



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:53 AM UTC

PDB ID : 9B00 / pdb_00009b00
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with berberine analog of chloramphenicol CAM-BER, mRNA, deacylated A- and E-site tRNA^{phe}, and deacylated P-site tRNA^{met} at 2.80Å resolution
Authors : Batool, Z.; Pavlova, J.A.; Paranjpe, M.N.; Tereshchenkov, A.G.; Lukianov, D.A.; Osterman, I.A.; Bogdanov, A.A.; Sumbatyan, N.V.; Polikanov, Y.S.
Deposited on : 2024-03-11
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

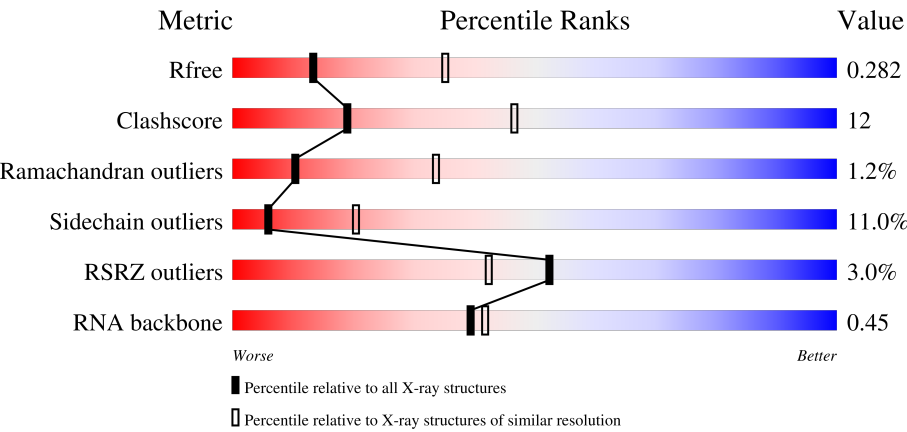
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



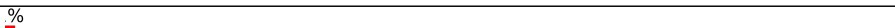
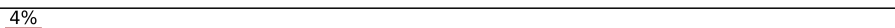
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114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

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

Mol	Chain	Length	Quality of chain
1	1A	2915	2% 54% 36% 8% .
1	2A	2915	% 47% 41% 8% .
2	1B	121	60% 37% ..
2	2B	121	% 31% 55% 14% .

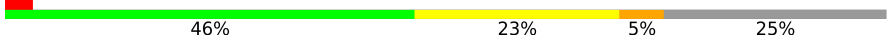
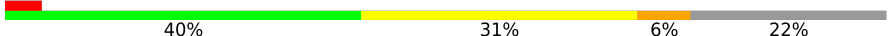
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
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	
27	25	60	

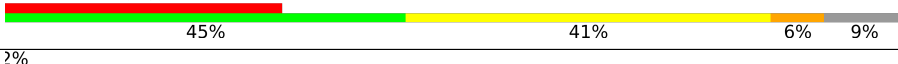
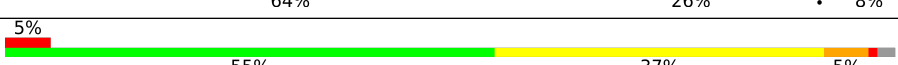
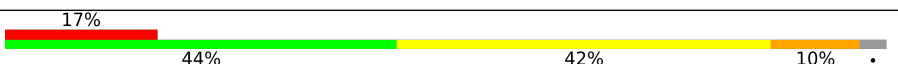
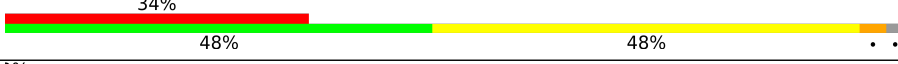
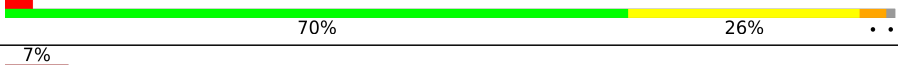
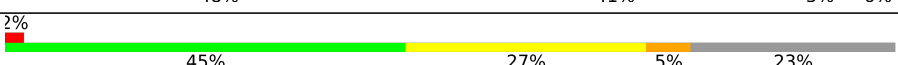
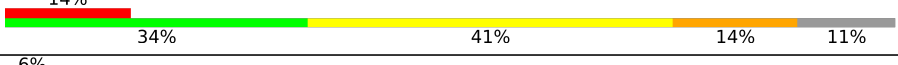
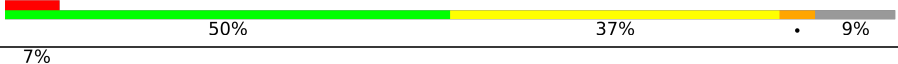
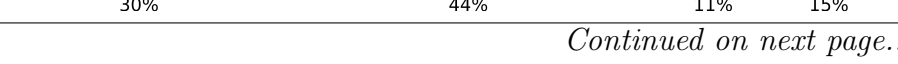
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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
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	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2v	102	-	-	-	X
56	MG	2v	103	-	-	-	X
60	SF4	1d	302	-	-	X	-
60	SF4	2d	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299897 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	0
			1587	1011	298	276	2			
5	2F	203	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site Deacylated tRNA^{phe}.

