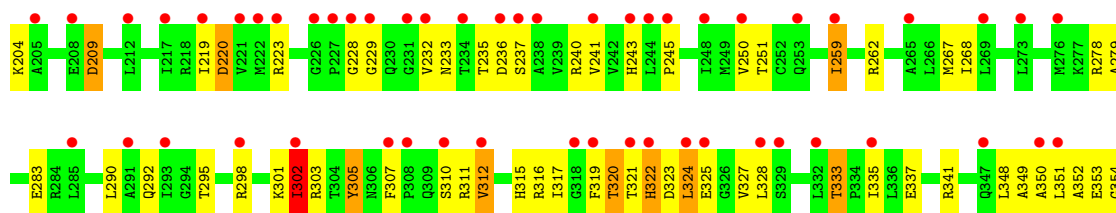
Chain 2v:

Category	Percentage
Red	29%
Green	29%
Yellow	17%
Orange	8%
Grey	46%

Legend:

Label	Color
G	Grey
C	Green
C	Green
A	Yellow
A	Yellow
G	Green
G	Green
G	Green
G	Green
G	Green
G	Green
U11	Red
A12	Orange
A13	Orange
A14	Yellow
A15	Yellow
A15	Yellow
A21	Yellow
U22	Yellow
A	Yellow
A	Yellow

[illegible][illegible]



● Molecule 55: P-site deacylated-tRNAcys



● Molecule 55: P-site deacylated-tRNAcys



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.05Å 450.80Å 622.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.39 – 2.60 188.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (188.39-2.60) 99.8 (188.39-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.224 , 0.271 0.224 , 0.270	Depositor DCC
R_{free} test set	89459 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	296938	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: 4OC, OMG, 2MG, 5MC, UR3, SF4, MA6, 2MA, ZN, M2G, OMU, 0TD, MG, MIA, MEQ, PSU, 5MU, 4SU, K, G7M, H2U, OMC

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	0.29	0/69011	0.47	2/107720 (0.0%)
1	2A	0.22	0/67295	0.41	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.34	0/4487
3	1D	0.26	0/2186	0.51	0/2944
3	2D	0.24	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.49	0/2149
4	2E	0.22	0/1592	0.43	0/2149
5	1F	0.26	0/1619	0.48	0/2193
5	2F	0.20	0/1615	0.42	0/2188
6	1G	0.21	0/1448	0.45	0/1957
6	2G	0.20	0/1453	0.44	0/1963
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.20	0/1112	0.47	0/1514
8	2I	0.19	0/1079	0.42	1/1475 (0.1%)
9	1N	0.25	0/1144	0.47	0/1543
9	2N	0.19	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.48	0/1269
10	2O	0.21	0/943	0.46	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.21	0/1152	0.48	1/1533 (0.1%)
12	1Q	0.26	0/1143	0.49	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.50	0/1312
13	2R	0.22	0/982	0.44	0/1312
14	1S	0.22	0/883	0.48	0/1176
14	2S	0.20	0/880	0.41	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.30	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.40	0/1301
17	1V	0.25	0/782	0.47	0/1049
17	2V	0.20	0/782	0.41	0/1049
18	1W	0.29	0/897	0.44	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.28	0/764	0.54	2/1025 (0.2%)
19	2X	0.20	0/764	0.47	2/1025 (0.2%)
20	1Y	0.23	0/819	0.46	0/1095
20	2Y	0.19	0/819	0.45	0/1095
21	1Z	0.23	0/1267	0.54	0/1717
21	2Z	0.21	0/1299	0.46	0/1763
22	10	0.28	0/612	0.51	0/816
22	20	0.21	0/612	0.46	0/816
23	11	0.26	0/762	0.45	0/1014
23	21	0.23	0/762	0.39	0/1014
24	12	0.24	0/590	0.41	0/781
24	22	0.19	0/590	0.38	0/781
25	13	0.27	0/474	0.47	0/635
25	23	0.20	0/469	0.47	0/630
26	14	0.24	0/565	0.51	0/761
26	24	0.24	0/545	0.50	0/737
27	15	0.30	0/469	0.51	0/635
27	25	0.22	0/469	0.43	0/635
28	16	0.27	0/460	0.50	0/613
28	26	0.20	0/456	0.42	0/608
29	17	0.32	0/426	0.57	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.28	0/525	0.50	0/691
30	28	0.20	0/525	0.41	0/691
31	19	0.25	0/310	0.61	1/407 (0.2%)
31	29	0.20	0/310	0.47	0/407
32	1a	0.20	1/35795 (0.0%)	0.38	3/55864 (0.0%)
32	2a	0.20	1/35886 (0.0%)	0.38	4/56005 (0.0%)
33	1b	0.24	0/1881	0.52	0/2542
33	2b	0.22	0/1860	0.49	0/2518
34	1c	0.21	0/1572	0.41	0/2126
34	2c	0.21	0/1566	0.45	0/2119
35	1d	0.23	0/1685	0.47	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.22	0/1145	0.49	0/1543
36	2e	0.21	0/1149	0.45	0/1548
37	1f	0.20	0/823	0.44	0/1115
37	2f	0.21	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.21	0/1250	0.44	0/1679
38	2g	0.20	0/1254	0.47	0/1683
39	1h	0.19	0/1108	0.43	0/1494
39	2h	0.19	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.44	0/1346
40	2i	0.22	0/997	0.47	1/1343 (0.1%)
41	1j	0.20	0/722	0.45	0/982
41	2j	0.21	0/727	0.46	0/988
42	1k	0.19	0/844	0.43	0/1145
42	2k	0.19	0/848	0.40	0/1149
43	1l	0.21	0/937	0.46	0/1260
43	2l	0.21	0/937	0.43	0/1260
44	1m	0.22	0/929	0.48	0/1250
44	2m	0.21	0/917	0.47	0/1234
45	1n	0.20	0/501	0.46	0/664
45	2n	0.21	0/501	0.46	0/664
46	1o	0.20	0/739	0.39	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.19	0/697	0.47	0/939
47	2p	0.21	0/693	0.44	0/935
48	1q	0.19	0/836	0.40	0/1117
48	2q	0.19	0/836	0.44	0/1117
49	1r	0.20	0/560	0.39	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.24	0/667	0.52	0/900
50	2s	0.20	0/661	0.43	0/893
51	1t	0.18	0/730	0.44	0/965
51	2t	0.19	0/729	0.43	0/965
52	1u	0.20	0/203	0.43	0/266
52	2u	0.24	0/203	0.50	0/266
53	1v	0.25	0/310	0.40	0/480
53	2v	0.24	0/310	0.42	0/480
54	1w	0.21	0/1956	0.41	1/2634 (0.0%)
54	2w	0.23	0/1974	0.43	1/2657 (0.0%)
55	1x	0.22	0/1580	0.34	0/2458
55	2x	0.22	1/1580 (0.1%)	0.33	0/2458
All	All	0.23	3/313795 (0.0%)	0.43	20/468848 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
21	1Z	0	1
33	1b	0	2
38	1g	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	O3'-P	5.46	1.61	1.56
32	2a	527	G7M	O3'-P	5.23	1.61	1.56
32	1a	527	G7M	O3'-P	5.03	1.61	1.56

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.54	119.30	109.50
54	2w	302	ILE	N-CA-C	-6.47	106.49	112.96
32	2a	1272	G	N1-C2-N2	-6.42	96.93	116.20
32	2a	1263	C	N1-C2-O2	6.16	137.39	118.90
1	2A	1992	G	C2'-C3'-O3'	6.02	118.54	109.50

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
33	1b	122	PHE	Peptide
33	1b	9	GLU	Peptide
38	1g	79	ARG	Peptide

5.2 Too-close contacts [i](#)

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31193	603	0
1	2A	60322	0	30424	632	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	39	0
3	1D	2136	0	2218	44	0
3	2D	2136	0	2218	51	0
4	1E	1559	0	1618	22	0
4	2E	1559	0	1618	32	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	39	0
6	1G	1423	0	1436	40	0
6	2G	1428	0	1438	56	0
7	1H	1330	0	1407	28	0
7	2H	1330	0	1407	32	0
8	1I	1097	0	1140	24	0
8	2I	1064	0	1082	28	0
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	15	0
10	2O	933	0	996	22	0
11	1P	1135	0	1212	19	0
11	2P	1135	0	1212	31	0
12	1Q	1122	0	1179	15	0
12	2Q	1122	0	1179	21	0
13	1R	968	0	1033	18	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	16	0
14	2S	870	0	923	22	0
15	1T	1091	0	1151	22	0
15	2T	1083	0	1136	21	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	13	0
17	1V	771	0	830	11	0
17	2V	771	0	830	16	0
18	1W	886	0	940	9	0
18	2W	886	0	940	11	0
19	1X	750	0	814	14	0
19	2X	750	0	814	17	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	8	0
21	1Z	1240	0	1240	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1271	0	1273	34	0
22	10	604	0	619	12	0
22	20	604	0	619	14	0
23	11	755	0	826	19	0
23	21	755	0	826	10	0
24	12	588	0	643	4	0
24	22	588	0	643	7	0
25	13	469	0	518	8	0
25	23	464	0	514	10	0
26	14	552	0	533	24	0
26	24	532	0	503	28	0
27	15	455	0	465	7	0
27	25	455	0	465	10	0
28	16	453	0	472	4	0
28	26	449	0	469	8	0
29	17	418	0	467	14	0
29	27	418	0	467	12	0
30	18	517	0	582	15	0
30	28	517	0	582	13	0
31	19	307	0	335	1	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	480	0
32	2a	32327	0	16338	448	0
33	1b	1846	0	1867	88	0
33	2b	1825	0	1828	67	0
34	1c	1548	0	1535	53	0
34	2c	1542	0	1517	53	0
35	1d	1655	0	1672	60	0
35	2d	1674	0	1714	51	0
36	1e	1129	0	1185	36	0
36	2e	1133	0	1191	29	0
37	1f	810	0	804	18	0
37	2f	816	0	808	27	0
38	1g	1231	0	1238	31	0
38	2g	1235	0	1249	53	0
39	1h	1088	0	1126	33	0
39	2h	1088	0	1126	25	0
40	1i	983	0	986	37	0
40	2i	978	0	966	37	0
41	1j	709	0	650	29	0
41	2j	714	0	672	23	0
42	1k	829	0	825	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	836	26	0
43	1l	932	0	981	18	0
43	2l	932	0	981	13	0
44	1m	919	0	951	38	0
44	2m	907	0	934	43	0
45	1n	492	0	529	16	0
45	2n	492	0	529	22	0
46	1o	728	0	760	14	0
46	2o	728	0	760	17	0
47	1p	681	0	697	26	0
47	2p	677	0	686	14	0
48	1q	823	0	891	15	0
48	2q	823	0	891	19	0
49	1r	555	0	618	14	0
49	2r	555	0	618	18	0
50	1s	652	0	662	24	0
50	2s	646	0	644	30	0
51	1t	728	0	798	22	0
51	2t	727	0	796	17	0
52	1u	199	0	208	7	0
52	2u	199	0	208	7	0
53	1v	277	0	140	8	0
53	2v	277	0	140	5	0
54	1w	1939	0	1922	54	0
54	2w	1957	0	1935	53	0
55	1x	1577	0	802	14	0
55	2x	1577	0	802	13	0
56	10	6	0	0	0	0
56	11	4	0	0	0	0
56	12	3	0	0	0	0
56	13	6	0	0	0	0
56	14	1	0	0	0	0
56	15	8	0	0	0	0
56	16	2	0	0	0	0
56	17	7	0	0	0	0
56	18	4	0	0	0	0
56	1A	1083	0	0	0	0
56	1B	37	0	0	0	0
56	1D	14	0	0	0	0
56	1E	17	0	0	0	0
56	1F	14	0	0	0	0
56	1G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1I	1	0	0	0	0
56	1N	8	0	0	0	0
56	1O	5	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	7	0	0	0	0
56	1R	4	0	0	0	0
56	1S	3	0	0	0	0
56	1T	3	0	0	0	0
56	1U	10	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	224	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	4	0	0	0	0
56	1f	2	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1p	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	4	0	0	0	0
56	1w	1	0	0	0	0
56	1x	13	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	3	0	0	0	0
56	25	5	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	3	0	0	0	0
56	2A	870	0	0	0	0
56	2B	20	0	0	0	0
56	2D	6	0	0	0	0
56	2E	7	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	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	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	3	0	0	0	0
56	2T	3	0	0	0	0
56	2U	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	4	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	176	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	2	0	0	0	0
56	2q	2	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2x	6	0	0	0	0
57	1A	1	0	0	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	2	0
59	2d	8	0	0	0	0
60	10	10	0	0	0	0
60	11	9	0	0	0	0
60	12	4	0	0	0	0
60	13	5	0	0	0	0
60	15	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	16	1	0	0	0	0
60	17	8	0	0	0	0
60	18	13	0	0	1	0
60	1A	1841	0	0	93	0
60	1B	66	0	0	2	0
60	1D	24	0	0	2	0
60	1E	27	0	0	2	0
60	1F	16	0	0	0	0
60	1G	3	0	0	3	0
60	1H	2	0	0	0	0
60	1N	5	0	0	0	0
60	1O	5	0	0	0	0
60	1P	20	0	0	2	0
60	1Q	5	0	0	0	0
60	1R	15	0	0	2	0
60	1S	4	0	0	1	0
60	1T	5	0	0	0	0
60	1U	15	0	0	1	0
60	1V	7	0	0	0	0
60	1W	12	0	0	0	0
60	1X	7	0	0	0	0
60	1Y	1	0	0	0	0
60	1Z	1	0	0	0	0
60	1a	274	0	0	17	0
60	1b	1	0	0	1	0
60	1g	1	0	0	0	0
60	1l	2	0	0	0	0
60	1n	1	0	0	0	0
60	1o	1	0	0	0	0
60	1q	1	0	0	0	0
60	1u	1	0	0	0	0
60	1v	3	0	0	0	0
60	1w	2	0	0	0	0
60	1x	15	0	0	2	0
60	20	5	0	0	1	0
60	21	10	0	0	0	0
60	23	2	0	0	0	0
60	25	2	0	0	1	0
60	27	6	0	0	0	0
60	28	3	0	0	0	0
60	29	1	0	0	0	0
60	2A	1163	0	0	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2B	25	0	0	2	0
60	2D	22	0	0	4	0
60	2E	15	0	0	1	0
60	2F	11	0	0	0	0
60	2I	1	0	0	0	0
60	2N	1	0	0	0	0
60	2O	2	0	0	1	0
60	2P	11	0	0	1	0
60	2Q	1	0	0	0	0
60	2R	5	0	0	2	0
60	2T	5	0	0	0	0
60	2U	2	0	0	0	0
60	2V	2	0	0	0	0
60	2W	4	0	0	0	0
60	2X	3	0	0	0	0
60	2Z	1	0	0	0	0
60	2a	138	0	0	10	0
60	2d	1	0	0	0	0
60	2e	1	0	0	0	0
60	2g	1	0	0	0	0
60	2j	3	0	0	0	0
60	2l	3	0	0	0	0
60	2q	1	0	0	0	0
60	2t	2	0	0	0	0
60	2v	1	0	0	0	0
60	2w	3	0	0	1	0
60	2x	8	0	0	0	0
All	All	296938	0	197070	4056	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 9.

The worst 5 of 4056 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:H61	1.02	1.00
1:1A:1082:U:H3	1:1A:1086:A:N6	1.59	1.00
1:2A:2104:G:H1	1:2A:2185:C:H42	1.05	0.98
1:1A:2427:C:OP1	60:1A:4104:HOH:O	1.81	0.96
1:1A:2138:C:H42	1:1A:2153:G:H1	1.11	0.96

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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	46
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	46
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	46
5	2F	201/210 (96%)	187 (93%)	10 (5%)	4 (2%)	6	12
6	1G	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	7	15
6	2G	179/182 (98%)	144 (80%)	29 (16%)	6 (3%)	3	4
7	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	21	42
7	2H	172/180 (96%)	154 (90%)	14 (8%)	4 (2%)	5	9
8	1I	144/148 (97%)	126 (88%)	18 (12%)	0	100	100
8	2I	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5	11
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	110 (92%)	7 (6%)	3 (2%)	4	8
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	34
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	18	38
11	2P	147/150 (98%)	135 (92%)	11 (8%)	1 (1%)	18	38
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	30
14	2S	108/112 (96%)	97 (90%)	9 (8%)	2 (2%)	6	13
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	28
17	2V	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	6	12
18	1W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	14	30
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	5	10
20	1Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	12	28
20	2Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	13
21	1Z	148/206 (72%)	127 (86%)	18 (12%)	3 (2%)	6	12
21	2Z	156/206 (76%)	139 (89%)	16 (10%)	1 (1%)	21	42
22	10	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
22	20	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	25
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	25
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	14
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	55 (82%)	9 (13%)	3 (4%)	2	2
26	24	67/71 (94%)	49 (73%)	15 (22%)	3 (4%)	2	2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	46 (100%)	0	0	100	100
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%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	185 (81%)	31 (14%)	13 (6%)	1	1
33	2b	229/256 (90%)	187 (82%)	30 (13%)	12 (5%)	1	2
34	1c	204/239 (85%)	173 (85%)	30 (15%)	1 (0%)	24	46
34	2c	204/239 (85%)	176 (86%)	23 (11%)	5 (2%)	4	8
35	1d	206/209 (99%)	173 (84%)	30 (15%)	3 (2%)	8	18
35	2d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	24	46
36	1e	146/162 (90%)	127 (87%)	16 (11%)	3 (2%)	5	11
36	2e	146/162 (90%)	131 (90%)	15 (10%)	0	100	100
37	1f	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
37	2f	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	12	28
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	21
38	2g	153/156 (98%)	127 (83%)	23 (15%)	3 (2%)	6	12
39	1h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	18	38
39	2h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
40	1i	125/128 (98%)	103 (82%)	20 (16%)	2 (2%)	7	16
40	2i	125/128 (98%)	104 (83%)	20 (16%)	1 (1%)	16	34
41	1j	95/105 (90%)	81 (85%)	12 (13%)	2 (2%)	5	11
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	5	11
42	1k	112/129 (87%)	97 (87%)	12 (11%)	3 (3%)	4	7
42	2k	112/129 (87%)	95 (85%)	15 (13%)	2 (2%)	6	14
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	116/126 (92%)	105 (90%)	10 (9%)	1 (1%)	14	30
44	2m	114/126 (90%)	96 (84%)	16 (14%)	2 (2%)	6	14
45	1n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	15
45	2n	58/61 (95%)	52 (90%)	4 (7%)	2 (3%)	3	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	62 (78%)	18 (22%)	0	100	100
47	2p	80/88 (91%)	68 (85%)	11 (14%)	1 (1%)	9	21
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	12	28
48	2q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	28
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8	18
50	1s	81/93 (87%)	64 (79%)	17 (21%)	0	100	100
50	2s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	4	8
51	1t	94/106 (89%)	81 (86%)	9 (10%)	4 (4%)	2	2
51	2t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5	11
52	1u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	2
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
54	1w	246/354 (70%)	229 (93%)	16 (6%)	1 (0%)	30	51
54	2w	250/354 (71%)	223 (89%)	25 (10%)	2 (1%)	16	34
All	All	11841/12836 (92%)	10743 (91%)	962 (8%)	136 (1%)	11	25

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
23	11	3	LYS
26	14	56	VAL
33	1b	17	PHE

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%)	204 (95%)	11 (5%)	21	45
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	45
4	1E	164/166 (99%)	159 (97%)	5 (3%)	36	64
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	33
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	16
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5	10
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	10
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	10
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	27
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	32
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	5
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	4
9	1N	118/119 (99%)	113 (96%)	5 (4%)	26	52
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	13
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	46
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	37
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	31
11	2P	115/116 (99%)	101 (88%)	14 (12%)	5	10
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	31	58
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	24
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	64
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	64
14	1S	86/88 (98%)	76 (88%)	10 (12%)	5	11
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	24
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32	59
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	25
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	42
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	35
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	46
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12	28
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	61
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	44
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11	26
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8	18
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	10	24
21	1Z	135/179 (75%)	113 (84%)	22 (16%)	2	4
21	2Z	137/179 (76%)	122 (89%)	15 (11%)	6	13
22	10	61/67 (91%)	57 (93%)	4 (7%)	15	34
22	20	61/67 (91%)	58 (95%)	3 (5%)	22	47
23	11	80/83 (96%)	73 (91%)	7 (9%)	9	21
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	16
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	36
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	16
26	14	59/63 (94%)	44 (75%)	15 (25%)	0	1
26	24	53/63 (84%)	44 (83%)	9 (17%)	2	4
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	55
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	37
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	38
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	10
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	29
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	29
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	29
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	29
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	29 (85%)	5 (15%)	3	6
33	1b	192/220 (87%)	158 (82%)	34 (18%)	2	3
33	2b	187/220 (85%)	152 (81%)	35 (19%)	1	3
34	1c	142/188 (76%)	131 (92%)	11 (8%)	12	27
34	2c	140/188 (74%)	130 (93%)	10 (7%)	13	31
35	1d	169/181 (93%)	151 (89%)	18 (11%)	6	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	36
36	2e	114/123 (93%)	96 (84%)	18 (16%)	2	4
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	14
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	14
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6	13
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8	19
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17	37
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	21
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3	6
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	7
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	6
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	13
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	23
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8	18
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	14
44	1m	89/101 (88%)	76 (85%)	13 (15%)	3	6
44	2m	88/101 (87%)	73 (83%)	15 (17%)	2	4
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	10
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	24
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	15
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	20
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3	6
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	51
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	43
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	7
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	60
50	1s	69/80 (86%)	57 (83%)	12 (17%)	2	3
50	2s	67/80 (84%)	62 (92%)	5 (8%)	12	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	11
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	11
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	12
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	40
54	1w	203/298 (68%)	175 (86%)	28 (14%)	3	7
54	2w	203/298 (68%)	171 (84%)	32 (16%)	2	4
All	All	9693/10660 (91%)	8764 (90%)	929 (10%)	8	17

5 of 929 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2E	134	ILE
50	2s	49	ILE
13	2R	6	SER
48	2q	57	VAL
39	2h	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	199	ASN
54	2w	189	GLN
37	2f	100	ASN
43	2l	8	ASN
38	1g	86	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	449 (15%)	36 (1%)
1	2A	2791/2915 (95%)	461 (16%)	22 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1497/1521 (98%)	319 (21%)	0
32	2a	1501/1521 (98%)	309 (20%)	0
53	1v	10/24 (41%)	4 (40%)	0
53	2v	10/24 (41%)	3 (30%)	0
55	1x	73/74 (98%)	10 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	73/74 (98%)	13 (17%)	0
All	All	9056/9310 (97%)	1599 (17%)	58 (0%)

5 of 1599 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	72	U

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2181	G
1	2A	2406	U
1	1A	2689	U
1	2A	2126	A
1	2A	1379	A

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

66 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	$\# Z > 2$
32	UR3	1a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.67	4 (15%)
32	4OC	1a	1402	56,32	20,23,24	0.76	0	25,32,35	1.04	2 (8%)
55	PSU	1x	55	55	18,21,22	1.31	2 (11%)	21,30,33	1.97	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	2.11	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	1.95	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.23	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1962	1,56	19,22,23	1.62	3 (15%)	26,32,35	1.08	2 (7%)
32	5MC	2a	967	56,32	19,22,23	1.68	3 (15%)	26,32,35	1.11	2 (7%)
32	M2G	2a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.91	6 (18%)
55	H2U	1x	21	55	18,21,22	0.87	2 (11%)	19,30,33	0.91	0
55	PSU	2x	32	55	18,21,22	1.35	2 (11%)	21,30,33	2.00	3 (14%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.36	3 (16%)	21,30,33	2.00	4 (19%)
1	OMG	1A	2251	55,1,56	23,26,27	1.25	3 (13%)	32,38,41	2.05	6 (18%)
32	PSU	1a	516	56,32	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
1	OMG	2A	2251	55,1,56	23,26,27	1.22	3 (13%)	32,38,41	1.92	6 (18%)
32	5MC	1a	1404	32	19,22,23	1.77	3 (15%)	26,32,35	1.24	4 (15%)
1	5MU	1A	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.16	6 (22%)
32	MA6	1a	1519	32	23,26,27	0.39	0	33,38,41	2.11	9 (27%)
1	OMC	1A	1920	1	19,22,23	0.84	0	25,31,34	0.94	0
55	MIA	1x	37	55	21,24,32	1.61	4 (19%)	30,35,47	2.06	7 (23%)
32	M2G	1a	966	32	24,27,28	1.34	3 (12%)	33,40,43	1.85	6 (18%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.09	9 (27%)
43	0TD	1l	92	43	8,9,10	4.63	2 (25%)	6,11,13	8.09	2 (33%)
54	MEQ	1w	230	54	8,9,10	0.60	0	5,10,12	1.27	1 (20%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.95	0
1	OMU	2A	2552	1,56	19,22,23	1.18	3 (15%)	25,31,34	1.81	5 (20%)
43	0TD	2l	92	43	8,9,10	4.69	2 (25%)	6,11,13	4.03	2 (33%)
55	H2U	2x	20	55	18,21,22	0.87	2 (11%)	19,30,33	1.01	1 (5%)
1	5MC	2A	1942	1,56	19,22,23	1.72	3 (15%)	26,32,35	1.13	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.79	3 (11%)
54	MEQ	2w	230	54	8,9,10	0.62	0	5,10,12	0.54	0
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.19	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	2.08	9 (27%)
55	4SU	1x	8	55	18,21,22	1.84	4 (22%)	25,30,33	1.89	4 (16%)
32	4OC	2a	1402	56,32	20,23,24	0.79	0	25,32,35	1.02	3 (12%)
32	5MC	1a	1407	32	19,22,23	1.72	3 (15%)	26,32,35	1.17	4 (15%)
1	2MA	2A	2503	1,56	22,25,26	1.43	3 (13%)	32,37,40	2.40	8 (25%)
55	H2U	2x	21	55	18,21,22	0.87	2 (11%)	19,30,33	0.77	0
55	4SU	2x	8	55	18,21,22	1.78	4 (22%)	25,30,33	1.95	5 (20%)
1	PSU	1A	1917	1	18,21,22	1.41	3 (16%)	21,30,33	2.13	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	1a	527	56,32	23,26,27	1.51	3 (13%)	34,39,42	1.73	5 (14%)
1	5MC	1A	1962	1,56	19,22,23	1.73	3 (15%)	26,32,35	1.16	3 (11%)
32	G7M	2a	527	32	23,26,27	1.53	3 (13%)	34,39,42	1.74	5 (14%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.18	10 (30%)
1	PSU	2A	1917	1,56	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
32	5MC	1a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.18	3 (11%)
1	5MC	1A	1942	1,56	19,22,23	1.55	2 (10%)	26,32,35	1.20	4 (15%)
32	5MC	1a	967	32	19,22,23	1.47	2 (10%)	26,32,35	1.06	2 (7%)
55	5MU	1x	54	55	19,22,23	1.45	4 (21%)	27,32,35	1.91	6 (22%)
1	5MU	2A	1939	1,56	19,22,23	1.47	5 (26%)	27,32,35	2.24	7 (25%)
1	PSU	1A	2605	1,56	18,21,22	1.46	4 (22%)	21,30,33	2.17	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.27	4 (17%)	33,38,41	2.24	8 (24%)
32	2MG	2a	1207	32	23,26,27	1.30	4 (17%)	33,38,41	2.11	5 (15%)
1	5MU	2A	1915	1	19,22,23	1.53	6 (31%)	27,32,35	2.13	6 (22%)
55	5MU	2x	54	55	19,22,23	1.39	4 (21%)	27,32,35	2.06	6 (22%)
1	5MU	1A	1915	1	19,22,23	1.40	6 (31%)	27,32,35	2.06	7 (25%)
1	2MA	1A	2503	1,56	22,25,26	1.42	5 (22%)	32,37,40	2.33	11 (34%)
55	H2U	1x	20	55	18,21,22	0.90	1 (5%)	19,30,33	1.11	1 (5%)
32	PSU	2a	516	32	18,21,22	1.36	3 (16%)	21,30,33	1.96	5 (23%)
1	OMU	1A	2552	1,56	19,22,23	1.29	4 (21%)	25,31,34	1.92	5 (20%)
55	MIA	2x	37	55	21,24,32	1.61	3 (14%)	30,35,47	2.05	9 (30%)
32	5MC	2a	1407	56,32	19,22,23	1.70	3 (15%)	26,32,35	1.25	3 (11%)
55	PSU	2x	39	55	18,21,22	1.40	2 (11%)	21,30,33	1.82	4 (19%)
55	PSU	1x	39	55	18,21,22	1.45	2 (11%)	21,30,33	1.74	3 (14%)
55	PSU	1x	32	55	18,21,22	1.31	2 (11%)	21,30,33	1.94	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	56,32	-	2/9/29/30	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	56,32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	H2U	1x	21	55	-	5/7/38/39	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	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	2251	55,1,56	-	0/9/27/28	0/3/3/3
32	PSU	1a	516	56,32	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1,56	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
55	MIA	1x	37	55	-	1/7/25/34	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
54	MEQ	1w	230	54	-	5/8/9/11	-
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
55	H2U	2x	20	55	-	2/7/38/39	0/2/2/2
1	5MC	2A	1942	1,56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	MEQ	2w	230	54	-	7/8/9/11	-
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	56,32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/7/25/26	0/3/3/3
55	H2U	2x	21	55	-	5/7/38/39	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	56,32	-	2/7/25/26	0/3/3/3
1	5MC	1A	1962	1,56	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	1917	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	1/7/25/26	0/3/3/3
55	H2U	1x	20	55	-	2/7/38/39	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
55	MIA	2x	37	55	-	2/7/25/34	0/3/3/3
32	5MC	2a	1407	56,32	-	0/7/25/26	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.57	1.69	1.82
43	1l	92	0TD	CB-SB	-12.53	1.69	1.82
32	1a	1404	5MC	C5-C4	6.55	1.49	1.44
32	1a	1407	5MC	C5-C4	6.39	1.49	1.44
1	2A	1942	5MC	C5-C4	6.28	1.48	1.44

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-19.43	67.44	102.36
43	2l	92	0TD	CSB-SB-CB	-9.09	86.02	102.36
1	2A	2503	2MA	C5-C4-N3	-8.22	118.52	127.18
1	1A	2503	2MA	C5-C4-N3	-7.71	119.06	127.18
32	2a	1498	UR3	C4-N3-C2	-7.32	118.69	124.58

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	230	MEQ	CG-CD-NE2-CE
32	2a	1400	5MC	O4'-C4'-C5'-O5'
54	2w	230	MEQ	N-CA-CB-CG
54	2w	230	MEQ	C-CA-CB-CG

There are no ring outliers.

24 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1402	4OC	2	0
32	2a	1400	5MC	1	0
32	2a	967	5MC	1	0
55	2x	55	PSU	1	0
32	1a	516	PSU	1	0
1	1A	1939	5MU	1	0
32	1a	1519	MA6	3	0
32	1a	966	M2G	1	0
32	2a	1518	MA6	1	0
1	2A	2552	OMU	1	0
43	2l	92	0TD	1	0
1	2A	1942	5MC	1	0
32	2a	1404	5MC	3	0
32	1a	1518	MA6	2	0
32	2a	1402	4OC	2	0
1	2A	2503	2MA	1	0
55	2x	21	H2U	1	0
32	2a	527	G7M	1	0
32	2a	1519	MA6	3	0
32	1a	967	5MC	1	0
32	1a	1207	2MG	1	0
32	2a	1207	2MG	1	0
1	2A	1915	5MU	1	0
1	1A	2552	OMU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2702 ligands modelled in this entry, 2700 are monoatomic - leaving 2 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	$\# Z > 2$
59	SF4	1d	302	35	0,12,12	-	-	-		
59	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	302	35	-	-	0/6/5/5
59	SF4	2d	303	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1d	302	SF4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.53	139 (4%) 35 29	18, 36, 93, 105	0
1	2A	2789/2915 (95%)	-0.14	102 (3%) 45 39	31, 55, 88, 103	0
2	1B	120/121 (99%)	-0.36	0 100 100	30, 52, 64, 84	0
2	2B	120/121 (99%)	0.54	6 (5%) 34 28	61, 74, 82, 87	0
3	1D	275/276 (99%)	-0.22	1 (0%) 88 86	20, 38, 54, 71	0
3	2D	275/276 (99%)	0.08	3 (1%) 78 74	27, 49, 60, 75	0
4	1E	204/206 (99%)	-0.20	0 100 100	20, 41, 59, 74	0
4	2E	204/206 (99%)	0.17	4 (1%) 65 60	32, 57, 72, 77	0
5	1F	203/210 (96%)	-0.19	0 100 100	17, 42, 66, 81	0
5	2F	203/210 (96%)	0.35	1 (0%) 87 85	34, 63, 75, 85	0
6	1G	181/182 (99%)	0.89	14 (7%) 19 15	48, 68, 78, 86	0
6	2G	181/182 (99%)	1.10	22 (12%) 8 6	67, 78, 84, 91	0
7	1H	174/180 (96%)	0.25	2 (1%) 78 74	39, 55, 66, 73	0
7	2H	174/180 (96%)	1.00	13 (7%) 20 16	66, 77, 84, 91	0
8	1I	146/148 (98%)	0.52	1 (0%) 84 82	40, 69, 76, 78	0
8	2I	146/148 (98%)	1.02	16 (10%) 10 8	57, 75, 80, 83	0
9	1N	140/140 (100%)	-0.18	0 100 100	25, 39, 61, 69	0
9	2N	140/140 (100%)	0.44	2 (1%) 73 69	46, 62, 75, 80	0
10	1O	122/122 (100%)	-0.15	0 100 100	29, 41, 58, 63	0
10	2O	122/122 (100%)	0.19	1 (0%) 82 80	40, 54, 65, 73	0
11	1P	149/150 (99%)	-0.12	0 100 100	20, 43, 66, 75	0
11	2P	149/150 (99%)	0.45	6 (4%) 42 37	36, 64, 77, 83	0
12	1Q	141/141 (100%)	-0.02	2 (1%) 73 69	26, 41, 53, 62	0
12	2Q	141/141 (100%)	0.56	3 (2%) 63 58	44, 62, 70, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.33	0 100 100	23, 36, 48, 58	0
13	2R	118/118 (100%)	0.13	0 100 100	40, 52, 61, 70	0
14	1S	110/112 (98%)	0.13	2 (1%) 67 63	38, 52, 63, 67	0
14	2S	110/112 (98%)	0.92	8 (7%) 21 17	60, 70, 79, 84	0
15	1T	131/146 (89%)	0.07	4 (3%) 51 45	34, 46, 67, 80	0
15	2T	131/146 (89%)	0.24	2 (1%) 72 68	48, 57, 72, 77	0
16	1U	116/118 (98%)	-0.38	0 100 100	22, 32, 48, 58	0
16	2U	116/118 (98%)	0.29	1 (0%) 81 78	41, 56, 70, 74	0
17	1V	101/101 (100%)	-0.24	1 (0%) 79 76	21, 43, 58, 67	0
17	2V	101/101 (100%)	0.60	2 (1%) 65 60	44, 65, 76, 81	0
18	1W	112/113 (99%)	-0.33	0 100 100	22, 31, 53, 76	0
18	2W	112/113 (99%)	0.08	1 (0%) 81 78	38, 50, 66, 80	0
19	1X	95/96 (98%)	-0.21	1 (1%) 78 74	24, 37, 56, 68	0
19	2X	95/96 (98%)	0.43	4 (4%) 40 35	46, 58, 74, 79	0
20	1Y	107/110 (97%)	0.16	1 (0%) 81 78	35, 49, 69, 73	0
20	2Y	107/110 (97%)	0.81	7 (6%) 25 19	56, 68, 80, 85	0
21	1Z	154/206 (74%)	0.36	4 (2%) 57 51	39, 57, 72, 79	0
21	2Z	160/206 (77%)	0.87	8 (5%) 34 28	62, 74, 80, 85	0
22	10	76/85 (89%)	-0.15	0 100 100	28, 38, 53, 57	0
22	20	76/85 (89%)	0.58	4 (5%) 32 26	43, 61, 70, 75	0
23	11	97/98 (98%)	0.07	2 (2%) 63 58	26, 42, 67, 72	0
23	21	97/98 (98%)	0.25	1 (1%) 79 76	40, 54, 72, 76	0
24	12	70/72 (97%)	0.01	0 100 100	33, 48, 58, 73	0
24	22	70/72 (97%)	0.65	4 (5%) 29 24	58, 68, 75, 83	0
25	13	59/60 (98%)	-0.40	0 100 100	25, 36, 62, 73	0
25	23	59/60 (98%)	0.31	0 100 100	49, 60, 72, 78	0
26	14	69/71 (97%)	1.07	12 (17%) 4 3	63, 79, 87, 94	0
26	24	69/71 (97%)	1.23	10 (14%) 6 4	75, 84, 90, 96	0
27	15	59/60 (98%)	-0.31	1 (1%) 69 64	18, 35, 62, 70	0
27	25	59/60 (98%)	0.05	1 (1%) 69 64	39, 50, 67, 77	0
28	16	53/54 (98%)	-0.18	0 100 100	31, 43, 54, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.42	1 (1%) 66 61	49, 59, 67, 68	0
29	17	48/49 (97%)	-0.29	1 (2%) 63 58	19, 26, 56, 62	0
29	27	48/49 (97%)	0.07	1 (2%) 63 58	30, 40, 65, 70	0
30	18	64/65 (98%)	-0.26	0 100 100	25, 34, 43, 51	0
30	28	64/65 (98%)	0.39	0 100 100	44, 53, 62, 66	0
31	19	37/37 (100%)	-0.04	0 100 100	32, 43, 56, 59	0
31	29	37/37 (100%)	0.93	2 (5%) 31 26	56, 64, 71, 71	0
32	1a	1488/1521 (97%)	0.61	85 (5%) 29 24	38, 76, 93, 102	0
32	2a	1491/1521 (98%)	0.46	58 (3%) 43 38	45, 75, 92, 104	0
33	1b	231/256 (90%)	1.17	32 (13%) 6 5	70, 78, 86, 91	0
33	2b	231/256 (90%)	1.13	35 (15%) 5 4	68, 80, 85, 90	0
34	1c	206/239 (86%)	1.20	31 (15%) 5 4	68, 79, 86, 91	0
34	2c	206/239 (86%)	1.08	22 (10%) 11 9	72, 79, 85, 90	0
35	1d	208/209 (99%)	1.13	21 (10%) 12 9	57, 75, 82, 87	0
35	2d	208/209 (99%)	0.92	12 (5%) 29 23	58, 70, 79, 84	0
36	1e	148/162 (91%)	0.63	6 (4%) 41 36	52, 68, 75, 78	0
36	2e	148/162 (91%)	0.69	5 (3%) 48 42	61, 70, 77, 84	0
37	1f	100/101 (99%)	0.65	4 (4%) 42 37	61, 69, 75, 78	0
37	2f	100/101 (99%)	0.71	3 (3%) 52 47	62, 71, 78, 81	0
38	1g	155/156 (99%)	0.99	10 (6%) 25 19	67, 77, 83, 86	0
38	2g	155/156 (99%)	1.09	23 (14%) 5 4	71, 79, 85, 87	0
39	1h	137/138 (99%)	0.78	8 (5%) 29 23	62, 72, 78, 83	0
39	2h	137/138 (99%)	0.75	5 (3%) 46 40	60, 70, 77, 79	0
40	1i	127/128 (99%)	1.55	33 (25%) 1 1	68, 79, 84, 86	0
40	2i	127/128 (99%)	1.94	53 (41%) 0 0	72, 83, 88, 91	0
41	1j	97/105 (92%)	1.44	20 (20%) 2 2	67, 81, 86, 87	0
41	2j	96/105 (91%)	1.79	39 (40%) 0 0	74, 83, 88, 90	0
42	1k	114/129 (88%)	0.60	4 (3%) 47 41	50, 70, 78, 79	0
42	2k	114/129 (88%)	0.78	8 (7%) 22 18	56, 73, 81, 85	0
43	1l	121/132 (91%)	0.57	4 (3%) 49 43	54, 64, 71, 77	0
43	2l	121/132 (91%)	0.57	3 (2%) 58 52	53, 64, 72, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	1.59	35 (29%) 1 1	70, 80, 85, 87	0
44	2m	116/126 (92%)	1.44	24 (20%) 2 2	73, 80, 86, 91	0
45	1n	60/61 (98%)	1.57	15 (25%) 2 1	72, 80, 84, 86	0
45	2n	60/61 (98%)	2.18	23 (38%) 1 0	72, 81, 86, 90	0
46	1o	88/89 (98%)	0.83	5 (5%) 29 24	51, 70, 80, 86	0
46	2o	88/89 (98%)	0.79	6 (6%) 23 19	61, 70, 78, 80	0
47	1p	82/88 (93%)	1.69	26 (31%) 1 1	65, 77, 83, 87	0
47	2p	82/88 (93%)	1.03	7 (8%) 16 13	62, 70, 77, 81	0
48	1q	99/105 (94%)	0.89	5 (5%) 33 28	59, 70, 77, 83	0
48	2q	99/105 (94%)	0.63	1 (1%) 79 76	56, 69, 76, 80	0
49	1r	68/88 (77%)	0.62	0 100 100	59, 68, 76, 82	0
49	2r	68/88 (77%)	0.78	2 (2%) 53 48	65, 73, 78, 84	0
50	1s	83/93 (89%)	1.81	31 (37%) 1 0	75, 82, 86, 87	0
50	2s	83/93 (89%)	1.69	30 (36%) 1 0	77, 84, 89, 92	0
51	1t	96/106 (90%)	1.17	13 (13%) 7 5	64, 75, 79, 85	0
51	2t	96/106 (90%)	0.68	2 (2%) 63 58	57, 69, 77, 81	0
52	1u	23/27 (85%)	2.37	15 (65%) 0 0	76, 79, 83, 84	0
52	2u	23/27 (85%)	1.85	10 (43%) 0 0	76, 80, 83, 84	0
53	1v	13/24 (54%)	1.61	4 (30%) 1 1	57, 81, 93, 94	0
53	2v	13/24 (54%)	1.76	7 (53%) 0 0	68, 85, 96, 98	0
54	1w	248/354 (70%)	1.09	35 (14%) 6 5	57, 78, 85, 91	0
54	2w	252/354 (71%)	1.68	77 (30%) 1 1	71, 83, 90, 92	0
55	1x	66/74 (89%)	0.17	1 (1%) 72 68	43, 74, 85, 88	0
55	2x	66/74 (89%)	0.40	1 (1%) 72 68	55, 78, 88, 90	0
All	All	21073/22146 (95%)	0.34	1323 (6%) 26 20	17, 64, 87, 105	0