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1083	Total	Mg	0	0
			1083	1083		
56	1B	38	Total	Mg	0	0
			38	38		
56	1D	11	Total	Mg	0	0
			11	11		
56	1E	12	Total	Mg	0	0
			12	12		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	4	Total	Mg	0	0
			4	4		
56	1H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	5	Total 5	Mg 5	0	0
56	1O	3	Total 3	Mg 3	0	0
56	1P	7	Total 7	Mg 7	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	5	Total 5	Mg 5	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1U	8	Total 8	Mg 8	0	0
56	1V	8	Total 8	Mg 8	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	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	6	Total 6	Mg 6	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	4	Total 4	Mg 4	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	5	Total 5	Mg 5	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	18	3	Total 3	Mg 3	0	0
56	19	2	Total 2	Mg 2	0	0
56	1a	226	Total 226	Mg 226	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	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	2	Total 2	Mg 2	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1w	7	Total 7	Mg 7	0	0
56	1x	12	Total 12	Mg 12	0	0
56	1y	1	Total 1	Mg 1	0	0
56	2A	849	Total 849	Mg 849	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	5	Total 5	Mg 5	0	0
56	2E	7	Total 7	Mg 7	0	0
56	2F	7	Total 7	Mg 7	0	0
56	2G	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	2Q	1	Total 1	Mg 1	0	0
56	2R	1	Total 1	Mg 1	0	0
56	2T	4	Total 4	Mg 4	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	2	Total 2	Mg 2	0	0
56	21	3	Total 3	Mg 3	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	2	Total 2	Mg 2	0	0
56	27	4	Total 4	Mg 4	0	0
56	28	6	Total 6	Mg 6	0	0
56	2a	246	Total 246	Mg 246	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	2	Total 2	Mg 2	0	0
56	2f	2	Total 2	Mg 2	0	0

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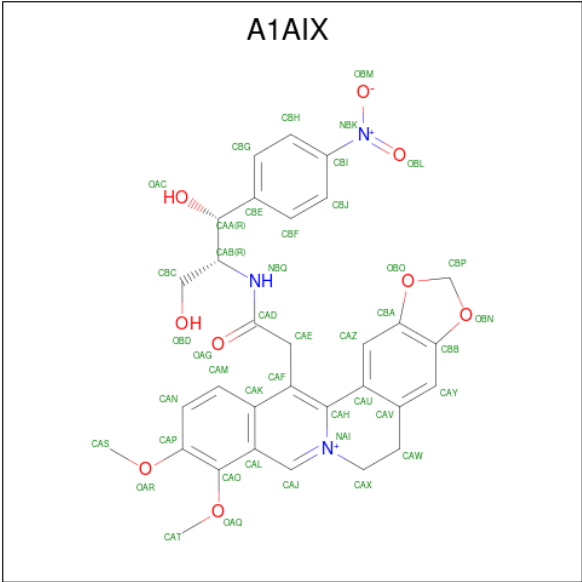
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2g	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2l	4	Total Mg 4 4	0	0
56	2q	3	Total Mg 3 3	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	1	Total Mg 1 1	0	0
56	2x	6	Total Mg 6 6	0	0
56	2y	4	Total Mg 4 4	0	0

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

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

- Molecule 58 is 13-(2-([(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]amino)-2-oxoethyl)-9,10-dimethoxy-5,6-dihydro-2H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-7-ium (CCD ID: A1AIX) (formula: C₃₁H₃₀N₃O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			43	31	3	9		
58	2A	1	Total	C	N	O	0	0
			43	31	3	9		