The worst 5 of 1323 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	6	GLY	9.3
1	2A	2147	G	8.2
45	1n	2	ALA	7.3
1	2A	2145	C	7.3
1	2A	2146	C	6.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	H2U	2x	21	20/21	0.64	0.15	85,95,104,117	0
55	H2U	2x	20	20/21	0.68	0.13	80,92,100,105	0
55	H2U	1x	21	20/21	0.74	0.15	90,94,100,109	0
55	PSU	2x	55	20/21	0.79	0.11	77,82,86,90	0
55	H2U	1x	20	20/21	0.80	0.11	78,87,93,97	0
55	5MU	2x	54	21/22	0.83	0.12	79,84,89,101	0
55	PSU	1x	55	20/21	0.86	0.11	74,78,85,92	0
55	5MU	1x	54	21/22	0.87	0.12	72,81,84,92	0
55	4SU	2x	8	20/21	0.87	0.11	79,83,87,88	0
1	5MU	2A	1915	21/22	0.88	0.11	67,76,83,92	0
55	MIA	2x	37	22/30	0.88	0.12	70,77,80,83	0
43	0TD	1l	92	10/11	0.89	0.13	55,62,65,75	0
32	2MG	1a	1207	24/25	0.89	0.13	73,81,90,91	0
55	PSU	1x	32	20/21	0.89	0.11	67,75,79,79	0
32	2MG	2a	1207	24/25	0.89	0.11	76,81,85,90	0
32	PSU	2a	516	20/21	0.90	0.10	66,78,82,82	0
55	PSU	2x	39	20/21	0.91	0.09	67,76,80,81	0
54	MEQ	1w	230	10/11	0.91	0.16	38,56,64,64	0
54	MEQ	2w	230	10/11	0.91	0.20	56,71,75,84	0
55	PSU	2x	32	20/21	0.91	0.10	71,75,80,81	0
32	M2G	2a	966	25/26	0.91	0.16	62,71,84,88	0
32	5MC	2a	967	21/22	0.92	0.14	61,69,77,87	0
1	PSU	2A	1911	20/21	0.92	0.10	56,61,68,69	0
32	4OC	2a	1402	22/23	0.93	0.12	56,65,70,76	0
1	5MU	1A	1915	21/22	0.93	0.10	52,63,68,74	0
55	4SU	1x	8	20/21	0.93	0.10	62,71,78,84	0
32	M2G	1a	966	25/26	0.93	0.10	59,66,75,79	0
32	5MC	1a	967	21/22	0.93	0.12	61,67,75,77	0
55	MIA	1x	37	22/30	0.93	0.10	59,65,70,73	0
32	G7M	2a	527	24/25	0.94	0.10	59,64,67,72	0
43	0TD	2l	92	10/11	0.94	0.10	61,66,68,84	0
32	5MC	1a	1400	21/22	0.94	0.12	53,61,68,69	0
32	G7M	1a	527	24/25	0.94	0.11	53,61,68,70	0
32	PSU	1a	516	20/21	0.94	0.09	65,74,78,81	0
32	5MC	2a	1400	21/22	0.94	0.12	68,71,75,78	0
1	PSU	1A	1911	20/21	0.95	0.09	41,54,60,62	0
32	5MC	2a	1404	21/22	0.95	0.09	52,56,63,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	2a	1518	24/25	0.95	0.10	47,63,66,69	0
32	5MC	1a	1404	21/22	0.95	0.10	44,49,54,57	0
32	4OC	1a	1402	22/23	0.96	0.09	48,54,58,60	0
1	PSU	1A	1917	20/21	0.96	0.07	48,56,60,61	0
1	OMC	2A	1920	21/22	0.96	0.09	56,61,66,69	0
55	PSU	1x	39	20/21	0.96	0.07	55,64,70,71	0
32	5MC	2a	1407	21/22	0.96	0.09	47,56,59,63	0
32	UR3	2a	1498	21/22	0.96	0.09	49,57,60,67	0
1	5MC	2A	1942	21/22	0.96	0.09	48,54,58,60	0
32	MA6	2a	1519	24/25	0.96	0.12	51,62,68,70	0
1	5MC	2A	1962	21/22	0.96	0.08	38,48,53,58	0
1	OMG	2A	2251	24/25	0.97	0.08	32,42,46,48	0
1	2MA	2A	2503	23/24	0.97	0.08	26,38,41,45	0
1	PSU	2A	2605	20/21	0.97	0.07	27,37,43,46	0
1	PSU	1A	2605	20/21	0.97	0.07	25,29,34,41	0
32	5MC	1a	1407	21/22	0.97	0.09	38,46,52,55	0
32	UR3	1a	1498	21/22	0.97	0.07	45,51,53,54	0
1	PSU	2A	1917	20/21	0.97	0.06	57,65,71,76	0
32	MA6	1a	1518	24/25	0.97	0.09	41,47,50,52	0
1	5MU	2A	1939	21/22	0.97	0.08	31,40,44,45	0
32	MA6	1a	1519	24/25	0.97	0.09	41,46,49,54	0
1	5MC	1A	1942	21/22	0.97	0.08	33,39,45,54	0
1	OMG	1A	2251	24/25	0.98	0.06	23,27,29,31	0
1	2MA	1A	2503	23/24	0.98	0.06	15,20,23,26	0
1	OMU	1A	2552	21/22	0.98	0.07	25,30,33,36	0
1	OMU	2A	2552	21/22	0.98	0.07	33,41,46,50	0
1	5MU	1A	1939	21/22	0.98	0.06	22,27,32,32	0
1	OMC	1A	1920	21/22	0.98	0.07	42,50,53,53	0
1	5MC	1A	1962	21/22	0.98	0.06	26,33,40,54	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	235	1/1	0.56	0.21	70,70,70,70	0
56	MG	1a	1781	1/1	0.57	0.18	91,91,91,91	0
56	MG	2A	3723	1/1	0.57	0.23	75,75,75,75	0
56	MG	2B	220	1/1	0.57	0.25	80,80,80,80	0
56	MG	2A	3656	1/1	0.62	0.21	79,79,79,79	0
56	MG	1A	4006	1/1	0.63	0.18	74,74,74,74	0
56	MG	2j	201	1/1	0.64	0.15	78,78,78,78	0
56	MG	1a	1664	1/1	0.65	0.19	83,83,83,83	0
56	MG	1a	1824	1/1	0.65	0.24	80,80,80,80	0
56	MG	1a	1813	1/1	0.66	0.16	89,89,89,89	0
56	MG	1a	1643	1/1	0.69	0.34	78,78,78,78	0
56	MG	2a	1750	1/1	0.69	0.22	92,92,92,92	0
56	MG	1l	202	1/1	0.69	0.11	75,75,75,75	0
56	MG	2A	3867	1/1	0.70	0.15	79,79,79,79	0
56	MG	1A	3028	1/1	0.70	0.20	69,69,69,69	0
56	MG	1a	1786	1/1	0.71	0.16	85,85,85,85	0
56	MG	1O	201	1/1	0.71	0.20	64,64,64,64	0
56	MG	1a	1676	1/1	0.72	0.24	73,73,73,73	0
56	MG	1a	1681	1/1	0.72	0.16	76,76,76,76	0
56	MG	1A	3829	1/1	0.72	0.18	54,54,54,54	0
56	MG	2A	3740	1/1	0.72	0.17	73,73,73,73	0
56	MG	1a	1700	1/1	0.73	0.29	76,76,76,76	0
56	MG	2A	3759	1/1	0.73	0.21	52,52,52,52	0
56	MG	1a	1734	1/1	0.73	0.28	90,90,90,90	0
56	MG	2A	3678	1/1	0.73	0.23	69,69,69,69	0
56	MG	2A	3707	1/1	0.73	0.18	57,57,57,57	0
56	MG	2g	201	1/1	0.73	0.15	78,78,78,78	0
56	MG	1A	3255	1/1	0.73	0.25	66,66,66,66	0
56	MG	1a	1733	1/1	0.74	0.56	87,87,87,87	0
56	MG	2A	3366	1/1	0.74	0.23	78,78,78,78	0
56	MG	2a	1657	1/1	0.74	0.30	64,64,64,64	0
56	MG	2a	1678	1/1	0.74	0.33	73,73,73,73	0
56	MG	2a	1694	1/1	0.74	0.44	76,76,76,76	0
56	MG	2A	3453	1/1	0.74	0.23	67,67,67,67	0
56	MG	2A	3464	1/1	0.74	0.34	83,83,83,83	0
56	MG	1A	3989	1/1	0.74	0.16	42,42,42,42	0
56	MG	1V	201	1/1	0.75	0.36	53,53,53,53	0
56	MG	2A	3216	1/1	0.75	0.18	67,67,67,67	0
56	MG	2A	3568	1/1	0.75	0.23	86,86,86,86	0
56	MG	2a	1681	1/1	0.75	0.21	78,78,78,78	0
56	MG	2A	3622	1/1	0.75	0.32	70,70,70,70	0
56	MG	1A	3344	1/1	0.75	0.20	70,70,70,70	0
56	MG	2A	3673	1/1	0.75	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	2B	209	1/1	0.75	0.24	69,69,69,69	0
56	MG	1a	1778	1/1	0.76	0.27	64,64,64,64	0
56	MG	2A	3869	1/1	0.76	0.19	80,80,80,80	0
56	MG	1A	3984	1/1	0.76	0.23	69,69,69,69	0
56	MG	1a	1711	1/1	0.76	0.35	74,74,74,74	0
56	MG	2a	1634	1/1	0.76	0.23	69,69,69,69	0
56	MG	1a	1796	1/1	0.76	0.14	64,64,64,64	0
56	MG	1A	3082	1/1	0.77	0.17	64,64,64,64	0
56	MG	1A	3515	1/1	0.77	0.21	73,73,73,73	0
56	MG	2A	3119	1/1	0.77	0.19	64,64,64,64	0
56	MG	2A	3853	1/1	0.77	0.24	76,76,76,76	0
56	MG	1a	1696	1/1	0.77	0.14	67,67,67,67	0
56	MG	2A	3360	1/1	0.77	0.14	68,68,68,68	0
56	MG	1a	1810	1/1	0.77	0.12	76,76,76,76	0
56	MG	1A	3647	1/1	0.77	0.21	74,74,74,74	0
56	MG	2j	202	1/1	0.77	0.10	76,76,76,76	0
56	MG	1A	3206	1/1	0.78	0.14	57,57,57,57	0
56	MG	1a	1607	1/1	0.78	0.12	80,80,80,80	0
56	MG	1a	1702	1/1	0.78	0.36	75,75,75,75	0
56	MG	2B	211	1/1	0.78	0.21	67,67,67,67	0
56	MG	2B	215	1/1	0.78	0.19	70,70,70,70	0
56	MG	1A	3716	1/1	0.78	0.23	76,76,76,76	0
56	MG	1a	1714	1/1	0.78	0.13	65,65,65,65	0
56	MG	1a	1652	1/1	0.78	0.36	77,77,77,77	0
56	MG	1v	102	1/1	0.78	0.16	81,81,81,81	0
56	MG	2A	3099	1/1	0.78	0.30	75,75,75,75	0
56	MG	2A	3713	1/1	0.78	0.26	69,69,69,69	0
56	MG	2a	1722	1/1	0.78	0.18	71,71,71,71	0
56	MG	2a	1735	1/1	0.78	0.18	84,84,84,84	0
56	MG	1A	3303	1/1	0.78	0.18	53,53,53,53	0
56	MG	1a	1769	1/1	0.78	0.24	73,73,73,73	0
56	MG	1A	3850	1/1	0.78	0.14	62,62,62,62	0
56	MG	1A	3968	1/1	0.78	0.18	72,72,72,72	0
56	MG	1G	204	1/1	0.79	0.13	61,61,61,61	0
56	MG	2B	207	1/1	0.79	0.18	72,72,72,72	0
56	MG	1A	3916	1/1	0.79	0.12	25,25,25,25	0
56	MG	1A	3752	1/1	0.79	0.19	51,51,51,51	0
56	MG	2A	3504	1/1	0.79	0.20	57,57,57,57	0
56	MG	1A	3409	1/1	0.79	0.38	53,53,53,53	0
56	MG	1A	3843	1/1	0.79	0.15	55,55,55,55	0
56	MG	1a	1645	1/1	0.79	0.18	78,78,78,78	0
56	MG	1A	3298	1/1	0.79	0.26	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	1B	230	1/1	0.79	0.23	65,65,65,65	0
56	MG	1a	1775	1/1	0.79	0.19	73,73,73,73	0
56	MG	1B	231	1/1	0.79	0.26	67,67,67,67	0
56	MG	2A	3280	1/1	0.79	0.14	48,48,48,48	0
56	MG	2A	3283	1/1	0.79	0.13	69,69,69,69	0
56	MG	2A	3290	1/1	0.79	0.20	56,56,56,56	0
56	MG	2A	3304	1/1	0.79	0.21	63,63,63,63	0
56	MG	1A	3888	1/1	0.79	0.19	52,52,52,52	0
56	MG	1A	3465	1/1	0.80	0.20	64,64,64,64	0
56	MG	1A	3869	1/1	0.80	0.21	64,64,64,64	0
56	MG	2A	3586	1/1	0.80	0.21	71,71,71,71	0
56	MG	2A	3267	1/1	0.80	0.18	81,81,81,81	0
56	MG	2A	3655	1/1	0.80	0.18	80,80,80,80	0
56	MG	1A	3199	1/1	0.80	0.20	56,56,56,56	0
56	MG	2A	3666	1/1	0.80	0.20	68,68,68,68	0
56	MG	2W	202	1/1	0.80	0.19	63,63,63,63	0
56	MG	1a	1760	1/1	0.80	0.28	77,77,77,77	0
56	MG	1A	4064	1/1	0.80	0.21	58,58,58,58	0
56	MG	2A	3298	1/1	0.80	0.24	73,73,73,73	0
56	MG	1A	3908	1/1	0.80	0.11	68,68,68,68	0
56	MG	1A	3524	1/1	0.80	0.13	72,72,72,72	0
56	MG	2a	1717	1/1	0.80	0.20	74,74,74,74	0
56	MG	2A	3737	1/1	0.80	0.15	64,64,64,64	0
56	MG	2A	3087	1/1	0.80	0.25	63,63,63,63	0
56	MG	2A	3750	1/1	0.80	0.19	71,71,71,71	0
56	MG	2A	3089	1/1	0.80	0.15	69,69,69,69	0
56	MG	2A	3781	1/1	0.80	0.16	78,78,78,78	0
56	MG	1A	3327	1/1	0.80	0.25	58,58,58,58	0
56	MG	2r	102	1/1	0.80	0.31	80,80,80,80	0
56	MG	1O	205	1/1	0.81	0.16	73,73,73,73	0
56	MG	1A	4000	1/1	0.81	0.12	31,31,31,31	0
56	MG	1a	1708	1/1	0.81	0.20	70,70,70,70	0
56	MG	2A	3760	1/1	0.81	0.17	69,69,69,69	0
56	MG	2A	3379	1/1	0.81	0.30	69,69,69,69	0
56	MG	2A	3789	1/1	0.81	0.14	85,85,85,85	0
56	MG	2A	3815	1/1	0.81	0.15	53,53,53,53	0
56	MG	2A	3391	1/1	0.81	0.31	54,54,54,54	0
56	MG	2A	3393	1/1	0.81	0.13	67,67,67,67	0
56	MG	2A	3451	1/1	0.81	0.36	80,80,80,80	0
56	MG	1Y	201	1/1	0.81	0.14	62,62,62,62	0
56	MG	1A	3759	1/1	0.81	0.22	66,66,66,66	0
56	MG	2A	3502	1/1	0.81	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	112	1/1	0.81	0.15	77,77,77,77	0
56	MG	2A	3535	1/1	0.81	0.17	65,65,65,65	0
56	MG	2A	3030	1/1	0.81	0.27	55,55,55,55	0
56	MG	1a	1728	1/1	0.81	0.27	75,75,75,75	0
56	MG	1a	1637	1/1	0.81	0.29	87,87,87,87	0
56	MG	2A	3650	1/1	0.81	0.20	59,59,59,59	0
56	MG	2A	3653	1/1	0.81	0.27	67,67,67,67	0
56	MG	1A	4023	1/1	0.81	0.17	60,60,60,60	0
56	MG	1A	3811	1/1	0.81	0.27	64,64,64,64	0
56	MG	2A	3197	1/1	0.81	0.27	69,69,69,69	0
56	MG	2a	1730	1/1	0.81	0.25	69,69,69,69	0
56	MG	1A	3661	1/1	0.81	0.17	57,57,57,57	0
56	MG	2a	1746	1/1	0.81	0.29	74,74,74,74	0
56	MG	1a	1653	1/1	0.81	0.24	81,81,81,81	0
56	MG	2a	1757	1/1	0.81	0.27	66,66,66,66	0
56	MG	1A	3934	1/1	0.81	0.11	21,21,21,21	0
56	MG	1A	3614	1/1	0.81	0.11	29,29,29,29	0
56	MG	1A	3717	1/1	0.81	0.23	61,61,61,61	0
56	MG	1A	3498	1/1	0.81	0.26	75,75,75,75	0
56	MG	2x	101	1/1	0.81	0.35	82,82,82,82	0
56	MG	1a	1602	1/1	0.82	0.38	75,75,75,75	0
56	MG	2A	3565	1/1	0.82	0.15	53,53,53,53	0
56	MG	1A	4059	1/1	0.82	0.15	46,46,46,46	0
56	MG	2A	3239	1/1	0.82	0.09	46,46,46,46	0
56	MG	2A	3589	1/1	0.82	0.26	74,74,74,74	0
56	MG	1A	3341	1/1	0.82	0.24	74,74,74,74	0
56	MG	1A	3535	1/1	0.82	0.09	61,61,61,61	0
56	MG	1A	3586	1/1	0.82	0.25	61,61,61,61	0
56	MG	2A	3286	1/1	0.82	0.19	76,76,76,76	0
56	MG	1A	3728	1/1	0.82	0.18	54,54,54,54	0
56	MG	2a	1654	1/1	0.82	0.28	79,79,79,79	0
56	MG	1A	3133	1/1	0.82	0.14	68,68,68,68	0
56	MG	2a	1665	1/1	0.82	0.28	62,62,62,62	0
56	MG	1A	3873	1/1	0.82	0.12	26,26,26,26	0
56	MG	2a	1679	1/1	0.82	0.42	68,68,68,68	0
56	MG	2A	3353	1/1	0.82	0.19	72,72,72,72	0
56	MG	2A	3699	1/1	0.82	0.18	69,69,69,69	0
56	MG	1a	1753	1/1	0.82	0.19	79,79,79,79	0
56	MG	2A	3020	1/1	0.82	0.19	55,55,55,55	0
56	MG	2A	3024	1/1	0.82	0.20	62,62,62,62	0
56	MG	1A	3184	1/1	0.82	0.22	59,59,59,59	0
56	MG	2A	3739	1/1	0.82	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3787	1/1	0.82	0.14	72,72,72,72	0
56	MG	1a	1682	1/1	0.82	0.41	74,74,74,74	0
56	MG	1A	4050	1/1	0.82	0.11	64,64,64,64	0
56	MG	1a	1780	1/1	0.82	0.23	76,76,76,76	0
56	MG	2A	3151	1/1	0.82	0.22	61,61,61,61	0
56	MG	2l	202	1/1	0.82	0.10	74,74,74,74	0
56	MG	2A	3170	1/1	0.82	0.22	80,80,80,80	0
56	MG	2A	3505	1/1	0.82	0.13	35,35,35,35	0
56	MG	1a	1741	1/1	0.83	0.18	58,58,58,58	0
56	MG	1A	3854	1/1	0.83	0.30	43,43,43,43	0
56	MG	1a	1679	1/1	0.83	0.21	72,72,72,72	0
56	MG	1A	3338	1/1	0.83	0.28	66,66,66,66	0
56	MG	1A	3644	1/1	0.83	0.17	52,52,52,52	0
56	MG	1B	217	1/1	0.83	0.14	54,54,54,54	0
56	MG	2a	1630	1/1	0.83	0.43	72,72,72,72	0
56	MG	2A	3100	1/1	0.83	0.34	66,66,66,66	0
56	MG	2A	3105	1/1	0.83	0.26	73,73,73,73	0
56	MG	1A	3512	1/1	0.83	0.16	65,65,65,65	0
56	MG	1a	1609	1/1	0.83	0.29	85,85,85,85	0
56	MG	2A	3167	1/1	0.83	0.14	71,71,71,71	0
56	MG	1A	3375	1/1	0.83	0.36	77,77,77,77	0
56	MG	1A	3909	1/1	0.83	0.13	63,63,63,63	0
56	MG	1E	312	1/1	0.83	0.21	52,52,52,52	0
56	MG	2A	3528	1/1	0.83	0.16	60,60,60,60	0
56	MG	1a	1727	1/1	0.83	0.32	75,75,75,75	0
56	MG	2A	3263	1/1	0.83	0.24	63,63,63,63	0
56	MG	1A	4015	1/1	0.83	0.21	75,75,75,75	0
56	MG	2A	3814	1/1	0.83	0.20	75,75,75,75	0
56	MG	1l	201	1/1	0.83	0.16	72,72,72,72	0
56	MG	2A	3842	1/1	0.83	0.23	70,70,70,70	0
56	MG	2a	1764	1/1	0.83	0.13	58,58,58,58	0
56	MG	2a	1774	1/1	0.83	0.11	65,65,65,65	0
56	MG	2A	3845	1/1	0.83	0.14	85,85,85,85	0
56	MG	2A	3851	1/1	0.83	0.17	50,50,50,50	0
56	MG	1A	3703	1/1	0.83	0.11	22,22,22,22	0
56	MG	1O	204	1/1	0.83	0.14	56,56,56,56	0
56	MG	1a	1737	1/1	0.83	0.43	73,73,73,73	0
56	MG	2B	202	1/1	0.83	0.16	67,67,67,67	0
56	MG	1a	1678	1/1	0.84	0.20	72,72,72,72	0
56	MG	2A	3680	1/1	0.84	0.24	67,67,67,67	0
56	MG	1A	3256	1/1	0.84	0.12	56,56,56,56	0
56	MG	2D	302	1/1	0.84	0.20	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	3714	1/1	0.84	0.27	65,65,65,65	0
56	MG	2a	1615	1/1	0.84	0.24	58,58,58,58	0
56	MG	2A	3712	1/1	0.84	0.13	75,75,75,75	0
56	MG	1A	3076	1/1	0.84	0.16	66,66,66,66	0
56	MG	1a	1694	1/1	0.84	0.22	63,63,63,63	0
56	MG	2A	3735	1/1	0.84	0.19	75,75,75,75	0
56	MG	1a	1614	1/1	0.84	0.16	75,75,75,75	0
56	MG	1a	1626	1/1	0.84	0.27	64,64,64,64	0
56	MG	2A	3282	1/1	0.84	0.10	66,66,66,66	0
56	MG	1A	3804	1/1	0.84	0.13	59,59,59,59	0
56	MG	2a	1692	1/1	0.84	0.40	73,73,73,73	0
56	MG	1A	3980	1/1	0.84	0.20	70,70,70,70	0
56	MG	2a	1715	1/1	0.84	0.18	68,68,68,68	0
56	MG	2A	3561	1/1	0.84	0.14	60,60,60,60	0
56	MG	2A	3764	1/1	0.84	0.21	71,71,71,71	0
56	MG	2A	3287	1/1	0.84	0.17	66,66,66,66	0
56	MG	1A	3393	1/1	0.84	0.10	67,67,67,67	0
56	MG	2A	3577	1/1	0.84	0.18	61,61,61,61	0
56	MG	1A	3827	1/1	0.84	0.21	45,45,45,45	0
56	MG	2A	3301	1/1	0.84	0.28	62,62,62,62	0
56	MG	1a	1725	1/1	0.84	0.34	80,80,80,80	0
56	MG	1B	229	1/1	0.84	0.20	67,67,67,67	0
56	MG	2A	3356	1/1	0.84	0.16	63,63,63,63	0
56	MG	2A	3358	1/1	0.84	0.29	70,70,70,70	0
56	MG	1A	3663	1/1	0.84	0.09	27,27,27,27	0
56	MG	2A	3164	1/1	0.84	0.28	52,52,52,52	0
56	MG	16	102	1/1	0.84	0.27	54,54,54,54	0
56	MG	2A	3675	1/1	0.84	0.23	79,79,79,79	0
56	MG	2A	3050	1/1	0.85	0.29	75,75,75,75	0
56	MG	2A	3581	1/1	0.85	0.22	61,61,61,61	0
56	MG	2A	3063	1/1	0.85	0.27	75,75,75,75	0
56	MG	2A	3296	1/1	0.85	0.12	61,61,61,61	0
56	MG	1A	3812	1/1	0.85	0.14	43,43,43,43	0
56	MG	1a	1766	1/1	0.85	0.20	68,68,68,68	0
56	MG	1A	3415	1/1	0.85	0.32	68,68,68,68	0
56	MG	2B	204	1/1	0.85	0.21	76,76,76,76	0
56	MG	2A	3330	1/1	0.85	0.15	74,74,74,74	0
56	MG	1B	202	1/1	0.85	0.23	62,62,62,62	0
56	MG	2A	3664	1/1	0.85	0.16	49,49,49,49	0
56	MG	2A	3665	1/1	0.85	0.15	54,54,54,54	0
56	MG	1B	211	1/1	0.85	0.24	53,53,53,53	0
56	MG	2A	3672	1/1	0.85	0.28	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2N	201	1/1	0.85	0.11	81,81,81,81	0
56	MG	1A	3541	1/1	0.85	0.29	68,68,68,68	0
56	MG	1A	3971	1/1	0.85	0.10	69,69,69,69	0
56	MG	2A	3362	1/1	0.85	0.13	65,65,65,65	0
56	MG	2A	3152	1/1	0.85	0.22	65,65,65,65	0
56	MG	2A	3692	1/1	0.85	0.17	82,82,82,82	0
56	MG	2A	3160	1/1	0.85	0.31	75,75,75,75	0
56	MG	1A	3979	1/1	0.85	0.09	28,28,28,28	0
56	MG	1A	3542	1/1	0.85	0.16	61,61,61,61	0
56	MG	2A	3396	1/1	0.85	0.10	71,71,71,71	0
56	MG	2A	3717	1/1	0.85	0.16	62,62,62,62	0
56	MG	2A	3720	1/1	0.85	0.22	68,68,68,68	0
56	MG	1A	3569	1/1	0.85	0.19	75,75,75,75	0
56	MG	2A	3731	1/1	0.85	0.14	48,48,48,48	0
56	MG	1A	3683	1/1	0.85	0.13	74,74,74,74	0
56	MG	1F	310	1/1	0.85	0.10	58,58,58,58	0
56	MG	2a	1723	1/1	0.85	0.16	74,74,74,74	0
56	MG	2A	3491	1/1	0.85	0.14	58,58,58,58	0
56	MG	1A	3775	1/1	0.85	0.17	59,59,59,59	0
56	MG	1A	3684	1/1	0.85	0.14	54,54,54,54	0
56	MG	2A	3753	1/1	0.85	0.14	74,74,74,74	0
56	MG	1a	1668	1/1	0.85	0.26	71,71,71,71	0
56	MG	1a	1735	1/1	0.85	0.40	69,69,69,69	0
56	MG	1A	3794	1/1	0.85	0.27	57,57,57,57	0
56	MG	2A	3773	1/1	0.85	0.20	59,59,59,59	0
56	MG	2A	3778	1/1	0.85	0.12	60,60,60,60	0
56	MG	2A	3551	1/1	0.85	0.24	75,75,75,75	0
56	MG	1A	3401	1/1	0.85	0.13	48,48,48,48	0
56	MG	2A	3284	1/1	0.85	0.13	65,65,65,65	0
56	MG	2v	101	1/1	0.85	0.35	70,70,70,70	0
56	MG	1A	3029	1/1	0.85	0.16	71,71,71,71	0
56	MG	1A	3233	1/1	0.86	0.17	57,57,57,57	0
56	MG	2A	3266	1/1	0.86	0.19	79,79,79,79	0
56	MG	1a	1821	1/1	0.86	0.13	68,68,68,68	0
56	MG	2A	3821	1/1	0.86	0.08	80,80,80,80	0
56	MG	2A	3570	1/1	0.86	0.15	72,72,72,72	0
56	MG	2A	3276	1/1	0.86	0.31	71,71,71,71	0
56	MG	1A	3905	1/1	0.86	0.12	43,43,43,43	0
56	MG	1A	3480	1/1	0.86	0.12	52,52,52,52	0
56	MG	2A	3855	1/1	0.86	0.15	56,56,56,56	0
56	MG	1A	3135	1/1	0.86	0.10	32,32,32,32	0
56	MG	1a	1723	1/1	0.86	0.09	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	1v	103	1/1	0.86	0.13	61,61,61,61	0
56	MG	1a	1624	1/1	0.86	0.32	71,71,71,71	0
56	MG	1A	3167	1/1	0.86	0.29	68,68,68,68	0
56	MG	1a	1633	1/1	0.86	0.28	66,66,66,66	0
56	MG	1a	1732	1/1	0.86	0.11	75,75,75,75	0
56	MG	1A	3358	1/1	0.86	0.12	48,48,48,48	0
56	MG	2B	216	1/1	0.86	0.12	70,70,70,70	0
56	MG	1B	224	1/1	0.86	0.10	57,57,57,57	0
56	MG	2A	3671	1/1	0.86	0.12	51,51,51,51	0
56	MG	2A	3073	1/1	0.86	0.24	69,69,69,69	0
56	MG	2A	3341	1/1	0.86	0.17	63,63,63,63	0
56	MG	2W	203	1/1	0.86	0.19	45,45,45,45	0
56	MG	2a	1603	1/1	0.86	0.29	81,81,81,81	0
56	MG	1A	3264	1/1	0.86	0.18	71,71,71,71	0
56	MG	2a	1624	1/1	0.86	0.35	72,72,72,72	0
56	MG	2A	3677	1/1	0.86	0.14	49,49,49,49	0
56	MG	1a	1736	1/1	0.86	0.30	65,65,65,65	0
56	MG	2a	1650	1/1	0.86	0.21	66,66,66,66	0
56	MG	2a	1651	1/1	0.86	0.23	69,69,69,69	0
56	MG	1A	3097	1/1	0.86	0.17	55,55,55,55	0
56	MG	2A	3689	1/1	0.86	0.17	58,58,58,58	0
56	MG	1A	3690	1/1	0.86	0.14	69,69,69,69	0
56	MG	1A	3694	1/1	0.86	0.11	27,27,27,27	0
56	MG	2A	3114	1/1	0.86	0.30	63,63,63,63	0
56	MG	1A	3982	1/1	0.86	0.14	54,54,54,54	0
56	MG	2a	1690	1/1	0.86	0.45	78,78,78,78	0
56	MG	2A	3388	1/1	0.86	0.18	60,60,60,60	0
56	MG	1a	1670	1/1	0.86	0.20	78,78,78,78	0
56	MG	2a	1713	1/1	0.86	0.24	56,56,56,56	0
56	MG	1A	3103	1/1	0.86	0.22	64,64,64,64	0
56	MG	1A	3709	1/1	0.86	0.13	33,33,33,33	0
56	MG	1A	3063	1/1	0.86	0.23	54,54,54,54	0
56	MG	2A	3732	1/1	0.86	0.11	57,57,57,57	0
56	MG	2A	3733	1/1	0.86	0.15	70,70,70,70	0
56	MG	1A	3337	1/1	0.86	0.21	57,57,57,57	0
56	MG	2a	1737	1/1	0.86	0.30	69,69,69,69	0
56	MG	2a	1738	1/1	0.86	0.12	71,71,71,71	0
56	MG	1A	4012	1/1	0.86	0.15	62,62,62,62	0
56	MG	2A	3484	1/1	0.86	0.19	63,63,63,63	0
56	MG	1A	3421	1/1	0.86	0.14	69,69,69,69	0
56	MG	2a	1759	1/1	0.86	0.28	58,58,58,58	0
56	MG	2a	1761	1/1	0.86	0.20	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1763	1/1	0.86	0.19	70,70,70,70	0
56	MG	1A	3603	1/1	0.86	0.13	59,59,59,59	0
56	MG	2A	3221	1/1	0.86	0.17	75,75,75,75	0
56	MG	2A	3754	1/1	0.86	0.17	68,68,68,68	0
56	MG	1A	4048	1/1	0.86	0.12	55,55,55,55	0
56	MG	2A	3517	1/1	0.86	0.37	81,81,81,81	0
56	MG	2A	3249	1/1	0.86	0.18	69,69,69,69	0
56	MG	2A	3255	1/1	0.86	0.19	62,62,62,62	0
56	MG	2A	3259	1/1	0.86	0.34	65,65,65,65	0
56	MG	2A	3554	1/1	0.86	0.15	38,38,38,38	0
56	MG	2x	104	1/1	0.86	0.12	77,77,77,77	0
56	MG	1A	3608	1/1	0.87	0.11	43,43,43,43	0
56	MG	2A	3367	1/1	0.87	0.14	70,70,70,70	0
56	MG	2B	213	1/1	0.87	0.27	67,67,67,67	0
56	MG	1a	1782	1/1	0.87	0.25	80,80,80,80	0
56	MG	1A	3837	1/1	0.87	0.13	39,39,39,39	0
56	MG	1a	1795	1/1	0.87	0.14	55,55,55,55	0
56	MG	1a	1707	1/1	0.87	0.20	58,58,58,58	0
56	MG	1A	3382	1/1	0.87	0.20	61,61,61,61	0
56	MG	2R	203	1/1	0.87	0.14	51,51,51,51	0
56	MG	2A	3694	1/1	0.87	0.20	67,67,67,67	0
56	MG	2A	3430	1/1	0.87	0.31	60,60,60,60	0
56	MG	1a	1638	1/1	0.87	0.25	74,74,74,74	0
56	MG	2a	1608	1/1	0.87	0.09	75,75,75,75	0
56	MG	2a	1612	1/1	0.87	0.26	67,67,67,67	0
56	MG	2A	3711	1/1	0.87	0.09	64,64,64,64	0
56	MG	2a	1616	1/1	0.87	0.18	56,56,56,56	0
56	MG	2a	1623	1/1	0.87	0.17	64,64,64,64	0
56	MG	2A	3242	1/1	0.87	0.21	74,74,74,74	0
56	MG	2A	3454	1/1	0.87	0.15	57,57,57,57	0
56	MG	1a	1641	1/1	0.87	0.34	61,61,61,61	0
56	MG	2a	1649	1/1	0.87	0.21	72,72,72,72	0
56	MG	2A	3719	1/1	0.87	0.12	55,55,55,55	0
56	MG	1A	4062	1/1	0.87	0.11	44,44,44,44	0
56	MG	1A	3534	1/1	0.87	0.12	38,38,38,38	0
56	MG	1a	1649	1/1	0.87	0.19	63,63,63,63	0
56	MG	2a	1664	1/1	0.87	0.26	58,58,58,58	0
56	MG	1A	4067	1/1	0.87	0.09	68,68,68,68	0
56	MG	2a	1667	1/1	0.87	0.21	66,66,66,66	0
56	MG	1a	1730	1/1	0.87	0.46	70,70,70,70	0
56	MG	2A	3273	1/1	0.87	0.15	70,70,70,70	0
56	MG	2A	3519	1/1	0.87	0.25	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	3853	1/1	0.87	0.14	59,59,59,59	0
56	MG	1a	1663	1/1	0.87	0.15	71,71,71,71	0
56	MG	2A	3747	1/1	0.87	0.23	66,66,66,66	0
56	MG	2A	3748	1/1	0.87	0.15	76,76,76,76	0
56	MG	1W	202	1/1	0.87	0.13	42,42,42,42	0
56	MG	1A	3917	1/1	0.87	0.10	45,45,45,45	0
56	MG	2A	3557	1/1	0.87	0.18	47,47,47,47	0
56	MG	13	105	1/1	0.87	0.10	28,28,28,28	0
56	MG	2a	1725	1/1	0.87	0.15	52,52,52,52	0
56	MG	1A	3387	1/1	0.87	0.14	55,55,55,55	0
56	MG	1a	1738	1/1	0.87	0.30	69,69,69,69	0
56	MG	1a	1601	1/1	0.87	0.35	72,72,72,72	0
56	MG	1a	1744	1/1	0.87	0.17	76,76,76,76	0
56	MG	1a	1747	1/1	0.87	0.11	60,60,60,60	0
56	MG	2a	1748	1/1	0.87	0.14	61,61,61,61	0
56	MG	1A	4009	1/1	0.87	0.17	62,62,62,62	0
56	MG	2a	1754	1/1	0.87	0.14	74,74,74,74	0
56	MG	1A	3963	1/1	0.87	0.16	54,54,54,54	0
56	MG	2A	3618	1/1	0.87	0.14	37,37,37,37	0
56	MG	2A	3315	1/1	0.87	0.14	67,67,67,67	0
56	MG	2A	3322	1/1	0.87	0.34	65,65,65,65	0
56	MG	2A	3109	1/1	0.87	0.19	60,60,60,60	0
56	MG	2a	1770	1/1	0.87	0.12	63,63,63,63	0
56	MG	2A	3332	1/1	0.87	0.22	66,66,66,66	0
56	MG	1A	3815	1/1	0.87	0.17	62,62,62,62	0
56	MG	2A	3659	1/1	0.87	0.14	59,59,59,59	0
56	MG	1A	3419	1/1	0.87	0.27	60,60,60,60	0
56	MG	2A	3149	1/1	0.87	0.17	58,58,58,58	0
56	MG	1a	1695	1/1	0.87	0.21	70,70,70,70	0
56	MG	1A	4045	1/1	0.87	0.17	57,57,57,57	0
56	MG	2B	205	1/1	0.87	0.22	59,59,59,59	0
56	MG	2x	103	1/1	0.87	0.27	75,75,75,75	0
56	MG	1a	1697	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3115	1/1	0.88	0.33	64,64,64,64	0
56	MG	2A	3761	1/1	0.88	0.14	68,68,68,68	0
56	MG	2A	3401	1/1	0.88	0.17	68,68,68,68	0
56	MG	2A	3423	1/1	0.88	0.24	66,66,66,66	0
56	MG	2A	3427	1/1	0.88	0.33	63,63,63,63	0
56	MG	2A	3429	1/1	0.88	0.29	60,60,60,60	0
56	MG	2A	3785	1/1	0.88	0.16	72,72,72,72	0
56	MG	1A	4033	1/1	0.88	0.16	45,45,45,45	0
56	MG	2A	3794	1/1	0.88	0.14	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	3431	1/1	0.88	0.31	58,58,58,58	0
56	MG	2A	3438	1/1	0.88	0.23	57,57,57,57	0
56	MG	2A	3133	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3832	1/1	0.88	0.18	66,66,66,66	0
56	MG	2A	3144	1/1	0.88	0.30	64,64,64,64	0
56	MG	1a	1661	1/1	0.88	0.10	70,70,70,70	0
56	MG	1a	1740	1/1	0.88	0.11	62,62,62,62	0
56	MG	1A	3302	1/1	0.88	0.28	56,56,56,56	0
56	MG	1A	3487	1/1	0.88	0.17	64,64,64,64	0
56	MG	2A	3860	1/1	0.88	0.12	49,49,49,49	0
56	MG	1a	1746	1/1	0.88	0.13	57,57,57,57	0
56	MG	1a	1666	1/1	0.88	0.19	75,75,75,75	0
56	MG	1A	3494	1/1	0.88	0.15	68,68,68,68	0
56	MG	2A	3182	1/1	0.88	0.21	56,56,56,56	0
56	MG	1A	3962	1/1	0.88	0.10	68,68,68,68	0
56	MG	2B	206	1/1	0.88	0.22	70,70,70,70	0
56	MG	2A	3198	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3531	1/1	0.88	0.20	49,49,49,49	0
56	MG	2A	3200	1/1	0.88	0.18	65,65,65,65	0
56	MG	2A	3210	1/1	0.88	0.14	70,70,70,70	0
56	MG	1a	1672	1/1	0.88	0.10	70,70,70,70	0
56	MG	2A	3219	1/1	0.88	0.13	62,62,62,62	0
56	MG	2B	219	1/1	0.88	0.30	68,68,68,68	0
56	MG	1a	1675	1/1	0.88	0.28	69,69,69,69	0
56	MG	2A	3235	1/1	0.88	0.15	49,49,49,49	0
56	MG	2F	301	1/1	0.88	0.18	46,46,46,46	0
56	MG	10	105	1/1	0.88	0.17	63,63,63,63	0
56	MG	1A	3578	1/1	0.88	0.14	69,69,69,69	0
56	MG	2A	3571	1/1	0.88	0.11	53,53,53,53	0
56	MG	2A	3247	1/1	0.88	0.08	59,59,59,59	0
56	MG	2Z	301	1/1	0.88	0.15	69,69,69,69	0
56	MG	25	101	1/1	0.88	0.11	54,54,54,54	0
56	MG	2A	3578	1/1	0.88	0.22	71,71,71,71	0
56	MG	1a	1779	1/1	0.88	0.19	95,95,95,95	0
56	MG	2a	1610	1/1	0.88	0.29	70,70,70,70	0
56	MG	14	101	1/1	0.88	0.17	61,61,61,61	0
56	MG	2A	3588	1/1	0.88	0.14	62,62,62,62	0
56	MG	1A	3392	1/1	0.88	0.32	74,74,74,74	0
56	MG	2A	3605	1/1	0.88	0.13	61,61,61,61	0
56	MG	2A	3610	1/1	0.88	0.12	35,35,35,35	0
56	MG	2A	3260	1/1	0.88	0.37	73,73,73,73	0
56	MG	2a	1631	1/1	0.88	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3599	1/1	0.88	0.25	61,61,61,61	0
56	MG	1a	1690	1/1	0.88	0.26	67,67,67,67	0
56	MG	1a	1692	1/1	0.88	0.14	62,62,62,62	0
56	MG	2A	3269	1/1	0.88	0.20	60,60,60,60	0
56	MG	1A	4083	1/1	0.88	0.17	66,66,66,66	0
56	MG	1A	3504	1/1	0.88	0.23	69,69,69,69	0
56	MG	2a	1658	1/1	0.88	0.43	69,69,69,69	0
56	MG	2a	1659	1/1	0.88	0.21	63,63,63,63	0
56	MG	2A	3660	1/1	0.88	0.12	69,69,69,69	0
56	MG	1a	1608	1/1	0.88	0.12	70,70,70,70	0
56	MG	1A	3430	1/1	0.88	0.08	45,45,45,45	0
56	MG	2a	1668	1/1	0.88	0.29	60,60,60,60	0
56	MG	1A	3514	1/1	0.88	0.15	53,53,53,53	0
56	MG	1a	1615	1/1	0.88	0.12	75,75,75,75	0
56	MG	1A	3638	1/1	0.88	0.16	74,74,74,74	0
56	MG	2a	1684	1/1	0.88	0.32	66,66,66,66	0
56	MG	2a	1689	1/1	0.88	0.29	71,71,71,71	0
56	MG	1A	3866	1/1	0.88	0.22	49,49,49,49	0
56	MG	1a	1710	1/1	0.88	0.11	78,78,78,78	0
56	MG	1x	104	1/1	0.88	0.36	70,70,70,70	0
56	MG	2a	1707	1/1	0.88	0.17	72,72,72,72	0
56	MG	1a	1631	1/1	0.88	0.19	62,62,62,62	0
56	MG	2A	3299	1/1	0.88	0.25	49,49,49,49	0
56	MG	2A	3683	1/1	0.88	0.10	48,48,48,48	0
56	MG	1A	3443	1/1	0.88	0.28	62,62,62,62	0
56	MG	2A	3691	1/1	0.88	0.14	74,74,74,74	0
56	MG	1a	1717	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3305	1/1	0.88	0.30	61,61,61,61	0
56	MG	1A	3454	1/1	0.88	0.21	62,62,62,62	0
56	MG	2A	3317	1/1	0.88	0.19	60,60,60,60	0
56	MG	2A	3033	1/1	0.88	0.18	52,52,52,52	0
56	MG	2A	3329	1/1	0.88	0.29	79,79,79,79	0
56	MG	1A	3781	1/1	0.88	0.10	33,33,33,33	0
56	MG	1A	3094	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3071	1/1	0.88	0.15	44,44,44,44	0
56	MG	1F	303	1/1	0.88	0.09	61,61,61,61	0
56	MG	1a	1644	1/1	0.88	0.18	68,68,68,68	0
56	MG	2a	1760	1/1	0.88	0.33	64,64,64,64	0
56	MG	1a	1731	1/1	0.88	0.40	66,66,66,66	0
56	MG	2A	3095	1/1	0.88	0.14	62,62,62,62	0
56	MG	1A	3467	1/1	0.88	0.14	68,68,68,68	0
56	MG	1a	1646	1/1	0.88	0.18	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	2A	3101	1/1	0.88	0.20	58,58,58,58	0
56	MG	2d	301	1/1	0.88	0.27	64,64,64,64	0
56	MG	2A	3373	1/1	0.88	0.25	60,60,60,60	0
56	MG	2A	3377	1/1	0.88	0.32	66,66,66,66	0
56	MG	2A	3746	1/1	0.88	0.13	69,69,69,69	0
56	MG	1a	1648	1/1	0.88	0.26	67,67,67,67	0
56	MG	2r	101	1/1	0.88	0.21	82,82,82,82	0
56	MG	2A	3383	1/1	0.88	0.23	72,72,72,72	0
56	MG	2A	3385	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3538	1/1	0.88	0.17	55,55,55,55	0
56	MG	2A	3110	1/1	0.88	0.17	53,53,53,53	0
56	MG	1A	4024	1/1	0.88	0.17	72,72,72,72	0
57	K	1A	3557	1/1	0.88	0.26	89,89,89,89	0
56	MG	1B	205	1/1	0.89	0.22	66,66,66,66	0
56	MG	2A	3132	1/1	0.89	0.14	59,59,59,59	0
56	MG	1A	3326	1/1	0.89	0.09	49,49,49,49	0
56	MG	2A	3336	1/1	0.89	0.09	76,76,76,76	0
56	MG	1A	3051	1/1	0.89	0.14	43,43,43,43	0
56	MG	2B	217	1/1	0.89	0.16	71,71,71,71	0
56	MG	1a	1616	1/1	0.89	0.10	75,75,75,75	0
56	MG	1a	1620	1/1	0.89	0.11	58,58,58,58	0
56	MG	1B	221	1/1	0.89	0.17	53,53,53,53	0
56	MG	2A	3663	1/1	0.89	0.13	62,62,62,62	0
56	MG	1a	1785	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3658	1/1	0.89	0.12	62,62,62,62	0
56	MG	2A	3166	1/1	0.89	0.20	62,62,62,62	0
56	MG	1B	226	1/1	0.89	0.16	61,61,61,61	0
56	MG	1A	3771	1/1	0.89	0.10	38,38,38,38	0
56	MG	1a	1803	1/1	0.89	0.22	63,63,63,63	0
56	MG	2A	3378	1/1	0.89	0.20	54,54,54,54	0
56	MG	1a	1804	1/1	0.89	0.11	58,58,58,58	0
56	MG	1A	3161	1/1	0.89	0.09	66,66,66,66	0
56	MG	2A	3199	1/1	0.89	0.21	61,61,61,61	0
56	MG	1a	1811	1/1	0.89	0.19	73,73,73,73	0
56	MG	2A	3204	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3026	1/1	0.89	0.12	44,44,44,44	0
56	MG	2A	3212	1/1	0.89	0.24	58,58,58,58	0
56	MG	2A	3214	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3416	1/1	0.89	0.30	61,61,61,61	0
56	MG	2A	3421	1/1	0.89	0.41	62,62,62,62	0
56	MG	2a	1637	1/1	0.89	0.23	56,56,56,56	0
56	MG	2a	1640	1/1	0.89	0.22	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1643	1/1	0.89	0.17	64,64,64,64	0
56	MG	1a	1818	1/1	0.89	0.10	72,72,72,72	0
56	MG	1A	3223	1/1	0.89	0.20	60,60,60,60	0
56	MG	1a	1712	1/1	0.89	0.20	59,59,59,59	0
56	MG	1e	204	1/1	0.89	0.21	83,83,83,83	0
56	MG	1A	4010	1/1	0.89	0.14	64,64,64,64	0
56	MG	1A	3172	1/1	0.89	0.29	57,57,57,57	0
56	MG	2A	3439	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3724	1/1	0.89	0.12	54,54,54,54	0
56	MG	2A	3727	1/1	0.89	0.11	72,72,72,72	0
56	MG	2A	3446	1/1	0.89	0.41	64,64,64,64	0
56	MG	2A	3246	1/1	0.89	0.19	65,65,65,65	0
56	MG	1A	3802	1/1	0.89	0.08	35,35,35,35	0
56	MG	1A	4022	1/1	0.89	0.14	56,56,56,56	0
56	MG	1A	3517	1/1	0.89	0.10	66,66,66,66	0
56	MG	1A	3520	1/1	0.89	0.18	44,44,44,44	0
56	MG	2A	3008	1/1	0.89	0.14	52,52,52,52	0
56	MG	1a	1650	1/1	0.89	0.18	58,58,58,58	0
56	MG	1A	3697	1/1	0.89	0.11	59,59,59,59	0
56	MG	1P	206	1/1	0.89	0.36	68,68,68,68	0
56	MG	2a	1696	1/1	0.89	0.18	80,80,80,80	0
56	MG	2A	3507	1/1	0.89	0.15	69,69,69,69	0
56	MG	2A	3514	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3516	1/1	0.89	0.13	58,58,58,58	0
56	MG	1a	1660	1/1	0.89	0.21	68,68,68,68	0
56	MG	2a	1719	1/1	0.89	0.17	54,54,54,54	0
56	MG	2A	3043	1/1	0.89	0.26	72,72,72,72	0
56	MG	1S	203	1/1	0.89	0.10	54,54,54,54	0
56	MG	2a	1724	1/1	0.89	0.16	82,82,82,82	0
56	MG	2A	3279	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3767	1/1	0.89	0.17	67,67,67,67	0
56	MG	2a	1732	1/1	0.89	0.24	61,61,61,61	0
56	MG	2a	1734	1/1	0.89	0.14	68,68,68,68	0
56	MG	2A	3058	1/1	0.89	0.18	66,66,66,66	0
56	MG	2A	3536	1/1	0.89	0.18	71,71,71,71	0
56	MG	2A	3542	1/1	0.89	0.11	42,42,42,42	0
56	MG	2a	1740	1/1	0.89	0.19	66,66,66,66	0
56	MG	2a	1745	1/1	0.89	0.21	67,67,67,67	0
56	MG	1A	4038	1/1	0.89	0.11	20,20,20,20	0
56	MG	1A	4039	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3792	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3601	1/1	0.89	0.24	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	3795	1/1	0.89	0.13	58,58,58,58	0
56	MG	1Y	202	1/1	0.89	0.07	60,60,60,60	0
56	MG	1A	3935	1/1	0.89	0.11	61,61,61,61	0
56	MG	1A	3942	1/1	0.89	0.12	65,65,65,65	0
56	MG	2A	3096	1/1	0.89	0.22	72,72,72,72	0
56	MG	2A	3834	1/1	0.89	0.11	41,41,41,41	0
56	MG	1A	3954	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3253	1/1	0.89	0.08	57,57,57,57	0
56	MG	2a	1775	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3527	1/1	0.89	0.27	60,60,60,60	0
56	MG	2d	302	1/1	0.89	0.07	73,73,73,73	0
56	MG	1A	3835	1/1	0.89	0.09	39,39,39,39	0
56	MG	1A	3531	1/1	0.89	0.36	70,70,70,70	0
56	MG	2A	3859	1/1	0.89	0.11	47,47,47,47	0
56	MG	1a	1761	1/1	0.89	0.18	69,69,69,69	0
56	MG	2q	202	1/1	0.89	0.23	77,77,77,77	0
56	MG	1A	3313	1/1	0.89	0.11	49,49,49,49	0
56	MG	2A	3595	1/1	0.89	0.14	65,65,65,65	0
56	MG	2t	201	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3599	1/1	0.89	0.11	51,51,51,51	0
56	MG	2A	3600	1/1	0.89	0.28	59,59,59,59	0
56	MG	2A	3318	1/1	0.89	0.25	74,74,74,74	0
56	MG	1a	1687	1/1	0.89	0.32	70,70,70,70	0
56	MG	2A	3617	1/1	0.89	0.24	77,77,77,77	0
56	MG	2A	3094	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	3516	1/1	0.90	0.17	84,84,84,84	0
56	MG	2A	3306	1/1	0.90	0.24	39,39,39,39	0
56	MG	2A	3308	1/1	0.90	0.16	59,59,59,59	0
56	MG	2A	3311	1/1	0.90	0.09	57,57,57,57	0
56	MG	1D	312	1/1	0.90	0.19	50,50,50,50	0
56	MG	1E	309	1/1	0.90	0.27	74,74,74,74	0
56	MG	1A	3844	1/1	0.90	0.23	60,60,60,60	0
56	MG	2E	305	1/1	0.90	0.07	30,30,30,30	0
56	MG	2A	3620	1/1	0.90	0.24	64,64,64,64	0
56	MG	1A	3845	1/1	0.90	0.12	58,58,58,58	0
56	MG	2R	202	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3326	1/1	0.90	0.23	63,63,63,63	0
56	MG	2T	203	1/1	0.90	0.15	72,72,72,72	0
56	MG	1F	304	1/1	0.90	0.13	50,50,50,50	0
56	MG	1A	3598	1/1	0.90	0.23	59,59,59,59	0
56	MG	1F	314	1/1	0.90	0.20	59,59,59,59	0
56	MG	2A	3333	1/1	0.90	0.15	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	28	101	1/1	0.90	0.18	67,67,67,67	0
56	MG	2a	1601	1/1	0.90	0.20	60,60,60,60	0
56	MG	1G	201	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3339	1/1	0.90	0.08	65,65,65,65	0
56	MG	1A	3332	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3404	1/1	0.90	0.10	54,54,54,54	0
56	MG	2a	1614	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3122	1/1	0.90	0.16	66,66,66,66	0
56	MG	1a	1763	1/1	0.90	0.08	64,64,64,64	0
56	MG	1O	203	1/1	0.90	0.28	69,69,69,69	0
56	MG	1A	3361	1/1	0.90	0.10	45,45,45,45	0
56	MG	1A	3212	1/1	0.90	0.17	61,61,61,61	0
56	MG	1A	3872	1/1	0.90	0.09	45,45,45,45	0
56	MG	2a	1632	1/1	0.90	0.21	58,58,58,58	0
56	MG	1Q	204	1/1	0.90	0.08	52,52,52,52	0
56	MG	2a	1636	1/1	0.90	0.26	56,56,56,56	0
56	MG	1A	3315	1/1	0.90	0.22	46,46,46,46	0
56	MG	1A	3884	1/1	0.90	0.16	72,72,72,72	0
56	MG	2A	3165	1/1	0.90	0.17	43,43,43,43	0
56	MG	2a	1647	1/1	0.90	0.22	70,70,70,70	0
56	MG	1V	206	1/1	0.90	0.06	51,51,51,51	0
56	MG	1A	3625	1/1	0.90	0.10	36,36,36,36	0
56	MG	2A	3168	1/1	0.90	0.26	67,67,67,67	0
56	MG	2a	1653	1/1	0.90	0.23	59,59,59,59	0
56	MG	1A	3249	1/1	0.90	0.16	65,65,65,65	0
56	MG	2A	3704	1/1	0.90	0.11	36,36,36,36	0
56	MG	2A	3171	1/1	0.90	0.16	48,48,48,48	0
56	MG	2A	3395	1/1	0.90	0.11	60,60,60,60	0
56	MG	1a	1792	1/1	0.90	0.16	56,56,56,56	0
56	MG	1A	3422	1/1	0.90	0.10	55,55,55,55	0
56	MG	2A	3403	1/1	0.90	0.10	56,56,56,56	0
56	MG	1a	1685	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3419	1/1	0.90	0.17	45,45,45,45	0
56	MG	1a	1686	1/1	0.90	0.27	72,72,72,72	0
56	MG	1A	3645	1/1	0.90	0.07	15,15,15,15	0
56	MG	2A	3201	1/1	0.90	0.20	55,55,55,55	0
56	MG	2A	3428	1/1	0.90	0.32	63,63,63,63	0
56	MG	12	101	1/1	0.90	0.09	48,48,48,48	0
56	MG	13	101	1/1	0.90	0.13	35,35,35,35	0
56	MG	1A	3783	1/1	0.90	0.13	37,37,37,37	0
56	MG	2A	3434	1/1	0.90	0.30	55,55,55,55	0
56	MG	2a	1703	1/1	0.90	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	3437	1/1	0.90	0.33	59,59,59,59	0
56	MG	1A	3424	1/1	0.90	0.13	59,59,59,59	0
56	MG	16	101	1/1	0.90	0.17	41,41,41,41	0
56	MG	2A	3217	1/1	0.90	0.08	56,56,56,56	0
56	MG	1A	4052	1/1	0.90	0.11	62,62,62,62	0
56	MG	1b	301	1/1	0.90	0.12	75,75,75,75	0
56	MG	2A	3231	1/1	0.90	0.30	65,65,65,65	0
56	MG	2A	3462	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3928	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3508	1/1	0.90	0.28	35,35,35,35	0
56	MG	2A	3487	1/1	0.90	0.15	59,59,59,59	0
56	MG	2a	1733	1/1	0.90	0.11	70,70,70,70	0
56	MG	1a	1706	1/1	0.90	0.25	67,67,67,67	0
56	MG	1a	1605	1/1	0.90	0.18	68,68,68,68	0
56	MG	2A	3503	1/1	0.90	0.15	58,58,58,58	0
56	MG	1a	1606	1/1	0.90	0.19	56,56,56,56	0
56	MG	1A	3085	1/1	0.90	0.24	43,43,43,43	0
56	MG	2A	3252	1/1	0.90	0.23	59,59,59,59	0
56	MG	2A	3786	1/1	0.90	0.25	61,61,61,61	0
56	MG	1x	105	1/1	0.90	0.22	69,69,69,69	0
56	MG	1A	3936	1/1	0.90	0.12	65,65,65,65	0
56	MG	2a	1751	1/1	0.90	0.21	68,68,68,68	0
56	MG	2a	1752	1/1	0.90	0.14	76,76,76,76	0
56	MG	2A	3002	1/1	0.90	0.32	55,55,55,55	0
56	MG	2A	3005	1/1	0.90	0.33	69,69,69,69	0
56	MG	2A	3524	1/1	0.90	0.09	37,37,37,37	0
56	MG	2A	3007	1/1	0.90	0.18	55,55,55,55	0
56	MG	2A	3820	1/1	0.90	0.11	51,51,51,51	0
56	MG	1A	4073	1/1	0.90	0.09	19,19,19,19	0
56	MG	2A	3268	1/1	0.90	0.10	78,78,78,78	0
56	MG	2A	3018	1/1	0.90	0.33	60,60,60,60	0
56	MG	2A	3841	1/1	0.90	0.17	55,55,55,55	0
56	MG	1A	3554	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3547	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3667	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3442	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3352	1/1	0.90	0.13	61,61,61,61	0
56	MG	1A	3688	1/1	0.90	0.08	42,42,42,42	0
56	MG	2A	3045	1/1	0.90	0.32	69,69,69,69	0
56	MG	1B	220	1/1	0.90	0.11	64,64,64,64	0
56	MG	1A	3579	1/1	0.90	0.09	49,49,49,49	0
56	MG	1A	3977	1/1	0.90	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3833	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3072	1/1	0.90	0.10	56,56,56,56	0
56	MG	1A	3580	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3981	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3584	1/1	0.90	0.11	50,50,50,50	0
56	MG	2B	210	1/1	0.90	0.08	68,68,68,68	0
56	MG	2A	3192	1/1	0.91	0.12	69,69,69,69	0
56	MG	1A	3499	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3440	1/1	0.91	0.24	53,53,53,53	0
56	MG	2A	3798	1/1	0.91	0.17	57,57,57,57	0
56	MG	1A	3921	1/1	0.91	0.15	48,48,48,48	0
56	MG	1A	3923	1/1	0.91	0.10	64,64,64,64	0
56	MG	1A	3745	1/1	0.91	0.17	44,44,44,44	0
56	MG	1A	3748	1/1	0.91	0.12	46,46,46,46	0
56	MG	2A	3460	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3461	1/1	0.91	0.25	55,55,55,55	0
56	MG	1A	3500	1/1	0.91	0.07	29,29,29,29	0
56	MG	1A	3754	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3479	1/1	0.91	0.23	65,65,65,65	0
56	MG	2A	3850	1/1	0.91	0.08	63,63,63,63	0
56	MG	1A	3757	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3944	1/1	0.91	0.18	60,60,60,60	0
56	MG	1D	304	1/1	0.91	0.29	41,41,41,41	0
56	MG	2A	3497	1/1	0.91	0.16	46,46,46,46	0
56	MG	1A	3952	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3866	1/1	0.91	0.13	47,47,47,47	0
56	MG	1a	1806	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	3953	1/1	0.91	0.35	50,50,50,50	0
56	MG	2A	3870	1/1	0.91	0.10	72,72,72,72	0
56	MG	2B	201	1/1	0.91	0.20	68,68,68,68	0
56	MG	1A	3501	1/1	0.91	0.11	61,61,61,61	0
56	MG	1A	3769	1/1	0.91	0.09	25,25,25,25	0
56	MG	1A	3503	1/1	0.91	0.08	47,47,47,47	0
56	MG	1A	3296	1/1	0.91	0.09	42,42,42,42	0
56	MG	1A	3507	1/1	0.91	0.19	45,45,45,45	0
56	MG	1a	1674	1/1	0.91	0.16	70,70,70,70	0
56	MG	1e	201	1/1	0.91	0.29	58,58,58,58	0
56	MG	2A	3526	1/1	0.91	0.07	33,33,33,33	0
56	MG	1e	203	1/1	0.91	0.11	57,57,57,57	0
56	MG	1A	3975	1/1	0.91	0.11	38,38,38,38	0
56	MG	1A	3091	1/1	0.91	0.14	48,48,48,48	0
56	MG	1N	203	1/1	0.91	0.07	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	1n	101	1/1	0.91	0.22	59,59,59,59	0
56	MG	1N	208	1/1	0.91	0.12	35,35,35,35	0
56	MG	1A	3509	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3366	1/1	0.91	0.10	43,43,43,43	0
56	MG	1A	3801	1/1	0.91	0.11	23,23,23,23	0
56	MG	2A	3271	1/1	0.91	0.37	67,67,67,67	0
56	MG	1x	107	1/1	0.91	0.20	72,72,72,72	0
56	MG	1A	3613	1/1	0.91	0.09	62,62,62,62	0
56	MG	2T	202	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3368	1/1	0.91	0.36	60,60,60,60	0
56	MG	1a	1688	1/1	0.91	0.30	72,72,72,72	0
56	MG	1A	3425	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3998	1/1	0.91	0.09	28,28,28,28	0
56	MG	23	102	1/1	0.91	0.17	59,59,59,59	0
56	MG	1A	3299	1/1	0.91	0.19	53,53,53,53	0
56	MG	1A	3643	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3818	1/1	0.91	0.08	37,37,37,37	0
56	MG	1A	3333	1/1	0.91	0.19	49,49,49,49	0
56	MG	2a	1604	1/1	0.91	0.33	67,67,67,67	0
56	MG	2A	3592	1/1	0.91	0.17	48,48,48,48	0
56	MG	2A	3594	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3292	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3031	1/1	0.91	0.10	64,64,64,64	0
56	MG	1A	3335	1/1	0.91	0.15	54,54,54,54	0
56	MG	2A	3042	1/1	0.91	0.27	66,66,66,66	0
56	MG	2A	3606	1/1	0.91	0.08	54,54,54,54	0
56	MG	2A	3607	1/1	0.91	0.13	66,66,66,66	0
56	MG	2a	1625	1/1	0.91	0.29	67,67,67,67	0
56	MG	2a	1626	1/1	0.91	0.16	55,55,55,55	0
56	MG	10	102	1/1	0.91	0.12	55,55,55,55	0
56	MG	2A	3303	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3448	1/1	0.91	0.18	66,66,66,66	0
56	MG	1A	4020	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3648	1/1	0.91	0.13	67,67,67,67	0
56	MG	2A	3635	1/1	0.91	0.12	41,41,41,41	0
56	MG	2A	3648	1/1	0.91	0.17	66,66,66,66	0
56	MG	2a	1642	1/1	0.91	0.27	67,67,67,67	0
56	MG	1A	3449	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3064	1/1	0.91	0.11	44,44,44,44	0
56	MG	2A	3654	1/1	0.91	0.17	70,70,70,70	0
56	MG	1A	3464	1/1	0.91	0.18	63,63,63,63	0
56	MG	1A	4034	1/1	0.91	0.10	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	3084	1/1	0.91	0.18	53,53,53,53	0
56	MG	2A	3319	1/1	0.91	0.18	62,62,62,62	0
56	MG	2a	1655	1/1	0.91	0.29	55,55,55,55	0
56	MG	18	103	1/1	0.91	0.09	54,54,54,54	0
56	MG	2A	3324	1/1	0.91	0.10	69,69,69,69	0
56	MG	2A	3325	1/1	0.91	0.39	72,72,72,72	0
56	MG	2a	1660	1/1	0.91	0.16	59,59,59,59	0
56	MG	1A	3248	1/1	0.91	0.13	56,56,56,56	0
56	MG	2A	3090	1/1	0.91	0.23	68,68,68,68	0
56	MG	2A	3093	1/1	0.91	0.12	53,53,53,53	0
56	MG	2A	3331	1/1	0.91	0.08	65,65,65,65	0
56	MG	2a	1674	1/1	0.91	0.20	65,65,65,65	0
56	MG	2a	1676	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3679	1/1	0.91	0.12	22,22,22,22	0
56	MG	2A	3676	1/1	0.91	0.15	64,64,64,64	0
56	MG	1a	1726	1/1	0.91	0.12	59,59,59,59	0
56	MG	2A	3334	1/1	0.91	0.28	70,70,70,70	0
56	MG	2a	1685	1/1	0.91	0.21	76,76,76,76	0
56	MG	1a	1603	1/1	0.91	0.10	55,55,55,55	0
56	MG	1A	3398	1/1	0.91	0.18	51,51,51,51	0
56	MG	2a	1691	1/1	0.91	0.32	59,59,59,59	0
56	MG	1A	4047	1/1	0.91	0.11	64,64,64,64	0
56	MG	2a	1693	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3344	1/1	0.91	0.25	51,51,51,51	0
56	MG	1A	3540	1/1	0.91	0.11	57,57,57,57	0
56	MG	2a	1699	1/1	0.91	0.23	61,61,61,61	0
56	MG	2a	1701	1/1	0.91	0.16	64,64,64,64	0
56	MG	2A	3103	1/1	0.91	0.24	54,54,54,54	0
56	MG	2A	3695	1/1	0.91	0.22	61,61,61,61	0
56	MG	2a	1708	1/1	0.91	0.15	53,53,53,53	0
56	MG	1A	3855	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	4051	1/1	0.91	0.11	36,36,36,36	0
56	MG	2A	3706	1/1	0.91	0.13	48,48,48,48	0
56	MG	1a	1610	1/1	0.91	0.15	73,73,73,73	0
56	MG	2A	3709	1/1	0.91	0.17	57,57,57,57	0
56	MG	2A	3364	1/1	0.91	0.16	72,72,72,72	0
56	MG	1a	1611	1/1	0.91	0.22	61,61,61,61	0
56	MG	1A	3306	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3368	1/1	0.91	0.08	62,62,62,62	0
56	MG	2A	3369	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3187	1/1	0.91	0.14	70,70,70,70	0
56	MG	2A	3721	1/1	0.91	0.11	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	1A	3543	1/1	0.91	0.11	69,69,69,69	0
56	MG	2A	3126	1/1	0.91	0.07	55,55,55,55	0
56	MG	2A	3726	1/1	0.91	0.13	51,51,51,51	0
56	MG	1a	1739	1/1	0.91	0.07	68,68,68,68	0
56	MG	2a	1742	1/1	0.91	0.21	56,56,56,56	0
56	MG	1a	1618	1/1	0.91	0.10	72,72,72,72	0
56	MG	1A	3266	1/1	0.91	0.12	53,53,53,53	0
56	MG	1a	1621	1/1	0.91	0.17	48,48,48,48	0
56	MG	1a	1623	1/1	0.91	0.21	63,63,63,63	0
56	MG	2A	3736	1/1	0.91	0.12	67,67,67,67	0
56	MG	1A	3566	1/1	0.91	0.10	39,39,39,39	0
56	MG	2A	3155	1/1	0.91	0.16	59,59,59,59	0
56	MG	2A	3158	1/1	0.91	0.11	47,47,47,47	0
56	MG	2A	3744	1/1	0.91	0.26	46,46,46,46	0
56	MG	2A	3397	1/1	0.91	0.11	72,72,72,72	0
56	MG	2A	3399	1/1	0.91	0.14	64,64,64,64	0
56	MG	1A	3495	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3163	1/1	0.91	0.40	71,71,71,71	0
56	MG	2A	3751	1/1	0.91	0.11	58,58,58,58	0
56	MG	2a	1772	1/1	0.91	0.20	78,78,78,78	0
56	MG	2A	3404	1/1	0.91	0.22	65,65,65,65	0
56	MG	2A	3405	1/1	0.91	0.17	61,61,61,61	0
56	MG	2a	1776	1/1	0.91	0.14	71,71,71,71	0
56	MG	2A	3755	1/1	0.91	0.14	66,66,66,66	0
56	MG	1a	1627	1/1	0.91	0.25	63,63,63,63	0
56	MG	1a	1630	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3712	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3572	1/1	0.91	0.20	58,58,58,58	0
56	MG	2l	201	1/1	0.91	0.11	70,70,70,70	0
56	MG	1A	3575	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3768	1/1	0.91	0.18	76,76,76,76	0
56	MG	1a	1772	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3774	1/1	0.91	0.09	81,81,81,81	0
56	MG	1B	209	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3173	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3176	1/1	0.91	0.13	68,68,68,68	0
56	MG	1A	3353	1/1	0.91	0.22	68,68,68,68	0
56	MG	2A	3185	1/1	0.91	0.08	53,53,53,53	0
56	MG	2A	3790	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3782	1/1	0.92	0.16	70,70,70,70	0
56	MG	1A	3896	1/1	0.92	0.12	52,52,52,52	0
56	MG	1a	1771	1/1	0.92	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3787	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3726	1/1	0.92	0.27	66,66,66,66	0
56	MG	1a	1774	1/1	0.92	0.12	63,63,63,63	0
56	MG	2A	3791	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3098	1/1	0.92	0.18	56,56,56,56	0
56	MG	2A	3436	1/1	0.92	0.14	52,52,52,52	0
56	MG	1B	203	1/1	0.92	0.22	51,51,51,51	0
56	MG	1A	3731	1/1	0.92	0.13	58,58,58,58	0
56	MG	2A	3806	1/1	0.92	0.14	70,70,70,70	0
56	MG	2A	3187	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3915	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3195	1/1	0.92	0.08	56,56,56,56	0
56	MG	2A	3447	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3822	1/1	0.92	0.17	40,40,40,40	0
56	MG	1B	210	1/1	0.92	0.08	46,46,46,46	0
56	MG	1a	1640	1/1	0.92	0.28	70,70,70,70	0
56	MG	2A	3838	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3840	1/1	0.92	0.08	74,74,74,74	0
56	MG	1a	1784	1/1	0.92	0.14	65,65,65,65	0
56	MG	1A	3151	1/1	0.92	0.23	34,34,34,34	0
56	MG	1A	3090	1/1	0.92	0.21	39,39,39,39	0
56	MG	2A	3849	1/1	0.92	0.10	70,70,70,70	0
56	MG	1a	1788	1/1	0.92	0.06	81,81,81,81	0
56	MG	2A	3205	1/1	0.92	0.09	46,46,46,46	0
56	MG	2A	3852	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3478	1/1	0.92	0.12	70,70,70,70	0