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

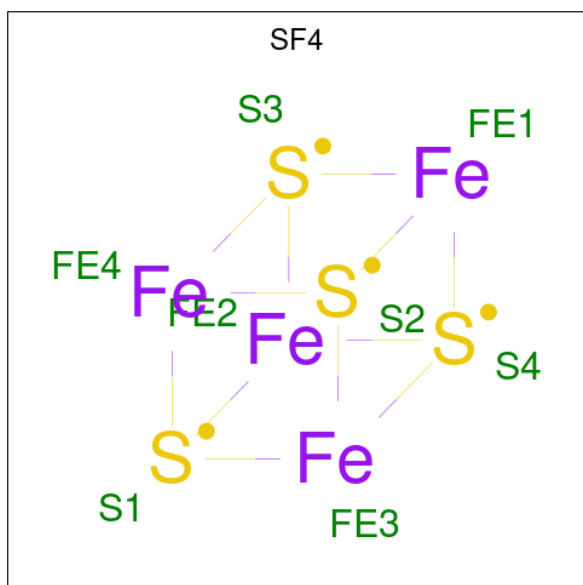
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0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

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1901	Total	O	0	0
			1901	1901		
61	1B	57	Total	O	0	0
			57	57		
61	1D	27	Total	O	0	0
			27	27		
61	1E	19	Total	O	0	0
			19	19		
61	1F	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	3	Total 3	O 3	0	0
61	1N	3	Total 3	O 3	0	0
61	1O	4	Total 4	O 4	0	0
61	1P	21	Total 21	O 21	0	0
61	1Q	8	Total 8	O 8	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	3	Total 3	O 3	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	11	Total 11	O 11	0	0
61	1V	5	Total 5	O 5	0	0
61	1W	10	Total 10	O 10	0	0
61	1X	4	Total 4	O 4	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	9	Total 9	O 9	0	0
61	11	6	Total 6	O 6	0	0
61	12	3	Total 3	O 3	0	0
61	13	4	Total 4	O 4	0	0
61	15	6	Total 6	O 6	0	0
61	16	2	Total 2	O 2	0	0
61	17	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	18	8	Total 8	O 8	0	0
61	1a	364	Total 364	O 364	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	2	Total 2	O 2	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	7	Total 7	O 7	0	0
61	1o	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	7	Total 7	O 7	0	0
61	1x	10	Total 10	O 10	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1097	Total 1097	O 1097	0	0
61	2B	22	Total 22	O 22	0	0
61	2D	19	Total 19	O 19	0	0
61	2E	13	Total 13	O 13	0	0
61	2F	13	Total 13	O 13	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	1	Total 1	O 1	0	0

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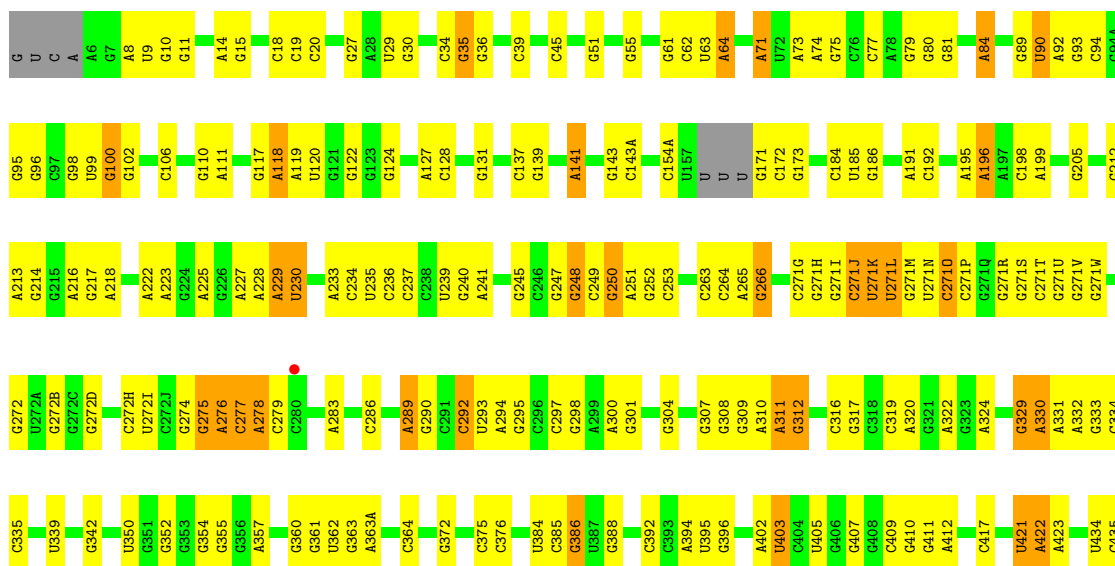
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2O	2	Total 2	O 2	0	0
61	2P	11	Total 11	O 11	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	5	Total 5	O 5	0	0
61	2T	3	Total 3	O 3	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	1	Total 1	O 1	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	2	Total 2	O 2	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	6	Total 6	O 6	0	0
61	21	7	Total 7	O 7	0	0
61	23	1	Total 1	O 1	0	0
61	26	1	Total 1	O 1	0	0
61	27	2	Total 2	O 2	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	260	Total 260	O 260	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	3	Total 3	O 3	0	0