56	MG	1A	3751	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3483	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3211	1/1	0.92	0.16	64,64,64,64	0
56	MG	1a	1793	1/1	0.92	0.20	56,56,56,56	0
56	MG	1A	3457	1/1	0.92	0.11	69,69,69,69	0
56	MG	2A	3868	1/1	0.92	0.13	35,35,35,35	0
56	MG	2A	3494	1/1	0.92	0.20	62,62,62,62	0
56	MG	2A	3495	1/1	0.92	0.23	57,57,57,57	0
56	MG	1A	3462	1/1	0.92	0.20	56,56,56,56	0
56	MG	1B	225	1/1	0.92	0.08	46,46,46,46	0
56	MG	1A	3399	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3113	1/1	0.92	0.06	40,40,40,40	0
56	MG	2A	3225	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3230	1/1	0.92	0.11	52,52,52,52	0
56	MG	2B	208	1/1	0.92	0.33	66,66,66,66	0
56	MG	1a	1809	1/1	0.92	0.08	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	2A	3232	1/1	0.92	0.17	68,68,68,68	0
56	MG	1a	1651	1/1	0.92	0.07	54,54,54,54	0
56	MG	2B	212	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	3403	1/1	0.92	0.09	51,51,51,51	0
56	MG	2A	3241	1/1	0.92	0.23	64,64,64,64	0
56	MG	2A	3525	1/1	0.92	0.09	45,45,45,45	0
56	MG	1A	3469	1/1	0.92	0.18	58,58,58,58	0
56	MG	2A	3243	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3244	1/1	0.92	0.28	57,57,57,57	0
56	MG	1a	1816	1/1	0.92	0.08	64,64,64,64	0
56	MG	2E	302	1/1	0.92	0.26	57,57,57,57	0
56	MG	1a	1657	1/1	0.92	0.09	44,44,44,44	0
56	MG	2E	306	1/1	0.92	0.08	52,52,52,52	0
56	MG	1B	234	1/1	0.92	0.08	33,33,33,33	0
56	MG	2F	305	1/1	0.92	0.19	40,40,40,40	0
56	MG	1A	3470	1/1	0.92	0.23	46,46,46,46	0
56	MG	2P	201	1/1	0.92	0.10	56,56,56,56	0
56	MG	2Q	203	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3947	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3780	1/1	0.92	0.15	45,45,45,45	0
56	MG	2T	201	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3131	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3558	1/1	0.92	0.14	55,55,55,55	0
56	MG	1a	1667	1/1	0.92	0.22	78,78,78,78	0
56	MG	2A	3564	1/1	0.92	0.10	46,46,46,46	0
56	MG	1f	201	1/1	0.92	0.17	52,52,52,52	0
56	MG	2A	3566	1/1	0.92	0.07	44,44,44,44	0
56	MG	1k	201	1/1	0.92	0.13	56,56,56,56	0
56	MG	1E	310	1/1	0.92	0.11	29,29,29,29	0
56	MG	1A	3482	1/1	0.92	0.21	61,61,61,61	0
56	MG	2A	3576	1/1	0.92	0.17	58,58,58,58	0
56	MG	1E	314	1/1	0.92	0.10	61,61,61,61	0
56	MG	2a	1606	1/1	0.92	0.20	54,54,54,54	0
56	MG	2a	1607	1/1	0.92	0.38	59,59,59,59	0
56	MG	1A	3539	1/1	0.92	0.22	55,55,55,55	0
56	MG	2A	3275	1/1	0.92	0.25	65,65,65,65	0
56	MG	1A	3790	1/1	0.92	0.14	60,60,60,60	0
56	MG	1x	101	1/1	0.92	0.08	64,64,64,64	0
56	MG	1x	102	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3281	1/1	0.92	0.11	55,55,55,55	0
56	MG	2a	1618	1/1	0.92	0.16	64,64,64,64	0
56	MG	2a	1621	1/1	0.92	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	3593	1/1	0.92	0.14	57,57,57,57	0
56	MG	1F	306	1/1	0.92	0.08	33,33,33,33	0
56	MG	1A	3965	1/1	0.92	0.07	72,72,72,72	0
56	MG	2A	3598	1/1	0.92	0.20	62,62,62,62	0
56	MG	1A	3486	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3654	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3602	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3972	1/1	0.92	0.08	54,54,54,54	0
56	MG	2a	1635	1/1	0.92	0.24	52,52,52,52	0
56	MG	2A	3289	1/1	0.92	0.27	69,69,69,69	0
56	MG	2A	3004	1/1	0.92	0.23	49,49,49,49	0
56	MG	1N	201	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3612	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3312	1/1	0.92	0.09	38,38,38,38	0
56	MG	2a	1645	1/1	0.92	0.21	69,69,69,69	0
56	MG	2A	3297	1/1	0.92	0.22	71,71,71,71	0
56	MG	1A	3414	1/1	0.92	0.21	53,53,53,53	0
56	MG	2A	3621	1/1	0.92	0.07	37,37,37,37	0
56	MG	1A	3807	1/1	0.92	0.06	22,22,22,22	0
56	MG	2A	3629	1/1	0.92	0.18	37,37,37,37	0
56	MG	1A	3662	1/1	0.92	0.15	47,47,47,47	0
56	MG	2A	3637	1/1	0.92	0.14	54,54,54,54	0
56	MG	2a	1656	1/1	0.92	0.40	72,72,72,72	0
56	MG	1A	3257	1/1	0.92	0.12	63,63,63,63	0
56	MG	1A	3665	1/1	0.92	0.06	19,19,19,19	0
56	MG	1A	3545	1/1	0.92	0.32	38,38,38,38	0
56	MG	1A	3986	1/1	0.92	0.09	38,38,38,38	0
56	MG	2A	3307	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3039	1/1	0.92	0.18	62,62,62,62	0
56	MG	2a	1666	1/1	0.92	0.19	56,56,56,56	0
56	MG	2A	3041	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3312	1/1	0.92	0.17	72,72,72,72	0
56	MG	2a	1669	1/1	0.92	0.12	68,68,68,68	0
56	MG	1S	201	1/1	0.92	0.28	46,46,46,46	0
56	MG	1a	1699	1/1	0.92	0.26	56,56,56,56	0
56	MG	2a	1677	1/1	0.92	0.34	66,66,66,66	0
56	MG	1S	202	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	1701	1/1	0.92	0.47	70,70,70,70	0
56	MG	2a	1680	1/1	0.92	0.13	63,63,63,63	0
56	MG	2A	3053	1/1	0.92	0.22	60,60,60,60	0
56	MG	2A	3056	1/1	0.92	0.19	66,66,66,66	0
56	MG	1A	3988	1/1	0.92	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1686	1/1	0.92	0.29	61,61,61,61	0
56	MG	1A	3674	1/1	0.92	0.07	33,33,33,33	0
56	MG	2A	3328	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3065	1/1	0.92	0.20	47,47,47,47	0
56	MG	1A	3678	1/1	0.92	0.05	21,21,21,21	0
56	MG	1A	3552	1/1	0.92	0.12	45,45,45,45	0
56	MG	1A	3834	1/1	0.92	0.12	35,35,35,35	0
56	MG	2A	3684	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3497	1/1	0.92	0.13	36,36,36,36	0
56	MG	2a	1700	1/1	0.92	0.22	59,59,59,59	0
56	MG	1A	3563	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	4011	1/1	0.92	0.11	42,42,42,42	0
56	MG	2A	3338	1/1	0.92	0.12	73,73,73,73	0
56	MG	1A	3838	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3696	1/1	0.92	0.08	74,74,74,74	0
56	MG	2A	3698	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3340	1/1	0.92	0.20	61,61,61,61	0
56	MG	1a	1718	1/1	0.92	0.31	66,66,66,66	0
56	MG	2A	3705	1/1	0.92	0.10	46,46,46,46	0
56	MG	1a	1720	1/1	0.92	0.12	52,52,52,52	0
56	MG	2A	3346	1/1	0.92	0.28	46,46,46,46	0
56	MG	2A	3350	1/1	0.92	0.12	54,54,54,54	0
56	MG	2a	1727	1/1	0.92	0.11	81,81,81,81	0
56	MG	2A	3352	1/1	0.92	0.19	60,60,60,60	0
56	MG	1A	4013	1/1	0.92	0.07	50,50,50,50	0
56	MG	1a	1724	1/1	0.92	0.14	64,64,64,64	0
56	MG	1A	3841	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3359	1/1	0.92	0.21	60,60,60,60	0
56	MG	1A	3263	1/1	0.92	0.25	52,52,52,52	0
56	MG	2A	3361	1/1	0.92	0.26	51,51,51,51	0
56	MG	15	108	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	3226	1/1	0.92	0.20	51,51,51,51	0
56	MG	2a	1743	1/1	0.92	0.17	63,63,63,63	0
56	MG	2A	3104	1/1	0.92	0.15	65,65,65,65	0
56	MG	1A	3367	1/1	0.92	0.20	53,53,53,53	0
56	MG	1A	3848	1/1	0.92	0.18	41,41,41,41	0
56	MG	2a	1749	1/1	0.92	0.23	56,56,56,56	0
56	MG	1A	3231	1/1	0.92	0.10	33,33,33,33	0
56	MG	2A	3371	1/1	0.92	0.20	61,61,61,61	0
56	MG	1A	3701	1/1	0.92	0.09	43,43,43,43	0
56	MG	2a	1753	1/1	0.92	0.13	66,66,66,66	0
56	MG	2A	3375	1/1	0.92	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1756	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	4036	1/1	0.92	0.12	33,33,33,33	0
56	MG	2A	3738	1/1	0.92	0.12	56,56,56,56	0
56	MG	2A	3118	1/1	0.92	0.18	58,58,58,58	0
56	MG	1A	3267	1/1	0.92	0.27	48,48,48,48	0
56	MG	2A	3121	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3291	1/1	0.92	0.10	44,44,44,44	0
56	MG	2a	1767	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	4043	1/1	0.92	0.10	56,56,56,56	0
56	MG	2a	1771	1/1	0.92	0.20	59,59,59,59	0
56	MG	2A	3129	1/1	0.92	0.12	62,62,62,62	0
56	MG	2a	1773	1/1	0.92	0.29	75,75,75,75	0
56	MG	2A	3392	1/1	0.92	0.26	71,71,71,71	0
56	MG	1A	3440	1/1	0.92	0.09	53,53,53,53	0
56	MG	1A	3867	1/1	0.92	0.16	31,31,31,31	0
56	MG	1A	3713	1/1	0.92	0.08	56,56,56,56	0
56	MG	1A	3870	1/1	0.92	0.10	37,37,37,37	0
56	MG	2A	3756	1/1	0.92	0.12	52,52,52,52	0
56	MG	2A	3757	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3871	1/1	0.92	0.11	43,43,43,43	0
56	MG	1A	3583	1/1	0.92	0.11	39,39,39,39	0
56	MG	1A	3385	1/1	0.92	0.29	24,24,24,24	0
56	MG	1A	3067	1/1	0.92	0.11	56,56,56,56	0
56	MG	1a	1756	1/1	0.92	0.20	71,71,71,71	0
56	MG	1A	4063	1/1	0.92	0.08	22,22,22,22	0
56	MG	1A	3885	1/1	0.92	0.18	44,44,44,44	0
56	MG	1a	1762	1/1	0.92	0.21	78,78,78,78	0
56	MG	2A	3777	1/1	0.92	0.08	58,58,58,58	0
56	MG	1A	3724	1/1	0.92	0.10	43,43,43,43	0
56	MG	2A	3779	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	4069	1/1	0.92	0.13	56,56,56,56	0
56	MG	2A	3435	1/1	0.93	0.20	59,59,59,59	0
56	MG	1A	3483	1/1	0.93	0.18	49,49,49,49	0
56	MG	1A	4017	1/1	0.93	0.08	41,41,41,41	0
56	MG	1A	4018	1/1	0.93	0.09	73,73,73,73	0
56	MG	2A	3188	1/1	0.93	0.15	75,75,75,75	0
56	MG	2A	3796	1/1	0.93	0.12	81,81,81,81	0
56	MG	1A	3270	1/1	0.93	0.21	59,59,59,59	0
56	MG	2A	3801	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3803	1/1	0.93	0.13	56,56,56,56	0
56	MG	2A	3194	1/1	0.93	0.32	68,68,68,68	0
56	MG	2A	3809	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3272	1/1	0.93	0.27	55,55,55,55	0
56	MG	2A	3450	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	3839	1/1	0.93	0.10	70,70,70,70	0
56	MG	1A	3491	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	4025	1/1	0.93	0.07	38,38,38,38	0
56	MG	2A	3457	1/1	0.93	0.07	54,54,54,54	0
56	MG	1A	4030	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	4032	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3339	1/1	0.93	0.06	33,33,33,33	0
56	MG	1A	3410	1/1	0.93	0.16	53,53,53,53	0
56	MG	2A	3466	1/1	0.93	0.08	51,51,51,51	0
56	MG	2A	3844	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3469	1/1	0.93	0.12	72,72,72,72	0
56	MG	2A	3473	1/1	0.93	0.09	68,68,68,68	0
56	MG	2A	3477	1/1	0.93	0.18	60,60,60,60	0
56	MG	2A	3208	1/1	0.93	0.08	65,65,65,65	0
56	MG	1A	3700	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3340	1/1	0.93	0.06	38,38,38,38	0
56	MG	2A	3854	1/1	0.93	0.10	35,35,35,35	0
56	MG	1A	3274	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3704	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3286	1/1	0.93	0.32	34,34,34,34	0
56	MG	2A	3864	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3350	1/1	0.93	0.24	54,54,54,54	0
56	MG	2A	3218	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3859	1/1	0.93	0.10	39,39,39,39	0
56	MG	2A	3220	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3863	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3223	1/1	0.93	0.17	69,69,69,69	0
56	MG	1A	3864	1/1	0.93	0.10	40,40,40,40	0
56	MG	1a	1798	1/1	0.93	0.16	53,53,53,53	0
56	MG	2A	3510	1/1	0.93	0.13	25,25,25,25	0
56	MG	1a	1800	1/1	0.93	0.19	62,62,62,62	0
56	MG	1a	1628	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3016	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3502	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3520	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3715	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3423	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3099	1/1	0.93	0.19	41,41,41,41	0
56	MG	2B	214	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3587	1/1	0.93	0.26	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	3529	1/1	0.93	0.06	32,32,32,32	0
56	MG	2A	3530	1/1	0.93	0.10	62,62,62,62	0
56	MG	2B	218	1/1	0.93	0.08	65,65,65,65	0
56	MG	1A	3589	1/1	0.93	0.12	45,45,45,45	0
56	MG	1a	1642	1/1	0.93	0.17	60,60,60,60	0
56	MG	1a	1820	1/1	0.93	0.23	62,62,62,62	0
56	MG	2A	3539	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	4072	1/1	0.93	0.09	58,58,58,58	0
56	MG	2A	3543	1/1	0.93	0.09	44,44,44,44	0
56	MG	2A	3544	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3546	1/1	0.93	0.07	34,34,34,34	0
56	MG	2A	3253	1/1	0.93	0.10	57,57,57,57	0
56	MG	2O	201	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3878	1/1	0.93	0.11	47,47,47,47	0
56	MG	2Q	201	1/1	0.93	0.17	59,59,59,59	0
56	MG	1A	4074	1/1	0.93	0.13	49,49,49,49	0
56	MG	1b	302	1/1	0.93	0.17	80,80,80,80	0
56	MG	1A	4080	1/1	0.93	0.10	36,36,36,36	0
56	MG	1a	1647	1/1	0.93	0.12	73,73,73,73	0
56	MG	1A	3590	1/1	0.93	0.17	33,33,33,33	0
56	MG	1A	3729	1/1	0.93	0.12	46,46,46,46	0
56	MG	2W	201	1/1	0.93	0.34	52,52,52,52	0
56	MG	1A	3591	1/1	0.93	0.08	32,32,32,32	0
56	MG	2A	3567	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3270	1/1	0.93	0.10	58,58,58,58	0
56	MG	20	101	1/1	0.93	0.13	75,75,75,75	0
56	MG	23	101	1/1	0.93	0.41	62,62,62,62	0
56	MG	2A	3569	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3889	1/1	0.93	0.10	49,49,49,49	0
56	MG	25	103	1/1	0.93	0.15	60,60,60,60	0
56	MG	1A	3892	1/1	0.93	0.13	43,43,43,43	0
56	MG	2A	3575	1/1	0.93	0.11	34,34,34,34	0
56	MG	2a	1602	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3736	1/1	0.93	0.18	60,60,60,60	0
56	MG	1A	3898	1/1	0.93	0.11	55,55,55,55	0
56	MG	2a	1605	1/1	0.93	0.11	60,60,60,60	0
56	MG	1A	3904	1/1	0.93	0.10	36,36,36,36	0
56	MG	1A	3739	1/1	0.93	0.09	53,53,53,53	0
56	MG	2A	3583	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	3743	1/1	0.93	0.10	51,51,51,51	0
56	MG	2a	1611	1/1	0.93	0.10	46,46,46,46	0
56	MG	1B	223	1/1	0.93	0.11	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	3593	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3237	1/1	0.93	0.07	59,59,59,59	0
56	MG	1x	111	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3429	1/1	0.93	0.17	49,49,49,49	0
56	MG	1A	3600	1/1	0.93	0.15	52,52,52,52	0
56	MG	2a	1622	1/1	0.93	0.33	49,49,49,49	0
56	MG	1a	1671	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	3192	1/1	0.93	0.28	35,35,35,35	0
56	MG	2A	3294	1/1	0.93	0.09	73,73,73,73	0
56	MG	1A	3198	1/1	0.93	0.25	31,31,31,31	0
56	MG	2A	3604	1/1	0.93	0.14	69,69,69,69	0
56	MG	1A	3093	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3013	1/1	0.93	0.07	43,43,43,43	0
56	MG	2a	1633	1/1	0.93	0.19	62,62,62,62	0
56	MG	2A	3017	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3300	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3611	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3933	1/1	0.93	0.11	26,26,26,26	0
56	MG	2A	3615	1/1	0.93	0.16	62,62,62,62	0
56	MG	2A	3302	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3760	1/1	0.93	0.21	44,44,44,44	0
56	MG	2A	3023	1/1	0.93	0.33	57,57,57,57	0
56	MG	2a	1646	1/1	0.93	0.35	59,59,59,59	0
56	MG	1D	310	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3765	1/1	0.93	0.11	22,22,22,22	0
56	MG	1D	314	1/1	0.93	0.11	31,31,31,31	0
56	MG	2A	3630	1/1	0.93	0.12	41,41,41,41	0
56	MG	1a	1684	1/1	0.93	0.23	58,58,58,58	0
56	MG	2A	3310	1/1	0.93	0.33	62,62,62,62	0
56	MG	2A	3639	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3612	1/1	0.93	0.10	23,23,23,23	0
56	MG	1A	3088	1/1	0.93	0.15	28,28,28,28	0
56	MG	2A	3313	1/1	0.93	0.11	60,60,60,60	0
56	MG	1E	311	1/1	0.93	0.09	26,26,26,26	0
56	MG	1A	3209	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3776	1/1	0.93	0.09	26,26,26,26	0
56	MG	2A	3657	1/1	0.93	0.09	59,59,59,59	0
56	MG	1E	316	1/1	0.93	0.07	58,58,58,58	0
56	MG	1A	3379	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3661	1/1	0.93	0.09	64,64,64,64	0
56	MG	2A	3662	1/1	0.93	0.13	43,43,43,43	0
56	MG	2a	1671	1/1	0.93	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1672	1/1	0.93	0.19	69,69,69,69	0
56	MG	2a	1673	1/1	0.93	0.21	56,56,56,56	0
56	MG	2A	3323	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3055	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3210	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3258	1/1	0.93	0.09	60,60,60,60	0
56	MG	2A	3059	1/1	0.93	0.23	54,54,54,54	0
56	MG	2A	3061	1/1	0.93	0.08	46,46,46,46	0
56	MG	1F	307	1/1	0.93	0.09	40,40,40,40	0
56	MG	2a	1682	1/1	0.93	0.18	62,62,62,62	0
56	MG	1a	1698	1/1	0.93	0.16	62,62,62,62	0
56	MG	1A	3958	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3786	1/1	0.93	0.11	27,27,27,27	0
56	MG	2a	1687	1/1	0.93	0.24	58,58,58,58	0
56	MG	1A	3526	1/1	0.93	0.21	43,43,43,43	0
56	MG	2A	3335	1/1	0.93	0.17	63,63,63,63	0
56	MG	2A	3682	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3078	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3082	1/1	0.93	0.14	54,54,54,54	0
56	MG	1A	3461	1/1	0.93	0.09	54,54,54,54	0
56	MG	2a	1695	1/1	0.93	0.23	62,62,62,62	0
56	MG	1a	1703	1/1	0.93	0.31	67,67,67,67	0
56	MG	2a	1698	1/1	0.93	0.25	64,64,64,64	0
56	MG	1a	1704	1/1	0.93	0.28	52,52,52,52	0
56	MG	2A	3693	1/1	0.93	0.07	68,68,68,68	0
56	MG	1A	3528	1/1	0.93	0.17	43,43,43,43	0
56	MG	1A	3969	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3347	1/1	0.93	0.20	57,57,57,57	0
56	MG	2A	3697	1/1	0.93	0.14	35,35,35,35	0
56	MG	1A	3796	1/1	0.93	0.14	47,47,47,47	0
56	MG	1a	1709	1/1	0.93	0.26	69,69,69,69	0
56	MG	2A	3701	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3800	1/1	0.93	0.10	16,16,16,16	0
56	MG	2A	3355	1/1	0.93	0.12	62,62,62,62	0
56	MG	1O	202	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3122	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3390	1/1	0.93	0.09	54,54,54,54	0
56	MG	2a	1726	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3102	1/1	0.93	0.08	29,29,29,29	0
56	MG	2a	1728	1/1	0.93	0.17	54,54,54,54	0
56	MG	2a	1729	1/1	0.93	0.11	62,62,62,62	0
56	MG	1A	3391	1/1	0.93	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	1731	1/1	0.93	0.15	66,66,66,66	0
56	MG	1A	3536	1/1	0.93	0.22	59,59,59,59	0
56	MG	2A	3715	1/1	0.93	0.15	62,62,62,62	0
56	MG	2A	3363	1/1	0.93	0.08	68,68,68,68	0
56	MG	1Q	201	1/1	0.93	0.23	37,37,37,37	0
56	MG	2a	1736	1/1	0.93	0.17	61,61,61,61	0
56	MG	1A	3466	1/1	0.93	0.27	62,62,62,62	0
56	MG	1A	3222	1/1	0.93	0.10	43,43,43,43	0
56	MG	2A	3113	1/1	0.93	0.23	62,62,62,62	0
56	MG	1A	3983	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3813	1/1	0.93	0.06	42,42,42,42	0
56	MG	2a	1744	1/1	0.93	0.27	59,59,59,59	0
56	MG	2A	3116	1/1	0.93	0.32	60,60,60,60	0
56	MG	2A	3117	1/1	0.93	0.17	48,48,48,48	0
56	MG	1T	202	1/1	0.93	0.14	63,63,63,63	0
56	MG	1U	203	1/1	0.93	0.14	43,43,43,43	0
56	MG	1a	1729	1/1	0.93	0.09	54,54,54,54	0
56	MG	2A	3380	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3265	1/1	0.93	0.15	74,74,74,74	0
56	MG	2A	3123	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3386	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3387	1/1	0.93	0.23	50,50,50,50	0
56	MG	1A	3987	1/1	0.93	0.07	64,64,64,64	0
56	MG	2A	3390	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3817	1/1	0.93	0.24	61,61,61,61	0
56	MG	1W	207	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3050	1/1	0.93	0.11	15,15,15,15	0
56	MG	1A	3991	1/1	0.93	0.13	27,27,27,27	0
56	MG	1Z	302	1/1	0.93	0.13	49,49,49,49	0
56	MG	1A	3822	1/1	0.93	0.07	27,27,27,27	0
56	MG	2A	3398	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3825	1/1	0.93	0.16	42,42,42,42	0
56	MG	11	104	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	4004	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3826	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3162	1/1	0.93	0.12	46,46,46,46	0
56	MG	2A	3413	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3414	1/1	0.93	0.18	50,50,50,50	0
56	MG	1a	1742	1/1	0.93	0.22	62,62,62,62	0
56	MG	2A	3771	1/1	0.93	0.08	68,68,68,68	0
56	MG	2A	3417	1/1	0.93	0.31	56,56,56,56	0
56	MG	13	104	1/1	0.93	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	3775	1/1	0.93	0.08	61,61,61,61	0
56	MG	2q	201	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3420	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3668	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3175	1/1	0.93	0.06	35,35,35,35	0
56	MG	1a	1748	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3831	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3336	1/1	0.93	0.22	46,46,46,46	0
56	MG	2x	102	1/1	0.93	0.26	61,61,61,61	0
56	MG	1a	1759	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	3544	1/1	0.93	0.18	63,63,63,63	0
56	MG	18	101	1/1	0.93	0.21	55,55,55,55	0
56	MG	1A	3428	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3345	1/1	0.94	0.19	45,45,45,45	0
56	MG	2A	3175	1/1	0.94	0.16	48,48,48,48	0
56	MG	1A	3518	1/1	0.94	0.27	47,47,47,47	0
56	MG	1A	3519	1/1	0.94	0.16	55,55,55,55	0
56	MG	2A	3184	1/1	0.94	0.27	63,63,63,63	0
56	MG	1a	1765	1/1	0.94	0.08	67,67,67,67	0
56	MG	2A	3442	1/1	0.94	0.10	40,40,40,40	0
56	MG	2A	3799	1/1	0.94	0.15	77,77,77,77	0
56	MG	2A	3443	1/1	0.94	0.35	54,54,54,54	0
56	MG	2A	3444	1/1	0.94	0.12	46,46,46,46	0
56	MG	2A	3804	1/1	0.94	0.13	67,67,67,67	0
56	MG	2A	3805	1/1	0.94	0.06	44,44,44,44	0
56	MG	2A	3445	1/1	0.94	0.33	59,59,59,59	0
56	MG	1A	3006	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3811	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3813	1/1	0.94	0.07	42,42,42,42	0
56	MG	1a	1768	1/1	0.94	0.11	66,66,66,66	0
56	MG	2A	3449	1/1	0.94	0.27	54,54,54,54	0
56	MG	1A	3431	1/1	0.94	0.06	51,51,51,51	0
56	MG	1a	1770	1/1	0.94	0.07	70,70,70,70	0
56	MG	2A	3452	1/1	0.94	0.24	48,48,48,48	0
56	MG	1A	3434	1/1	0.94	0.18	62,62,62,62	0
56	MG	2A	3196	1/1	0.94	0.26	60,60,60,60	0
56	MG	2A	3835	1/1	0.94	0.08	48,48,48,48	0
56	MG	2A	3456	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3671	1/1	0.94	0.07	26,26,26,26	0
56	MG	1A	3435	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3436	1/1	0.94	0.17	29,29,29,29	0
56	MG	1a	1777	1/1	0.94	0.17	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	3463	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3846	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3529	1/1	0.94	0.23	42,42,42,42	0
56	MG	1a	1604	1/1	0.94	0.14	74,74,74,74	0
56	MG	2A	3467	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3468	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3152	1/1	0.94	0.14	31,31,31,31	0
56	MG	2A	3206	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3474	1/1	0.94	0.21	57,57,57,57	0
56	MG	1A	3009	1/1	0.94	0.10	28,28,28,28	0
56	MG	2A	3209	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3861	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	4031	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3480	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3481	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3356	1/1	0.94	0.08	50,50,50,50	0
56	MG	1A	3445	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3485	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3290	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3052	1/1	0.94	0.09	25,25,25,25	0
56	MG	2A	3493	1/1	0.94	0.25	61,61,61,61	0
56	MG	1A	3856	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3168	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	4041	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3500	1/1	0.94	0.13	55,55,55,55	0