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

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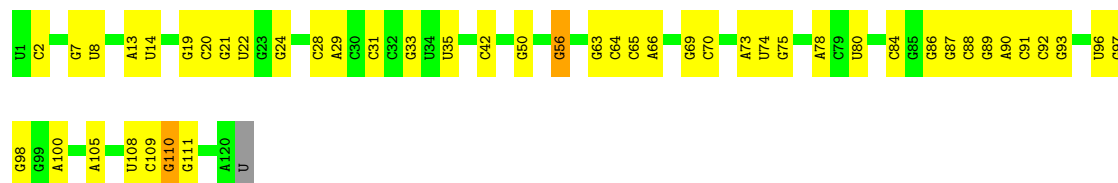






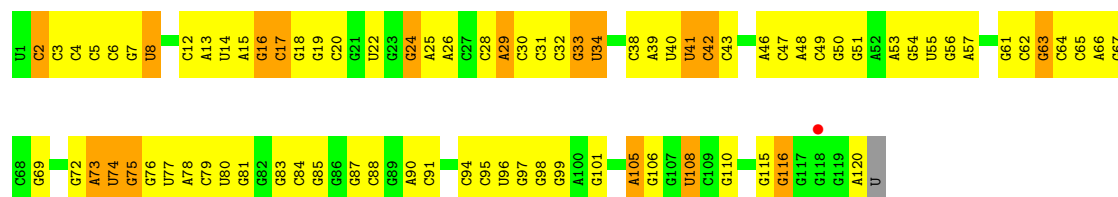
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 60% 37% ..



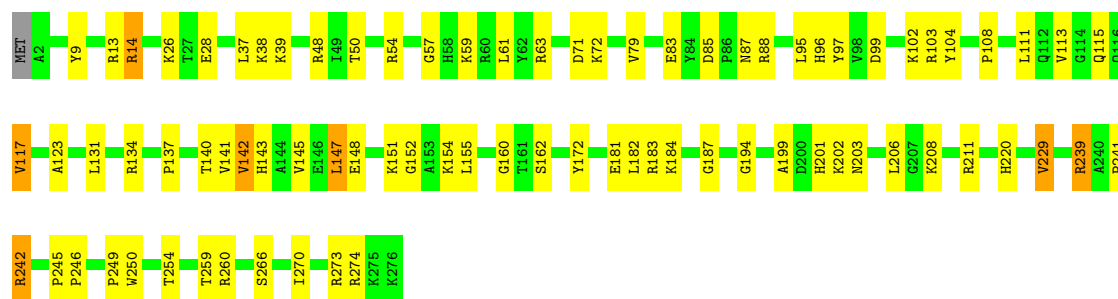
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 31% 55% 14% .



• Molecule 3: 50S ribosomal protein L2

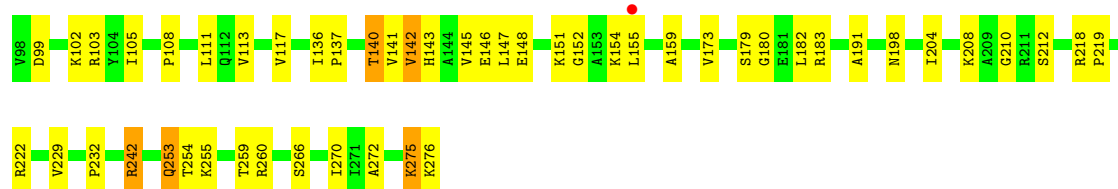
Chain 1D: 70% 27% .