56	MG	1a	1617	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3861	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3862	1/1	0.94	0.10	34,34,34,34	0
56	MG	2A	3224	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3455	1/1	0.94	0.24	59,59,59,59	0
56	MG	2A	3229	1/1	0.94	0.29	44,44,44,44	0
56	MG	1A	3105	1/1	0.94	0.27	64,64,64,64	0
56	MG	1A	3234	1/1	0.94	0.06	42,42,42,42	0
56	MG	1a	1808	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3708	1/1	0.94	0.06	23,23,23,23	0
56	MG	2A	3237	1/1	0.94	0.12	58,58,58,58	0
56	MG	2A	3522	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3868	1/1	0.94	0.10	26,26,26,26	0
56	MG	2D	303	1/1	0.94	0.09	53,53,53,53	0
56	MG	2E	301	1/1	0.94	0.12	61,61,61,61	0
56	MG	1A	4057	1/1	0.94	0.07	54,54,54,54	0
56	MG	2E	303	1/1	0.94	0.21	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	1a	1629	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3372	1/1	0.94	0.09	46,46,46,46	0
56	MG	2E	307	1/1	0.94	0.10	31,31,31,31	0
56	MG	1A	3235	1/1	0.94	0.08	56,56,56,56	0
56	MG	2F	304	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3547	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3550	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3248	1/1	0.94	0.06	60,60,60,60	0
56	MG	1a	1822	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3251	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	3173	1/1	0.94	0.18	45,45,45,45	0
56	MG	2R	201	1/1	0.94	0.20	64,64,64,64	0
56	MG	1a	1639	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3875	1/1	0.94	0.13	30,30,30,30	0
56	MG	2A	3258	1/1	0.94	0.14	69,69,69,69	0
56	MG	1A	4070	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3548	1/1	0.94	0.09	42,42,42,42	0
56	MG	2A	3550	1/1	0.94	0.17	49,49,49,49	0
56	MG	1e	202	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3876	1/1	0.94	0.11	41,41,41,41	0
56	MG	2X	101	1/1	0.94	0.10	72,72,72,72	0
56	MG	1A	3244	1/1	0.94	0.23	35,35,35,35	0
56	MG	1A	3879	1/1	0.94	0.12	25,25,25,25	0
56	MG	1f	202	1/1	0.94	0.26	64,64,64,64	0
56	MG	1A	3561	1/1	0.94	0.11	33,33,33,33	0
56	MG	1A	4081	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	4082	1/1	0.94	0.07	42,42,42,42	0
56	MG	25	105	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3311	1/1	0.94	0.08	48,48,48,48	0
56	MG	28	102	1/1	0.94	0.23	61,61,61,61	0
56	MG	28	103	1/1	0.94	0.16	57,57,57,57	0
56	MG	1A	3246	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3053	1/1	0.94	0.16	28,28,28,28	0
56	MG	2A	3277	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3570	1/1	0.94	0.21	44,44,44,44	0
56	MG	1B	207	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3730	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	3471	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3900	1/1	0.94	0.25	39,39,39,39	0
56	MG	1x	110	1/1	0.94	0.12	66,66,66,66	0
56	MG	2A	3285	1/1	0.94	0.14	67,67,67,67	0
56	MG	2A	3584	1/1	0.94	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	2a	1613	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3574	1/1	0.94	0.24	37,37,37,37	0
56	MG	1A	3476	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3907	1/1	0.94	0.17	42,42,42,42	0
56	MG	2a	1617	1/1	0.94	0.15	60,60,60,60	0
56	MG	2A	3003	1/1	0.94	0.25	53,53,53,53	0
56	MG	2A	3291	1/1	0.94	0.07	53,53,53,53	0
56	MG	1a	1665	1/1	0.94	0.14	70,70,70,70	0
56	MG	1B	222	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3576	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3577	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3011	1/1	0.94	0.13	42,42,42,42	0
56	MG	2a	1629	1/1	0.94	0.16	58,58,58,58	0
56	MG	1a	1669	1/1	0.94	0.10	65,65,65,65	0
56	MG	1A	3479	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3750	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3314	1/1	0.94	0.22	52,52,52,52	0
56	MG	1a	1673	1/1	0.94	0.09	80,80,80,80	0
56	MG	2A	3609	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3920	1/1	0.94	0.07	37,37,37,37	0
56	MG	1A	3481	1/1	0.94	0.19	48,48,48,48	0
56	MG	1B	233	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3032	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3117	1/1	0.94	0.07	38,38,38,38	0
56	MG	2A	3036	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3755	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3932	1/1	0.94	0.06	43,43,43,43	0
56	MG	1A	3316	1/1	0.94	0.20	52,52,52,52	0
56	MG	2A	3627	1/1	0.94	0.20	51,51,51,51	0
56	MG	1a	1683	1/1	0.94	0.11	61,61,61,61	0
56	MG	2a	1652	1/1	0.94	0.31	53,53,53,53	0
56	MG	2A	3316	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3631	1/1	0.94	0.06	32,32,32,32	0
56	MG	2A	3634	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3044	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3636	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3485	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3048	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3641	1/1	0.94	0.16	62,62,62,62	0
56	MG	2a	1663	1/1	0.94	0.19	62,62,62,62	0
56	MG	2A	3646	1/1	0.94	0.22	57,57,57,57	0
56	MG	1A	3395	1/1	0.94	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3649	1/1	0.94	0.12	61,61,61,61	0
56	MG	1E	305	1/1	0.94	0.12	29,29,29,29	0
56	MG	1A	3764	1/1	0.94	0.18	42,42,42,42	0
56	MG	1A	3939	1/1	0.94	0.11	54,54,54,54	0
56	MG	2a	1670	1/1	0.94	0.21	55,55,55,55	0
56	MG	2A	3057	1/1	0.94	0.28	69,69,69,69	0
56	MG	1A	3396	1/1	0.94	0.17	52,52,52,52	0
56	MG	1a	1691	1/1	0.94	0.10	74,74,74,74	0
56	MG	1A	3943	1/1	0.94	0.07	46,46,46,46	0
56	MG	2a	1675	1/1	0.94	0.27	58,58,58,58	0
56	MG	2A	3062	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3488	1/1	0.94	0.30	51,51,51,51	0
56	MG	1A	3318	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	3948	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3949	1/1	0.94	0.06	32,32,32,32	0
56	MG	1A	3774	1/1	0.94	0.08	17,17,17,17	0
56	MG	2A	3075	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3492	1/1	0.94	0.26	50,50,50,50	0
56	MG	2A	3081	1/1	0.94	0.21	54,54,54,54	0
56	MG	1A	3596	1/1	0.94	0.23	51,51,51,51	0
56	MG	2A	3342	1/1	0.94	0.26	51,51,51,51	0
56	MG	2a	1688	1/1	0.94	0.27	68,68,68,68	0
56	MG	1F	311	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3345	1/1	0.94	0.11	56,56,56,56	0
56	MG	1F	312	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3777	1/1	0.94	0.05	18,18,18,18	0
56	MG	2A	3348	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3961	1/1	0.94	0.07	53,53,53,53	0
56	MG	1a	1705	1/1	0.94	0.26	61,61,61,61	0
56	MG	2A	3685	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	3493	1/1	0.94	0.08	64,64,64,64	0
56	MG	2A	3690	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3354	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3323	1/1	0.94	0.08	51,51,51,51	0
56	MG	2a	1702	1/1	0.94	0.12	71,71,71,71	0
56	MG	1A	3325	1/1	0.94	0.07	42,42,42,42	0
56	MG	2a	1704	1/1	0.94	0.12	62,62,62,62	0
56	MG	2a	1705	1/1	0.94	0.16	68,68,68,68	0
56	MG	2A	3357	1/1	0.94	0.13	50,50,50,50	0
56	MG	1N	206	1/1	0.94	0.10	48,48,48,48	0
56	MG	2a	1710	1/1	0.94	0.12	40,40,40,40	0
56	MG	2a	1711	1/1	0.94	0.20	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	3251	1/1	0.94	0.07	45,45,45,45	0
56	MG	2a	1714	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3186	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3408	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3004	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	1720	1/1	0.94	0.15	57,57,57,57	0
56	MG	1a	1715	1/1	0.94	0.38	70,70,70,70	0
56	MG	1A	3191	1/1	0.94	0.16	52,52,52,52	0
56	MG	2A	3107	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3030	1/1	0.94	0.17	32,32,32,32	0
56	MG	1a	1719	1/1	0.94	0.15	69,69,69,69	0
56	MG	1A	3617	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3195	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3626	1/1	0.94	0.09	34,34,34,34	0
56	MG	1Q	207	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3636	1/1	0.94	0.07	32,32,32,32	0
56	MG	2A	3716	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3810	1/1	0.94	0.21	24,24,24,24	0
56	MG	1A	3637	1/1	0.94	0.07	24,24,24,24	0
56	MG	1T	201	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3036	1/1	0.94	0.23	33,33,33,33	0
56	MG	1T	203	1/1	0.94	0.28	59,59,59,59	0
56	MG	1A	3642	1/1	0.94	0.12	44,44,44,44	0
56	MG	1U	209	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3047	1/1	0.94	0.05	27,27,27,27	0
56	MG	2A	3729	1/1	0.94	0.17	62,62,62,62	0
56	MG	2A	3389	1/1	0.94	0.07	70,70,70,70	0
56	MG	1A	3201	1/1	0.94	0.18	40,40,40,40	0
56	MG	2A	3134	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3135	1/1	0.94	0.09	42,42,42,42	0
56	MG	2A	3136	1/1	0.94	0.19	53,53,53,53	0
56	MG	2A	3394	1/1	0.94	0.11	54,54,54,54	0
56	MG	2A	3138	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3140	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3990	1/1	0.94	0.08	13,13,13,13	0
56	MG	2A	3741	1/1	0.94	0.12	65,65,65,65	0
56	MG	2A	3145	1/1	0.94	0.14	61,61,61,61	0
56	MG	2A	3147	1/1	0.94	0.28	50,50,50,50	0
56	MG	1W	205	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3402	1/1	0.94	0.11	43,43,43,43	0
56	MG	2A	3749	1/1	0.94	0.16	59,59,59,59	0
56	MG	2a	1762	1/1	0.94	0.14	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	3139	1/1	0.94	0.17	28,28,28,28	0
56	MG	1A	3995	1/1	0.94	0.21	64,64,64,64	0
56	MG	2A	3752	1/1	0.94	0.09	52,52,52,52	0
56	MG	2a	1768	1/1	0.94	0.25	64,64,64,64	0
56	MG	2A	3153	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3407	1/1	0.94	0.21	51,51,51,51	0
56	MG	2A	3408	1/1	0.94	0.20	41,41,41,41	0
56	MG	2A	3409	1/1	0.94	0.23	45,45,45,45	0
56	MG	2A	3411	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3154	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3142	1/1	0.94	0.25	36,36,36,36	0
56	MG	1Y	203	1/1	0.94	0.22	47,47,47,47	0
56	MG	2A	3763	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3159	1/1	0.94	0.21	63,63,63,63	0
56	MG	2A	3418	1/1	0.94	0.17	34,34,34,34	0
56	MG	1Z	301	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3769	1/1	0.94	0.17	68,68,68,68	0
56	MG	1A	3999	1/1	0.94	0.07	19,19,19,19	0
56	MG	1A	3824	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3422	1/1	0.94	0.27	54,54,54,54	0
56	MG	10	103	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3424	1/1	0.94	0.29	52,52,52,52	0
56	MG	2A	3426	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3145	1/1	0.94	0.14	49,49,49,49	0
56	MG	2v	102	1/1	0.94	0.10	60,60,60,60	0
56	MG	1a	1752	1/1	0.94	0.06	40,40,40,40	0
56	MG	1A	3652	1/1	0.94	0.07	21,21,21,21	0
56	MG	1A	4008	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3427	1/1	0.94	0.09	46,46,46,46	0
56	MG	2x	105	1/1	0.94	0.15	71,71,71,71	0
56	MG	2A	3433	1/1	0.94	0.17	58,58,58,58	0
58	ZN	14	102	1/1	0.94	0.12	125,125,125,125	0
56	MG	1A	3733	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	4079	1/1	0.95	0.05	38,38,38,38	0
56	MG	2A	3492	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3245	1/1	0.95	0.13	70,70,70,70	0
56	MG	1A	3397	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3843	1/1	0.95	0.07	61,61,61,61	0
56	MG	1A	3897	1/1	0.95	0.09	44,44,44,44	0
56	MG	1v	101	1/1	0.95	0.11	64,64,64,64	0
56	MG	2A	3499	1/1	0.95	0.13	47,47,47,47	0
56	MG	2A	3847	1/1	0.95	0.06	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3240	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3250	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3741	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	4084	1/1	0.95	0.09	49,49,49,49	0
56	MG	1B	201	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3506	1/1	0.95	0.16	45,45,45,45	0
56	MG	1x	103	1/1	0.95	0.05	58,58,58,58	0
56	MG	2A	3857	1/1	0.95	0.06	37,37,37,37	0
56	MG	2A	3508	1/1	0.95	0.08	34,34,34,34	0
56	MG	2A	3256	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3257	1/1	0.95	0.12	62,62,62,62	0
56	MG	1A	3588	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3865	1/1	0.95	0.07	62,62,62,62	0
56	MG	1A	3242	1/1	0.95	0.24	37,37,37,37	0
56	MG	1A	3906	1/1	0.95	0.12	54,54,54,54	0
56	MG	2A	3262	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3521	1/1	0.95	0.09	56,56,56,56	0
56	MG	1x	109	1/1	0.95	0.12	67,67,67,67	0
56	MG	2A	3265	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3243	1/1	0.95	0.19	33,33,33,33	0
56	MG	2B	203	1/1	0.95	0.15	57,57,57,57	0
56	MG	1A	3115	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3018	1/1	0.95	0.16	32,32,32,32	0
56	MG	1x	113	1/1	0.95	0.17	78,78,78,78	0
56	MG	1A	3912	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3913	1/1	0.95	0.07	57,57,57,57	0
56	MG	1B	218	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3274	1/1	0.95	0.14	52,52,52,52	0
56	MG	1B	219	1/1	0.95	0.17	40,40,40,40	0
56	MG	2A	3541	1/1	0.95	0.12	40,40,40,40	0
56	MG	2A	3006	1/1	0.95	0.26	61,61,61,61	0
56	MG	1A	3405	1/1	0.95	0.10	53,53,53,53	0
56	MG	1a	1662	1/1	0.95	0.13	66,66,66,66	0
56	MG	1A	3247	1/1	0.95	0.20	58,58,58,58	0
56	MG	1A	3120	1/1	0.95	0.13	28,28,28,28	0
56	MG	2A	3016	1/1	0.95	0.20	65,65,65,65	0
56	MG	1A	3919	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3319	1/1	0.95	0.15	50,50,50,50	0
56	MG	2D	301	1/1	0.95	0.11	38,38,38,38	0
56	MG	2A	3019	1/1	0.95	0.04	32,32,32,32	0
56	MG	1A	3758	1/1	0.95	0.10	24,24,24,24	0
56	MG	1A	3185	1/1	0.95	0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3288	1/1	0.95	0.35	65,65,65,65	0
56	MG	1A	3602	1/1	0.95	0.09	35,35,35,35	0
56	MG	2A	3027	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3929	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3763	1/1	0.95	0.14	40,40,40,40	0
56	MG	2A	3293	1/1	0.95	0.17	59,59,59,59	0
56	MG	1B	232	1/1	0.95	0.07	50,50,50,50	0
56	MG	2A	3295	1/1	0.95	0.11	53,53,53,53	0
56	MG	2F	306	1/1	0.95	0.21	48,48,48,48	0
56	MG	1A	3031	1/1	0.95	0.07	32,32,32,32	0
56	MG	2A	3034	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3127	1/1	0.95	0.16	38,38,38,38	0
56	MG	1A	3768	1/1	0.95	0.09	37,37,37,37	0
56	MG	2A	3040	1/1	0.95	0.09	49,49,49,49	0
56	MG	1B	236	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3582	1/1	0.95	0.20	59,59,59,59	0
56	MG	1A	3254	1/1	0.95	0.16	49,49,49,49	0
56	MG	1D	306	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3330	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3772	1/1	0.95	0.10	38,38,38,38	0
56	MG	2U	202	1/1	0.95	0.12	54,54,54,54	0
56	MG	2V	201	1/1	0.95	0.25	46,46,46,46	0
56	MG	1D	313	1/1	0.95	0.16	31,31,31,31	0
56	MG	1A	3511	1/1	0.95	0.06	40,40,40,40	0
56	MG	1E	302	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3001	1/1	0.95	0.08	31,31,31,31	0
56	MG	1E	306	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3945	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1689	1/1	0.95	0.16	57,57,57,57	0
56	MG	1A	3621	1/1	0.95	0.11	9,9,9,9	0
56	MG	23	103	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3623	1/1	0.95	0.10	42,42,42,42	0
56	MG	25	102	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3624	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3951	1/1	0.95	0.05	15,15,15,15	0
56	MG	26	101	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3132	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3066	1/1	0.95	0.27	56,56,56,56	0
56	MG	2A	3068	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3334	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3632	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3956	1/1	0.95	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3633	1/1	0.95	0.05	27,27,27,27	0
56	MG	1F	309	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3080	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3789	1/1	0.95	0.07	31,31,31,31	0
56	MG	1A	3635	1/1	0.95	0.05	24,24,24,24	0
56	MG	2a	1609	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3791	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3624	1/1	0.95	0.12	61,61,61,61	0
56	MG	2A	3625	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3626	1/1	0.95	0.09	50,50,50,50	0
56	MG	1F	313	1/1	0.95	0.12	57,57,57,57	0
56	MG	2A	3628	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3792	1/1	0.95	0.05	38,38,38,38	0
56	MG	1A	3966	1/1	0.95	0.08	57,57,57,57	0
56	MG	2A	3337	1/1	0.95	0.11	45,45,45,45	0
56	MG	2a	1619	1/1	0.95	0.12	52,52,52,52	0
56	MG	2a	1620	1/1	0.95	0.06	61,61,61,61	0
56	MG	2A	3632	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3633	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3426	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3043	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3134	1/1	0.95	0.10	40,40,40,40	0
56	MG	1N	205	1/1	0.95	0.21	40,40,40,40	0
56	MG	2a	1628	1/1	0.95	0.22	58,58,58,58	0
56	MG	2A	3097	1/1	0.95	0.13	45,45,45,45	0
56	MG	2A	3343	1/1	0.95	0.09	69,69,69,69	0
56	MG	2A	3642	1/1	0.95	0.19	38,38,38,38	0
56	MG	2A	3645	1/1	0.95	0.17	52,52,52,52	0
56	MG	1A	3640	1/1	0.95	0.06	22,22,22,22	0
56	MG	1N	207	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3262	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3976	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3046	1/1	0.95	0.05	39,39,39,39	0
56	MG	2a	1638	1/1	0.95	0.33	60,60,60,60	0
56	MG	1A	3806	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3351	1/1	0.95	0.15	56,56,56,56	0
56	MG	1A	3054	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3106	1/1	0.95	0.05	46,46,46,46	0
56	MG	1A	3140	1/1	0.95	0.29	29,29,29,29	0
56	MG	1a	1722	1/1	0.95	0.29	45,45,45,45	0
56	MG	1A	3100	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3112	1/1	0.95	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3342	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3102	1/1	0.95	0.07	46,46,46,46	0
56	MG	1Q	205	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3269	1/1	0.95	0.14	48,48,48,48	0
56	MG	2A	3667	1/1	0.95	0.12	35,35,35,35	0
56	MG	2A	3668	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3657	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	3086	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3821	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3674	1/1	0.95	0.07	52,52,52,52	0
56	MG	2a	1661	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3365	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3660	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3351	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3213	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3679	1/1	0.95	0.18	56,56,56,56	0
56	MG	2A	3124	1/1	0.95	0.24	68,68,68,68	0
56	MG	2A	3125	1/1	0.95	0.31	57,57,57,57	0
56	MG	1A	3220	1/1	0.95	0.36	39,39,39,39	0
56	MG	2A	3127	1/1	0.95	0.10	61,61,61,61	0
56	MG	2A	3376	1/1	0.95	0.22	52,52,52,52	0
56	MG	2A	3686	1/1	0.95	0.08	61,61,61,61	0
56	MG	2A	3128	1/1	0.95	0.21	58,58,58,58	0
56	MG	1A	3450	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3131	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3452	1/1	0.95	0.16	43,43,43,43	0
56	MG	2A	3382	1/1	0.95	0.10	53,53,53,53	0
56	MG	1V	205	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3384	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3830	1/1	0.95	0.19	47,47,47,47	0
56	MG	1W	201	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3277	1/1	0.95	0.06	43,43,43,43	0
56	MG	1W	203	1/1	0.95	0.06	38,38,38,38	0
56	MG	2A	3700	1/1	0.95	0.20	61,61,61,61	0
56	MG	2A	3139	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	4007	1/1	0.95	0.11	47,47,47,47	0
56	MG	2A	3141	1/1	0.95	0.26	50,50,50,50	0
56	MG	2A	3142	1/1	0.95	0.15	40,40,40,40	0
56	MG	2A	3143	1/1	0.95	0.15	48,48,48,48	0
56	MG	1W	206	1/1	0.95	0.12	29,29,29,29	0
56	MG	1A	3280	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3360	1/1	0.95	0.13	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	3676	1/1	0.95	0.05	19,19,19,19	0
56	MG	1A	3459	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3282	1/1	0.95	0.13	34,34,34,34	0
56	MG	2A	3400	1/1	0.95	0.06	59,59,59,59	0
56	MG	1A	3681	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3363	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3283	1/1	0.95	0.51	44,44,44,44	0
56	MG	10	104	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	3685	1/1	0.95	0.08	27,27,27,27	0
56	MG	11	101	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	4019	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3728	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3686	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3410	1/1	0.95	0.21	47,47,47,47	0
56	MG	2a	1712	1/1	0.95	0.09	56,56,56,56	0
56	MG	1a	1767	1/1	0.95	0.18	49,49,49,49	0
56	MG	2A	3412	1/1	0.95	0.21	44,44,44,44	0
56	MG	12	102	1/1	0.95	0.08	49,49,49,49	0
56	MG	2a	1716	1/1	0.95	0.30	53,53,53,53	0
56	MG	1A	3846	1/1	0.95	0.15	46,46,46,46	0
56	MG	2a	1718	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3104	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3553	1/1	0.95	0.23	33,33,33,33	0
56	MG	1A	3155	1/1	0.95	0.10	45,45,45,45	0
56	MG	15	103	1/1	0.95	0.32	44,44,44,44	0
56	MG	15	106	1/1	0.95	0.15	45,45,45,45	0
56	MG	1a	1776	1/1	0.95	0.06	59,59,59,59	0
56	MG	1A	4028	1/1	0.95	0.10	57,57,57,57	0
56	MG	2A	3179	1/1	0.95	0.27	60,60,60,60	0
56	MG	2A	3181	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3555	1/1	0.95	0.31	51,51,51,51	0
56	MG	2A	3183	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3699	1/1	0.95	0.08	36,36,36,36	0
56	MG	17	104	1/1	0.95	0.09	39,39,39,39	0
56	MG	17	106	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3556	1/1	0.95	0.22	44,44,44,44	0
56	MG	2A	3189	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3559	1/1	0.95	0.19	33,33,33,33	0
56	MG	18	104	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3702	1/1	0.95	0.11	38,38,38,38	0
56	MG	2a	1739	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	4035	1/1	0.95	0.07	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	1741	1/1	0.95	0.13	53,53,53,53	0
56	MG	1a	1789	1/1	0.95	0.12	70,70,70,70	0
56	MG	1A	3370	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3562	1/1	0.95	0.35	41,41,41,41	0
56	MG	2A	3766	1/1	0.95	0.11	56,56,56,56	0
56	MG	2A	3441	1/1	0.95	0.19	50,50,50,50	0
56	MG	2a	1747	1/1	0.95	0.18	65,65,65,65	0
56	MG	1A	3705	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	4040	1/1	0.95	0.11	37,37,37,37	0
56	MG	1a	1797	1/1	0.95	0.10	68,68,68,68	0
56	MG	1A	3865	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	4042	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3371	1/1	0.95	0.11	58,58,58,58	0
56	MG	2A	3448	1/1	0.95	0.24	56,56,56,56	0
56	MG	1A	4044	1/1	0.95	0.09	22,22,22,22	0
56	MG	1a	1805	1/1	0.95	0.18	71,71,71,71	0
56	MG	2a	1758	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3158	1/1	0.95	0.12	33,33,33,33	0
56	MG	1a	1807	1/1	0.95	0.14	57,57,57,57	0
56	MG	2A	3213	1/1	0.95	0.17	54,54,54,54	0
56	MG	1a	1612	1/1	0.95	0.17	58,58,58,58	0
56	MG	1A	3711	1/1	0.95	0.09	32,32,32,32	0
56	MG	2A	3788	1/1	0.95	0.17	41,41,41,41	0
56	MG	2a	1766	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3229	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3297	1/1	0.95	0.07	45,45,45,45	0
56	MG	2a	1769	1/1	0.95	0.10	70,70,70,70	0
56	MG	1A	3060	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3107	1/1	0.95	0.15	34,34,34,34	0
56	MG	2A	3793	1/1	0.95	0.07	72,72,72,72	0
56	MG	1A	4055	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3222	1/1	0.95	0.25	40,40,40,40	0
56	MG	1A	3300	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3389	1/1	0.95	0.19	37,37,37,37	0
56	MG	1A	3719	1/1	0.95	0.18	53,53,53,53	0
56	MG	2A	3800	1/1	0.95	0.07	53,53,53,53	0
56	MG	2A	3228	1/1	0.95	0.23	44,44,44,44	0
56	MG	2A	3471	1/1	0.95	0.16	62,62,62,62	0
56	MG	2A	3472	1/1	0.95	0.23	48,48,48,48	0
56	MG	1a	1625	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3110	1/1	0.95	0.16	36,36,36,36	0
56	MG	1A	3171	1/1	0.95	0.28	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	1A	3883	1/1	0.95	0.06	14,14,14,14	0
56	MG	2A	3812	1/1	0.95	0.06	41,41,41,41	0
56	MG	1A	4068	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	3305	1/1	0.95	0.29	40,40,40,40	0
56	MG	2A	3238	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3816	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3482	1/1	0.95	0.17	66,66,66,66	0
56	MG	1A	3062	1/1	0.95	0.09	31,31,31,31	0
56	MG	1A	3308	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3823	1/1	0.95	0.09	28,28,28,28	0
56	MG	1A	3309	1/1	0.95	0.14	36,36,36,36	0
56	MG	2x	106	1/1	0.95	0.10	76,76,76,76	0
56	MG	2A	3833	1/1	0.95	0.14	63,63,63,63	0
56	MG	2A	3486	1/1	0.95	0.11	48,48,48,48	0
58	ZN	24	501	1/1	0.95	0.17	131,131,131,131	0
56	MG	1A	3400	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3515	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3001	1/1	0.96	0.43	60,60,60,60	0
56	MG	1A	3740	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3594	1/1	0.96	0.16	29,29,29,29	0
56	MG	2A	3264	1/1	0.96	0.09	49,49,49,49	0
56	MG	1B	214	1/1	0.96	0.05	48,48,48,48	0
56	MG	1A	3595	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3523	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3329	1/1	0.96	0.22	49,49,49,49	0
56	MG	1A	3746	1/1	0.96	0.05	21,21,21,21	0
56	MG	1A	3597	1/1	0.96	0.11	44,44,44,44	0
56	MG	1A	3402	1/1	0.96	0.23	43,43,43,43	0
56	MG	1A	3128	1/1	0.96	0.37	33,33,33,33	0
56	MG	2A	3272	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3858	1/1	0.96	0.05	48,48,48,48	0
56	MG	2A	3014	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3533	1/1	0.96	0.13	44,44,44,44	0
56	MG	2A	3015	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3863	1/1	0.96	0.06	60,60,60,60	0
56	MG	1a	1658	1/1	0.96	0.06	49,49,49,49	0
56	MG	2A	3538	1/1	0.96	0.14	61,61,61,61	0
56	MG	1A	3918	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3496	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3278	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	3753	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3331	1/1	0.96	0.21	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3022	1/1	0.96	0.14	31,31,31,31	0
56	MG	1A	3922	1/1	0.96	0.06	15,15,15,15	0
56	MG	1A	3066	1/1	0.96	0.12	43,43,43,43	0
56	MG	2A	3025	1/1	0.96	0.43	48,48,48,48	0
56	MG	1A	3924	1/1	0.96	0.10	56,56,56,56	0
56	MG	2A	3553	1/1	0.96	0.09	34,34,34,34	0
56	MG	2A	3029	1/1	0.96	0.14	58,58,58,58	0
56	MG	2A	3555	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3556	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3224	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3605	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3559	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3560	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	3169	1/1	0.96	0.20	40,40,40,40	0
56	MG	1A	3049	1/1	0.96	0.07	31,31,31,31	0
56	MG	1A	3411	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3035	1/1	0.96	0.14	42,42,42,42	0
56	MG	1D	302	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3070	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3615	1/1	0.96	0.09	50,50,50,50	0
56	MG	1D	307	1/1	0.96	0.14	37,37,37,37	0
56	MG	1D	308	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3572	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3573	1/1	0.96	0.08	37,37,37,37	0
56	MG	2A	3574	1/1	0.96	0.10	25,25,25,25	0
56	MG	1a	1677	1/1	0.96	0.15	55,55,55,55	0
56	MG	1D	309	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3092	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3046	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3579	1/1	0.96	0.09	24,24,24,24	0
56	MG	2F	303	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3580	1/1	0.96	0.06	52,52,52,52	0
56	MG	1a	1680	1/1	0.96	0.07	82,82,82,82	0
56	MG	2A	3049	1/1	0.96	0.05	29,29,29,29	0
56	MG	2G	201	1/1	0.96	0.13	66,66,66,66	0
56	MG	1A	3940	1/1	0.96	0.11	83,83,83,83	0
56	MG	2A	3051	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3618	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3770	1/1	0.96	0.08	28,28,28,28	0
56	MG	2Q	202	1/1	0.96	0.22	53,53,53,53	0
56	MG	1E	301	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3619	1/1	0.96	0.07	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3620	1/1	0.96	0.05	37,37,37,37	0
56	MG	1A	3946	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3506	1/1	0.96	0.11	33,33,33,33	0
56	MG	2A	3597	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3416	1/1	0.96	0.13	37,37,37,37	0
56	MG	2U	201	1/1	0.96	0.16	59,59,59,59	0
56	MG	1A	3418	1/1	0.96	0.13	53,53,53,53	0
56	MG	2A	3064	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3279	1/1	0.96	0.05	40,40,40,40	0
56	MG	2A	3603	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3420	1/1	0.96	0.10	52,52,52,52	0
56	MG	2W	204	1/1	0.96	0.04	53,53,53,53	0
56	MG	2A	3067	1/1	0.96	0.09	42,42,42,42	0
56	MG	1a	1693	1/1	0.96	0.34	62,62,62,62	0
56	MG	2A	3069	1/1	0.96	0.14	50,50,50,50	0
56	MG	2I	101	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3608	1/1	0.96	0.11	55,55,55,55	0
56	MG	2A	3070	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3628	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3782	1/1	0.96	0.04	23,23,23,23	0
56	MG	1A	3955	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3614	1/1	0.96	0.15	48,48,48,48	0
56	MG	25	104	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3630	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3616	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3784	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3079	1/1	0.96	0.13	55,55,55,55	0
56	MG	1F	308	1/1	0.96	0.18	23,23,23,23	0
56	MG	1A	3073	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3513	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3623	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3634	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3086	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3136	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3088	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3236	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3967	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3092	1/1	0.96	0.37	52,52,52,52	0
56	MG	1A	3284	1/1	0.96	0.24	31,31,31,31	0
56	MG	1G	203	1/1	0.96	0.07	80,80,80,80	0
56	MG	1A	3793	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3970	1/1	0.96	0.08	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	3343	1/1	0.96	0.23	44,44,44,44	0
56	MG	2A	3098	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3349	1/1	0.96	0.14	62,62,62,62	0
56	MG	1N	204	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3640	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3639	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	3973	1/1	0.96	0.09	55,55,55,55	0
56	MG	2A	3644	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3061	1/1	0.96	0.19	48,48,48,48	0
56	MG	1a	1716	1/1	0.96	0.17	57,57,57,57	0
56	MG	2A	3647	1/1	0.96	0.10	57,57,57,57	0
56	MG	1A	3287	1/1	0.96	0.11	39,39,39,39	0
56	MG	2a	1627	1/1	0.96	0.20	56,56,56,56	0
56	MG	1A	3288	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3803	1/1	0.96	0.05	32,32,32,32	0
56	MG	2A	3651	1/1	0.96	0.06	59,59,59,59	0
56	MG	2A	3652	1/1	0.96	0.06	61,61,61,61	0
56	MG	1A	3522	1/1	0.96	0.24	41,41,41,41	0
56	MG	1a	1721	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3805	1/1	0.96	0.15	52,52,52,52	0
56	MG	1A	3238	1/1	0.96	0.17	32,32,32,32	0
56	MG	1P	202	1/1	0.96	0.23	30,30,30,30	0
56	MG	2A	3658	1/1	0.96	0.06	38,38,38,38	0
56	MG	1P	203	1/1	0.96	0.20	31,31,31,31	0
56	MG	2a	1639	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3646	1/1	0.96	0.07	16,16,16,16	0
56	MG	1A	3239	1/1	0.96	0.09	20,20,20,20	0
56	MG	1A	3985	1/1	0.96	0.05	43,43,43,43	0
56	MG	1A	3292	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3649	1/1	0.96	0.10	25,25,25,25	0
56	MG	1R	202	1/1	0.96	0.18	43,43,43,43	0
56	MG	2a	1648	1/1	0.96	0.13	64,64,64,64	0
56	MG	1A	3354	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	3653	1/1	0.96	0.07	24,24,24,24	0
56	MG	1A	3816	1/1	0.96	0.19	47,47,47,47	0
56	MG	2A	3669	1/1	0.96	0.13	55,55,55,55	0
56	MG	2A	3670	1/1	0.96	0.25	77,77,77,77	0
56	MG	1A	3114	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3655	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3656	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3530	1/1	0.96	0.21	49,49,49,49	0
56	MG	1U	205	1/1	0.96	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3381	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3077	1/1	0.96	0.05	27,27,27,27	0
56	MG	1A	4003	1/1	0.96	0.10	55,55,55,55	0
56	MG	2a	1662	1/1	0.96	0.17	58,58,58,58	0
56	MG	1V	202	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	3532	1/1	0.96	0.24	49,49,49,49	0
56	MG	2A	3681	1/1	0.96	0.07	58,58,58,58	0
56	MG	1a	1745	1/1	0.96	0.23	55,55,55,55	0
56	MG	1A	3437	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3439	1/1	0.96	0.13	31,31,31,31	0
56	MG	1A	3011	1/1	0.96	0.10	33,33,33,33	0
56	MG	1a	1751	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3687	1/1	0.96	0.06	62,62,62,62	0
56	MG	1A	3664	1/1	0.96	0.09	21,21,21,21	0
56	MG	1A	3537	1/1	0.96	0.18	42,42,42,42	0
56	MG	1a	1754	1/1	0.96	0.06	60,60,60,60	0
56	MG	1a	1755	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3146	1/1	0.96	0.12	54,54,54,54	0
56	MG	1a	1758	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3362	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3150	1/1	0.96	0.11	51,51,51,51	0
56	MG	1X	101	1/1	0.96	0.05	23,23,23,23	0
56	MG	1X	103	1/1	0.96	0.14	40,40,40,40	0
56	MG	1X	105	1/1	0.96	0.20	41,41,41,41	0
56	MG	2a	1683	1/1	0.96	0.09	63,63,63,63	0
56	MG	1A	3670	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	4014	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3702	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3245	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3673	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3446	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3447	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3364	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3150	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3197	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3451	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3714	1/1	0.96	0.07	35,35,35,35	0
56	MG	1I	103	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3118	1/1	0.96	0.12	34,34,34,34	0
56	MG	2A	3415	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	3551	1/1	0.96	0.12	27,27,27,27	0
56	MG	1A	3851	1/1	0.96	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3172	1/1	0.96	0.09	57,57,57,57	0
56	MG	2A	3722	1/1	0.96	0.18	64,64,64,64	0
56	MG	1A	3453	1/1	0.96	0.27	62,62,62,62	0
56	MG	2A	3174	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3725	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3687	1/1	0.96	0.05	20,20,20,20	0
56	MG	2a	1709	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3084	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3178	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3153	1/1	0.96	0.25	35,35,35,35	0
56	MG	1a	1783	1/1	0.96	0.11	54,54,54,54	0
56	MG	15	102	1/1	0.96	0.27	29,29,29,29	0
56	MG	1A	3857	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3693	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	4037	1/1	0.96	0.09	27,27,27,27	0
56	MG	2A	3186	1/1	0.96	0.05	60,60,60,60	0
56	MG	1A	3860	1/1	0.96	0.06	23,23,23,23	0
56	MG	1a	1790	1/1	0.96	0.08	76,76,76,76	0
56	MG	1a	1791	1/1	0.96	0.18	61,61,61,61	0
56	MG	2A	3191	1/1	0.96	0.06	65,65,65,65	0
56	MG	2A	3742	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3252	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3193	1/1	0.96	0.10	55,55,55,55	0
56	MG	17	103	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3373	1/1	0.96	0.23	39,39,39,39	0
56	MG	17	105	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3558	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3374	1/1	0.96	0.12	34,34,34,34	0
56	MG	18	102	1/1	0.96	0.10	33,33,33,33	0
56	MG	1a	1801	1/1	0.96	0.13	57,57,57,57	0
56	MG	1a	1802	1/1	0.96	0.06	68,68,68,68	0
56	MG	2A	3202	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3310	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3463	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3376	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3378	1/1	0.96	0.19	40,40,40,40	0
56	MG	1A	3205	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3762	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3381	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3154	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3035	1/1	0.96	0.17	23,23,23,23	0
56	MG	1A	4054	1/1	0.96	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3458	1/1	0.96	0.20	44,44,44,44	0
56	MG	1A	3126	1/1	0.96	0.13	49,49,49,49	0
56	MG	2A	3770	1/1	0.96	0.05	46,46,46,46	0
56	MG	1a	1815	1/1	0.96	0.16	63,63,63,63	0
56	MG	1A	4056	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3388	1/1	0.96	0.23	45,45,45,45	0
56	MG	1A	3477	1/1	0.96	0.06	48,48,48,48	0
56	MG	2A	3776	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	4060	1/1	0.96	0.05	11,11,11,11	0
56	MG	2a	1755	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3160	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3055	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3780	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3881	1/1	0.96	0.08	22,22,22,22	0
56	MG	2A	3470	1/1	0.96	0.15	53,53,53,53	0
56	MG	1A	3259	1/1	0.96	0.10	25,25,25,25	0
56	MG	1A	3261	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3226	1/1	0.96	0.07	30,30,30,30	0
56	MG	1A	3723	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3475	1/1	0.96	0.15	55,55,55,55	0
56	MG	2A	3476	1/1	0.96	0.09	69,69,69,69	0
56	MG	1A	3886	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3887	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3320	1/1	0.96	0.18	59,59,59,59	0
56	MG	1A	3585	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	4075	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3236	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3890	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3322	1/1	0.96	0.23	37,37,37,37	0
56	MG	1m	3001	1/1	0.96	0.06	74,74,74,74	0
56	MG	2A	3240	1/1	0.96	0.07	68,68,68,68	0
56	MG	1A	3894	1/1	0.96	0.04	35,35,35,35	0
56	MG	2e	201	1/1	0.96	0.06	57,57,57,57	0
56	MG	2f	201	1/1	0.96	0.11	51,51,51,51	0
56	MG	2A	3490	1/1	0.96	0.16	46,46,46,46	0
56	MG	1p	101	1/1	0.96	0.23	61,61,61,61	0
56	MG	1A	3895	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3216	1/1	0.96	0.09	38,38,38,38	0
56	MG	1a	1632	1/1	0.96	0.18	64,64,64,64	0
56	MG	1v	104	1/1	0.96	0.10	70,70,70,70	0
56	MG	1w	401	1/1	0.96	0.08	59,59,59,59	0
56	MG	1A	3218	1/1	0.96	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1636	1/1	0.96	0.25	62,62,62,62	0
56	MG	2A	3501	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3817	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3166	1/1	0.96	0.04	40,40,40,40	0
56	MG	1A	3490	1/1	0.96	0.24	34,34,34,34	0
56	MG	1A	3901	1/1	0.96	0.07	28,28,28,28	0
56	MG	1B	204	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3221	1/1	0.96	0.26	68,68,68,68	0
56	MG	1B	206	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3738	1/1	0.96	0.06	44,44,44,44	0
56	MG	1B	208	1/1	0.96	0.10	69,69,69,69	0
56	MG	2A	3511	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3512	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3370	1/1	0.97	0.24	56,56,56,56	0
56	MG	2A	3146	1/1	0.97	0.21	46,46,46,46	0
56	MG	2A	3372	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3193	1/1	0.97	0.21	23,23,23,23	0
56	MG	2A	3374	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3148	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3137	1/1	0.97	0.09	33,33,33,33	0
56	MG	2D	304	1/1	0.97	0.04	29,29,29,29	0
56	MG	2D	305	1/1	0.97	0.17	37,37,37,37	0
56	MG	2D	306	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3024	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3045	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3761	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3762	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3141	1/1	0.97	0.09	36,36,36,36	0
56	MG	1a	1794	1/1	0.97	0.13	60,60,60,60	0
56	MG	1A	3627	1/1	0.97	0.09	22,22,22,22	0
56	MG	1A	3200	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3766	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3767	1/1	0.97	0.04	20,20,20,20	0
56	MG	1a	1799	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3025	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3202	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3204	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3144	1/1	0.97	0.07	16,16,16,16	0
56	MG	1a	1613	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3169	1/1	0.97	0.08	58,58,58,58	0
56	MG	1A	3068	1/1	0.97	0.12	37,37,37,37	0
56	MG	2Q	204	1/1	0.97	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3643	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3523	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3208	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3007	1/1	0.97	0.08	37,37,37,37	0
56	MG	1B	212	1/1	0.97	0.16	31,31,31,31	0
56	MG	1a	1619	1/1	0.97	0.10	50,50,50,50	0
56	MG	1B	213	1/1	0.97	0.08	46,46,46,46	0
56	MG	2A	3177	1/1	0.97	0.08	65,65,65,65	0
56	MG	1a	1812	1/1	0.97	0.06	69,69,69,69	0
56	MG	2V	202	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	3931	1/1	0.97	0.06	53,53,53,53	0
56	MG	1A	3148	1/1	0.97	0.13	28,28,28,28	0
56	MG	1A	3778	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3406	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3211	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3641	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3271	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3937	1/1	0.97	0.07	37,37,37,37	0
56	MG	1a	1823	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3347	1/1	0.97	0.19	38,38,38,38	0
56	MG	1A	3048	1/1	0.97	0.06	32,32,32,32	0
56	MG	2A	3190	1/1	0.97	0.33	59,59,59,59	0
56	MG	1A	3785	1/1	0.97	0.09	56,56,56,56	0
56	MG	1d	301	1/1	0.97	0.19	39,39,39,39	0
56	MG	1A	3273	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3533	1/1	0.97	0.11	23,23,23,23	0
56	MG	1a	1634	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3108	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3275	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3214	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3650	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3651	1/1	0.97	0.06	25,25,25,25	0
56	MG	2A	3425	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3950	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3441	1/1	0.97	0.09	32,32,32,32	0
56	MG	2A	3203	1/1	0.97	0.06	56,56,56,56	0
56	MG	1D	301	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3278	1/1	0.97	0.13	35,35,35,35	0
56	MG	1t	201	1/1	0.97	0.16	62,62,62,62	0
56	MG	2A	3432	1/1	0.97	0.11	57,57,57,57	0
56	MG	1D	303	1/1	0.97	0.04	38,38,38,38	0
56	MG	1A	3798	1/1	0.97	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3799	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3357	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3444	1/1	0.97	0.20	34,34,34,34	0
56	MG	1A	3957	1/1	0.97	0.05	30,30,30,30	0
56	MG	2A	3688	1/1	0.97	0.10	48,48,48,48	0
56	MG	1A	3215	1/1	0.97	0.23	31,31,31,31	0
56	MG	2A	3215	1/1	0.97	0.19	56,56,56,56	0
56	MG	1A	3959	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3960	1/1	0.97	0.08	41,41,41,41	0
56	MG	1a	1654	1/1	0.97	0.11	56,56,56,56	0
56	MG	1x	106	1/1	0.97	0.16	45,45,45,45	0
56	MG	1a	1656	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3359	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3074	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3659	1/1	0.97	0.06	32,32,32,32	0
56	MG	1E	303	1/1	0.97	0.08	32,32,32,32	0
56	MG	1E	304	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3964	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3217	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3111	1/1	0.97	0.22	34,34,34,34	0
56	MG	1A	3546	1/1	0.97	0.16	31,31,31,31	0
56	MG	2A	3455	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3219	1/1	0.97	0.22	39,39,39,39	0
56	MG	2A	3708	1/1	0.97	0.17	61,61,61,61	0
56	MG	1A	3549	1/1	0.97	0.16	32,32,32,32	0
56	MG	1E	313	1/1	0.97	0.10	20,20,20,20	0
56	MG	1A	3027	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3010	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3666	1/1	0.97	0.04	21,21,21,21	0
56	MG	1E	317	1/1	0.97	0.05	50,50,50,50	0
56	MG	2a	1644	1/1	0.97	0.11	36,36,36,36	0
56	MG	1F	301	1/1	0.97	0.18	28,28,28,28	0
56	MG	2A	3465	1/1	0.97	0.11	22,22,22,22	0
56	MG	1F	302	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3365	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3013	1/1	0.97	0.08	22,22,22,22	0
56	MG	1A	3974	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3156	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3819	1/1	0.97	0.04	47,47,47,47	0
56	MG	2A	3021	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	3157	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3672	1/1	0.97	0.08	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3369	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3458	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3730	1/1	0.97	0.05	69,69,69,69	0
56	MG	1A	3079	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3028	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3460	1/1	0.97	0.17	44,44,44,44	0
56	MG	2A	3734	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3828	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3560	1/1	0.97	0.04	21,21,21,21	0
56	MG	1A	3225	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3294	1/1	0.97	0.14	42,42,42,42	0
56	MG	1N	202	1/1	0.97	0.19	37,37,37,37	0
56	MG	2A	3261	1/1	0.97	0.13	52,52,52,52	0
56	MG	1A	3832	1/1	0.97	0.11	52,52,52,52	0
56	MG	1A	3015	1/1	0.97	0.15	25,25,25,25	0
56	MG	2A	3488	1/1	0.97	0.15	44,44,44,44	0
56	MG	2A	3745	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3565	1/1	0.97	0.22	32,32,32,32	0
56	MG	1A	3228	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3567	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3002	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3689	1/1	0.97	0.06	28,28,28,28	0
56	MG	1A	3840	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	4001	1/1	0.97	0.11	23,23,23,23	0
56	MG	1A	3230	1/1	0.97	0.09	40,40,40,40	0
56	MG	2A	3047	1/1	0.97	0.21	50,50,50,50	0
56	MG	1A	3165	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3468	1/1	0.97	0.16	48,48,48,48	0
56	MG	1A	3695	1/1	0.97	0.06	19,19,19,19	0
56	MG	2A	3758	1/1	0.97	0.11	32,32,32,32	0
56	MG	1P	205	1/1	0.97	0.10	41,41,41,41	0
56	MG	2A	3052	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3696	1/1	0.97	0.06	21,21,21,21	0
56	MG	1A	3847	1/1	0.97	0.06	14,14,14,14	0
56	MG	1Q	202	1/1	0.97	0.10	33,33,33,33	0
56	MG	2A	3509	1/1	0.97	0.09	56,56,56,56	0
56	MG	1Q	203	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3301	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3232	1/1	0.97	0.28	31,31,31,31	0
56	MG	2A	3060	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3119	1/1	0.97	0.11	38,38,38,38	0
56	MG	2a	1697	1/1	0.97	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1R	201	1/1	0.97	0.06	40,40,40,40	0
56	MG	2A	3772	1/1	0.97	0.06	54,54,54,54	0
56	MG	1a	1713	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3852	1/1	0.97	0.10	23,23,23,23	0
56	MG	1R	204	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3472	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3474	1/1	0.97	0.16	35,35,35,35	0
56	MG	1A	4016	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3383	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3581	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3582	1/1	0.97	0.04	31,31,31,31	0
56	MG	2A	3527	1/1	0.97	0.14	67,67,67,67	0
56	MG	2A	3783	1/1	0.97	0.06	34,34,34,34	0
56	MG	1U	202	1/1	0.97	0.35	35,35,35,35	0
56	MG	1A	3858	1/1	0.97	0.09	43,43,43,43	0
56	MG	1U	204	1/1	0.97	0.18	37,37,37,37	0
56	MG	2A	3076	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	4021	1/1	0.97	0.09	39,39,39,39	0
56	MG	2A	3534	1/1	0.97	0.20	58,58,58,58	0
56	MG	1U	207	1/1	0.97	0.32	28,28,28,28	0
56	MG	1U	208	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3384	1/1	0.97	0.35	24,24,24,24	0
56	MG	2a	1721	1/1	0.97	0.09	48,48,48,48	0
56	MG	1U	210	1/1	0.97	0.21	32,32,32,32	0
56	MG	2A	3540	1/1	0.97	0.05	60,60,60,60	0
56	MG	2A	3083	1/1	0.97	0.13	55,55,55,55	0
56	MG	1A	3304	1/1	0.97	0.18	31,31,31,31	0
56	MG	2A	3085	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3386	1/1	0.97	0.17	21,21,21,21	0
56	MG	2A	3545	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3309	1/1	0.97	0.07	54,54,54,54	0
56	MG	1V	204	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3017	1/1	0.97	0.08	62,62,62,62	0
56	MG	2A	3549	1/1	0.97	0.08	36,36,36,36	0
56	MG	2A	3807	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3032	1/1	0.97	0.17	30,30,30,30	0
56	MG	1A	3124	1/1	0.97	0.13	48,48,48,48	0
56	MG	2A	3552	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3125	1/1	0.97	0.18	29,29,29,29	0
56	MG	1A	3010	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3056	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3718	1/1	0.97	0.04	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3174	1/1	0.97	0.09	49,49,49,49	0
56	MG	2A	3819	1/1	0.97	0.04	32,32,32,32	0
56	MG	2A	3320	1/1	0.97	0.05	49,49,49,49	0
56	MG	2A	3321	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3720	1/1	0.97	0.08	29,29,29,29	0
56	MG	1A	3394	1/1	0.97	0.16	40,40,40,40	0
56	MG	2A	3825	1/1	0.97	0.04	43,43,43,43	0
56	MG	2A	3830	1/1	0.97	0.05	44,44,44,44	0
56	MG	2A	3831	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3562	1/1	0.97	0.04	36,36,36,36	0
56	MG	1a	1743	1/1	0.97	0.16	63,63,63,63	0
56	MG	1A	3241	1/1	0.97	0.13	35,35,35,35	0
56	MG	1X	106	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3057	1/1	0.97	0.07	24,24,24,24	0
56	MG	1A	3179	1/1	0.97	0.06	25,25,25,25	0
56	MG	1A	3180	1/1	0.97	0.13	29,29,29,29	0
56	MG	1a	1749	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3317	1/1	0.97	0.17	48,48,48,48	0
56	MG	1A	3058	1/1	0.97	0.16	44,44,44,44	0
56	MG	2A	3108	1/1	0.97	0.07	40,40,40,40	0
56	MG	10	101	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3880	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3111	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3059	1/1	0.97	0.08	17,17,17,17	0
56	MG	2a	1765	1/1	0.97	0.11	68,68,68,68	0
56	MG	1A	4046	1/1	0.97	0.04	16,16,16,16	0
56	MG	1a	1757	1/1	0.97	0.08	59,59,59,59	0
56	MG	1A	3882	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3735	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	4049	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3856	1/1	0.97	0.11	52,52,52,52	0
56	MG	1A	3019	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3321	1/1	0.97	0.11	25,25,25,25	0
56	MG	1A	3604	1/1	0.97	0.08	46,46,46,46	0
56	MG	2A	3587	1/1	0.97	0.09	58,58,58,58	0
56	MG	1a	1764	1/1	0.97	0.07	64,64,64,64	0
56	MG	2A	3862	1/1	0.97	0.14	60,60,60,60	0
56	MG	12	103	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3037	1/1	0.97	0.05	39,39,39,39	0
56	MG	13	102	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3188	1/1	0.97	0.04	40,40,40,40	0
56	MG	1A	3609	1/1	0.97	0.12	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	3596	1/1	0.97	0.16	59,59,59,59	0
56	MG	13	106	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3744	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3406	1/1	0.97	0.18	46,46,46,46	0
56	MG	1a	1773	1/1	0.97	0.08	60,60,60,60	0
56	MG	2A	3601	1/1	0.97	0.06	57,57,57,57	0
56	MG	1A	3324	1/1	0.97	0.09	31,31,31,31	0
56	MG	15	105	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3250	1/1	0.97	0.26	30,30,30,30	0
56	MG	1A	3505	1/1	0.97	0.18	21,21,21,21	0
56	MG	2A	3137	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3616	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3189	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3899	1/1	0.97	0.13	29,29,29,29	0
56	MG	1A	3040	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3413	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3903	1/1	0.97	0.06	20,20,20,20	0
56	MG	17	107	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3042	1/1	0.97	0.04	39,39,39,39	0
56	MG	1a	1622	1/1	0.98	0.06	56,56,56,56	0
56	MG	2A	3227	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3432	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3710	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3433	1/1	0.98	0.20	34,34,34,34	0
56	MG	1A	4027	1/1	0.98	0.05	50,50,50,50	0
56	MG	1A	3910	1/1	0.98	0.09	53,53,53,53	0
56	MG	2A	3233	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3234	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	4029	1/1	0.98	0.05	50,50,50,50	0
56	MG	2A	3765	1/1	0.98	0.06	60,60,60,60	0
56	MG	1A	3911	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3183	1/1	0.98	0.03	25,25,25,25	0
56	MG	1A	3081	1/1	0.98	0.05	44,44,44,44	0
56	MG	1G	202	1/1	0.98	0.10	55,55,55,55	0
56	MG	2A	3074	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3914	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3631	1/1	0.98	0.07	17,17,17,17	0
56	MG	2A	3077	1/1	0.98	0.07	26,26,26,26	0
56	MG	2A	3591	1/1	0.98	0.04	38,38,38,38	0
56	MG	1a	1635	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3293	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3814	1/1	0.98	0.05	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3071	1/1	0.98	0.11	23,23,23,23	0
56	MG	1A	3438	1/1	0.98	0.15	32,32,32,32	0
56	MG	1A	3295	1/1	0.98	0.15	28,28,28,28	0
56	MG	1A	3095	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3130	1/1	0.98	0.18	31,31,31,31	0
56	MG	1a	1787	1/1	0.98	0.14	63,63,63,63	0
56	MG	2A	3784	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3820	1/1	0.98	0.30	29,29,29,29	0
56	MG	2A	3254	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3721	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	3927	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3564	1/1	0.98	0.10	23,23,23,23	0
56	MG	2A	3091	1/1	0.98	0.12	39,39,39,39	0
56	MG	1A	3823	1/1	0.98	0.04	25,25,25,25	0
56	MG	2a	1641	1/1	0.98	0.12	52,52,52,52	0
56	MG	1A	3930	1/1	0.98	0.03	50,50,50,50	0
56	MG	1P	201	1/1	0.98	0.20	29,29,29,29	0
56	MG	1A	3096	1/1	0.98	0.12	23,23,23,23	0
56	MG	1A	3112	1/1	0.98	0.17	32,32,32,32	0
56	MG	1P	204	1/1	0.98	0.26	29,29,29,29	0
56	MG	2A	3797	1/1	0.98	0.12	61,61,61,61	0
56	MG	2A	3613	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	3021	1/1	0.98	0.03	16,16,16,16	0
56	MG	1A	3568	1/1	0.98	0.14	34,34,34,34	0
56	MG	1a	1655	1/1	0.98	0.09	48,48,48,48	0
56	MG	1A	3260	1/1	0.98	0.03	32,32,32,32	0
56	MG	1A	4053	1/1	0.98	0.03	32,32,32,32	0
56	MG	2A	3619	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3227	1/1	0.98	0.05	42,42,42,42	0
56	MG	1a	1659	1/1	0.98	0.06	72,72,72,72	0
56	MG	2A	3808	1/1	0.98	0.08	60,60,60,60	0
56	MG	1A	3732	1/1	0.98	0.07	43,43,43,43	0
56	MG	2A	3810	1/1	0.98	0.07	53,53,53,53	0
56	MG	1A	3938	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3571	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	3039	1/1	0.98	0.09	15,15,15,15	0
56	MG	1A	3941	1/1	0.98	0.11	58,58,58,58	0
56	MG	1R	203	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3573	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	3346	1/1	0.98	0.21	38,38,38,38	0
56	MG	2A	3818	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3005	1/1	0.98	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1814	1/1	0.98	0.07	68,68,68,68	0
56	MG	1A	4065	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	4066	1/1	0.98	0.04	30,30,30,30	0
56	MG	1a	1817	1/1	0.98	0.08	70,70,70,70	0
56	MG	2A	3824	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3836	1/1	0.98	0.18	53,53,53,53	0
56	MG	2A	3826	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3827	1/1	0.98	0.10	46,46,46,46	0
56	MG	2A	3828	1/1	0.98	0.04	65,65,65,65	0
56	MG	2A	3829	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3348	1/1	0.98	0.14	33,33,33,33	0
56	MG	2A	3120	1/1	0.98	0.07	31,31,31,31	0
56	MG	2A	3638	1/1	0.98	0.08	42,42,42,42	0
56	MG	1U	201	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	3510	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3742	1/1	0.98	0.05	58,58,58,58	0
56	MG	2A	3836	1/1	0.98	0.04	36,36,36,36	0
56	MG	2A	3837	1/1	0.98	0.06	50,50,50,50	0
56	MG	2A	3459	1/1	0.98	0.17	51,51,51,51	0
56	MG	1A	4071	1/1	0.98	0.05	59,59,59,59	0
56	MG	1A	3349	1/1	0.98	0.12	39,39,39,39	0
56	MG	1A	3194	1/1	0.98	0.18	32,32,32,32	0
56	MG	1A	3842	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3116	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	4077	1/1	0.98	0.03	42,42,42,42	0
56	MG	2A	3130	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3307	1/1	0.98	0.12	28,28,28,28	0
56	MG	1A	3041	1/1	0.98	0.19	30,30,30,30	0
56	MG	1A	3749	1/1	0.98	0.06	15,15,15,15	0
56	MG	1A	3456	1/1	0.98	0.08	34,34,34,34	0
56	MG	1A	3162	1/1	0.98	0.17	33,33,33,33	0
56	MG	1A	3849	1/1	0.98	0.14	51,51,51,51	0
56	MG	1A	3355	1/1	0.98	0.21	61,61,61,61	0
56	MG	1A	3163	1/1	0.98	0.19	38,38,38,38	0
56	MG	1A	3164	1/1	0.98	0.21	33,33,33,33	0
56	MG	1A	3521	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3756	1/1	0.98	0.04	45,45,45,45	0
56	MG	2a	1706	1/1	0.98	0.03	44,44,44,44	0
56	MG	1A	3138	1/1	0.98	0.06	43,43,43,43	0
56	MG	1X	102	1/1	0.98	0.24	42,42,42,42	0
56	MG	1A	3407	1/1	0.98	0.08	47,47,47,47	0
56	MG	1X	104	1/1	0.98	0.08	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	1A	3101	1/1	0.98	0.11	17,17,17,17	0
56	MG	2A	3314	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3592	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3525	1/1	0.98	0.19	38,38,38,38	0
56	MG	1A	3089	1/1	0.98	0.27	35,35,35,35	0
56	MG	1A	3078	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3121	1/1	0.98	0.07	39,39,39,39	0
56	MG	2A	3489	1/1	0.98	0.08	32,32,32,32	0
56	MG	1A	3276	1/1	0.98	0.15	32,32,32,32	0
56	MG	1B	215	1/1	0.98	0.06	40,40,40,40	0
56	MG	1x	108	1/1	0.98	0.25	48,48,48,48	0
56	MG	1A	3143	1/1	0.98	0.08	17,17,17,17	0
56	MG	2A	3156	1/1	0.98	0.10	31,31,31,31	0
56	MG	2A	3157	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3020	1/1	0.98	0.11	40,40,40,40	0
56	MG	2A	3327	1/1	0.98	0.11	46,46,46,46	0
56	MG	1A	3675	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3123	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3161	1/1	0.98	0.12	52,52,52,52	0
56	MG	10	106	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3677	1/1	0.98	0.06	19,19,19,19	0
56	MG	11	102	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3978	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3417	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3080	1/1	0.98	0.10	30,30,30,30	0
56	MG	1A	3773	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3680	1/1	0.98	0.05	26,26,26,26	0
56	MG	1B	228	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3473	1/1	0.98	0.09	43,43,43,43	0
56	MG	2A	3513	1/1	0.98	0.09	43,43,43,43	0
56	MG	13	103	1/1	0.98	0.04	37,37,37,37	0
56	MG	2A	3012	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3874	1/1	0.98	0.08	28,28,28,28	0
56	MG	1A	3281	1/1	0.98	0.13	23,23,23,23	0
56	MG	2A	3518	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3475	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	3877	1/1	0.98	0.11	62,62,62,62	0
56	MG	2E	304	1/1	0.98	0.13	31,31,31,31	0
56	MG	15	101	1/1	0.98	0.15	26,26,26,26	0
56	MG	1A	3606	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3779	1/1	0.98	0.10	64,64,64,64	0
56	MG	1A	3607	1/1	0.98	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2F	302	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3147	1/1	0.98	0.05	24,24,24,24	0
56	MG	15	107	1/1	0.98	0.15	45,45,45,45	0
56	MG	1A	3992	1/1	0.98	0.07	17,17,17,17	0
56	MG	1A	3994	1/1	0.98	0.04	58,58,58,58	0
56	MG	1A	3176	1/1	0.98	0.08	27,27,27,27	0
56	MG	2A	3026	1/1	0.98	0.13	40,40,40,40	0
56	MG	17	101	1/1	0.98	0.07	34,34,34,34	0
56	MG	2O	202	1/1	0.98	0.06	52,52,52,52	0
56	MG	2A	3532	1/1	0.98	0.11	42,42,42,42	0
56	MG	17	102	1/1	0.98	0.15	31,31,31,31	0
56	MG	1A	3996	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3997	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3610	1/1	0.98	0.13	28,28,28,28	0
56	MG	2A	3537	1/1	0.98	0.07	51,51,51,51	0
56	MG	1A	3611	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3692	1/1	0.98	0.06	25,25,25,25	0
56	MG	1D	311	1/1	0.98	0.20	23,23,23,23	0
56	MG	1A	3478	1/1	0.98	0.12	50,50,50,50	0
56	MG	1A	4002	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3037	1/1	0.98	0.03	35,35,35,35	0
56	MG	2A	3038	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	3177	1/1	0.98	0.22	20,20,20,20	0
56	MG	1A	3285	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	4005	1/1	0.98	0.08	31,31,31,31	0
56	MG	1A	3106	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	3328	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3891	1/1	0.98	0.07	39,39,39,39	0
56	MG	2A	3207	1/1	0.98	0.06	46,46,46,46	0
56	MG	2X	102	1/1	0.98	0.11	46,46,46,46	0
56	MG	1A	3698	1/1	0.98	0.10	25,25,25,25	0
56	MG	1a	1750	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3893	1/1	0.98	0.09	50,50,50,50	0
56	MG	1A	3149	1/1	0.98	0.11	23,23,23,23	0
56	MG	1A	3181	1/1	0.98	0.04	16,16,16,16	0
56	MG	1A	3795	1/1	0.98	0.07	51,51,51,51	0
56	MG	1A	3377	1/1	0.98	0.17	27,27,27,27	0
56	MG	1A	3797	1/1	0.98	0.07	56,56,56,56	0
56	MG	1E	315	1/1	0.98	0.21	46,46,46,46	0
56	MG	2A	3054	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3548	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3289	1/1	0.98	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	27	101	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	3182	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	3489	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3706	1/1	0.98	0.04	19,19,19,19	0
56	MG	1A	3707	1/1	0.98	0.04	10,10,10,10	0
56	MG	1F	305	1/1	0.98	0.11	31,31,31,31	0
58	ZN	1n	102	1/1	0.98	0.04	89,89,89,89	0
56	MG	1A	3380	1/1	0.98	0.12	36,36,36,36	0
59	SF4	2d	303	8/8	0.98	0.04	64,76,84,86	0
56	MG	1A	3170	1/1	0.99	0.03	26,26,26,26	0
56	MG	2A	3180	1/1	0.99	0.10	47,47,47,47	0
56	MG	1B	227	1/1	0.99	0.03	37,37,37,37	0
56	MG	2A	3710	1/1	0.99	0.07	39,39,39,39	0
56	MG	1A	4061	1/1	0.99	0.09	22,22,22,22	0
56	MG	1W	204	1/1	0.99	0.17	33,33,33,33	0
56	MG	1A	3190	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3075	1/1	0.99	0.06	9,9,9,9	0
56	MG	1A	3012	1/1	0.99	0.04	28,28,28,28	0
56	MG	1I	201	1/1	0.99	0.04	64,64,64,64	0
56	MG	1A	3808	1/1	0.99	0.04	30,30,30,30	0
56	MG	2A	3718	1/1	0.99	0.03	42,42,42,42	0
56	MG	1A	3809	1/1	0.99	0.04	18,18,18,18	0
56	MG	1A	3008	1/1	0.99	0.09	23,23,23,23	0
56	MG	1A	3734	1/1	0.99	0.06	27,27,27,27	0
56	MG	1A	3669	1/1	0.99	0.06	36,36,36,36	0
56	MG	1B	237	1/1	0.99	0.06	30,30,30,30	0
56	MG	1A	3065	1/1	0.99	0.20	42,42,42,42	0
56	MG	1A	3737	1/1	0.99	0.05	36,36,36,36	0
56	MG	2A	3585	1/1	0.99	0.09	34,34,34,34	0
56	MG	1A	3038	1/1	0.99	0.06	23,23,23,23	0
56	MG	1A	4026	1/1	0.99	0.03	25,25,25,25	0
56	MG	1D	305	1/1	0.99	0.03	17,17,17,17	0
56	MG	2A	3802	1/1	0.99	0.03	55,55,55,55	0
56	MG	2A	3009	1/1	0.99	0.04	39,39,39,39	0
56	MG	2A	3590	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3484	1/1	0.99	0.12	31,31,31,31	0
56	MG	1A	3196	1/1	0.99	0.23	35,35,35,35	0
56	MG	1A	4076	1/1	0.99	0.02	43,43,43,43	0
56	MG	1A	3003	1/1	0.99	0.02	23,23,23,23	0
56	MG	1A	4078	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3159	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	3412	1/1	0.99	0.08	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	3268	1/1	0.99	0.12	32,32,32,32	0
56	MG	1A	3902	1/1	0.99	0.03	35,35,35,35	0
56	MG	1A	3178	1/1	0.99	0.12	29,29,29,29	0
56	MG	1A	3622	1/1	0.99	0.09	36,36,36,36	0
56	MG	2A	3743	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3747	1/1	0.99	0.04	25,25,25,25	0
56	MG	1A	3022	1/1	0.99	0.07	38,38,38,38	0
56	MG	1Q	206	1/1	0.99	0.17	39,39,39,39	0
56	MG	1a	1819	1/1	0.99	0.02	55,55,55,55	0
56	MG	1A	3993	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3069	1/1	0.99	0.07	35,35,35,35	0
56	MG	1E	307	1/1	0.99	0.13	45,45,45,45	0
56	MG	1E	308	1/1	0.99	0.03	27,27,27,27	0
56	MG	1A	3682	1/1	0.99	0.04	26,26,26,26	0
56	MG	1A	3788	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3129	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3203	1/1	0.99	0.10	23,23,23,23	0
56	MG	15	104	1/1	0.99	0.21	24,24,24,24	0
56	MG	1A	3083	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3033	1/1	0.99	0.04	24,24,24,24	0
56	MG	1A	3629	1/1	0.99	0.06	55,55,55,55	0
56	MG	1A	3034	1/1	0.99	0.10	27,27,27,27	0
56	MG	1A	3207	1/1	0.99	0.04	20,20,20,20	0
56	MG	1A	3072	1/1	0.99	0.04	18,18,18,18	0
56	MG	1A	3722	1/1	0.99	0.05	42,42,42,42	0
56	MG	1B	216	1/1	0.99	0.05	43,43,43,43	0
56	MG	1U	206	1/1	0.99	0.09	30,30,30,30	0
56	MG	2A	3839	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	3691	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3087	1/1	0.99	0.05	25,25,25,25	0
56	MG	1A	3725	1/1	0.99	0.06	23,23,23,23	0
56	MG	1A	3023	1/1	0.99	0.05	15,15,15,15	0
56	MG	1A	3727	1/1	0.99	0.06	43,43,43,43	0
56	MG	1A	3044	1/1	0.99	0.06	24,24,24,24	0
56	MG	1V	203	1/1	0.99	0.15	29,29,29,29	0
56	MG	2A	3496	1/1	0.99	0.07	74,74,74,74	0
56	MG	2A	3848	1/1	0.99	0.03	23,23,23,23	0
56	MG	2A	3563	1/1	0.99	0.06	33,33,33,33	0
58	ZN	1Y	204	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3925	1/1	0.99	0.05	30,30,30,30	0
58	ZN	15	109	1/1	0.99	0.03	57,57,57,57	0
56	MG	2A	3498	1/1	0.99	0.04	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	2Y	501	1/1	0.99	0.03	85,85,85,85	0
56	MG	1A	4058	1/1	0.99	0.05	36,36,36,36	0
58	ZN	25	106	1/1	0.99	0.03	62,62,62,62	0
58	ZN	26	102	1/1	0.99	0.05	61,61,61,61	0
58	ZN	29	501	1/1	0.99	0.04	71,71,71,71	0
58	ZN	2n	501	1/1	0.99	0.05	85,85,85,85	0
59	SF4	1d	302	8/8	0.99	0.04	67,80,86,86	0
56	MG	1A	3926	1/1	0.99	0.04	33,33,33,33	0
58	ZN	19	501	1/1	1.00	0.03	42,42,42,42	0
56	MG	2A	3703	1/1	1.00	0.04	22,22,22,22	0
56	MG	1A	3014	1/1	1.00	0.03	23,23,23,23	0
56	MG	1A	3109	1/1	1.00	0.09	27,27,27,27	0
58	ZN	16	103	1/1	1.00	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.