• Molecule 3: 50S ribosomal protein L2

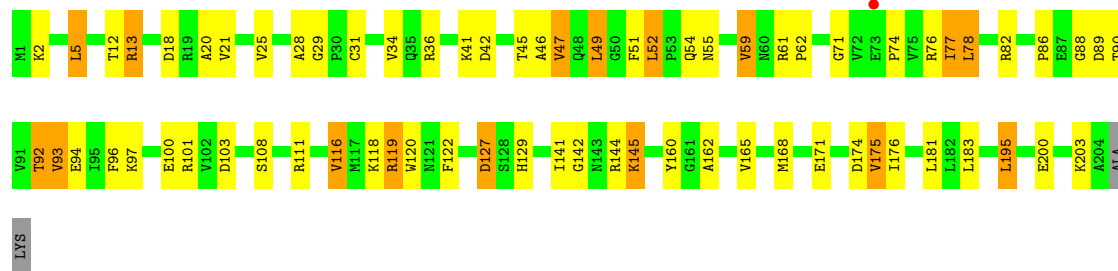
Chain 2D: 69% 28% .





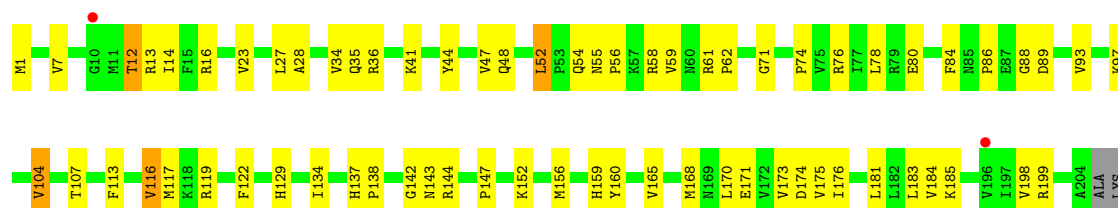
• Molecule 4: 50S ribosomal protein L3

Chain 1E: .



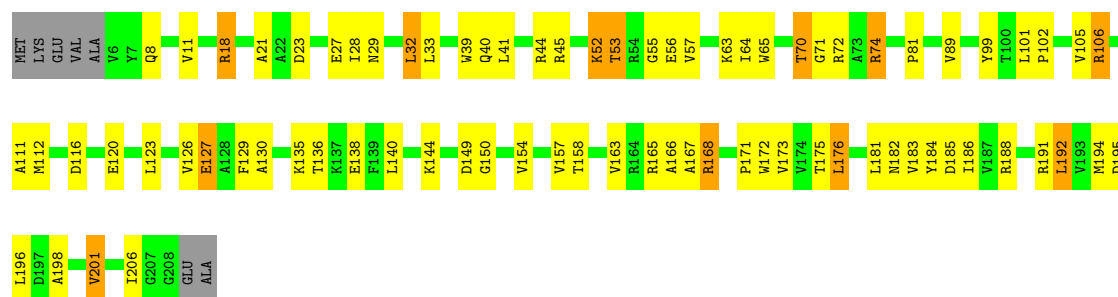
• Molecule 4: 50S ribosomal protein L3

Chain 2E: .



• Molecule 5: 50S ribosomal protein L4

Chain 1F: .

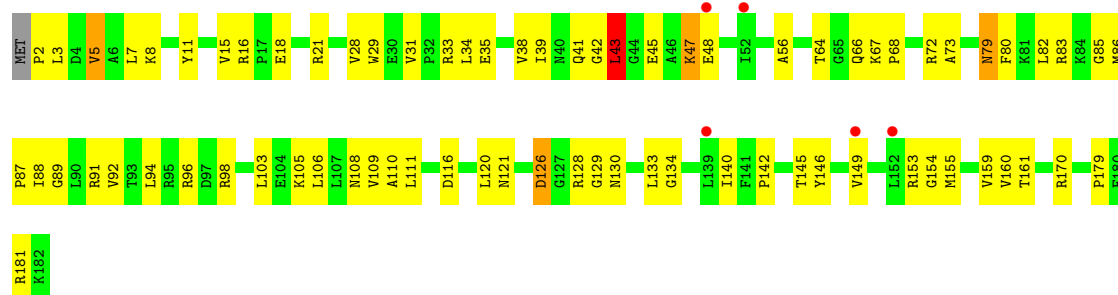


• Molecule 5: 50S ribosomal protein L4

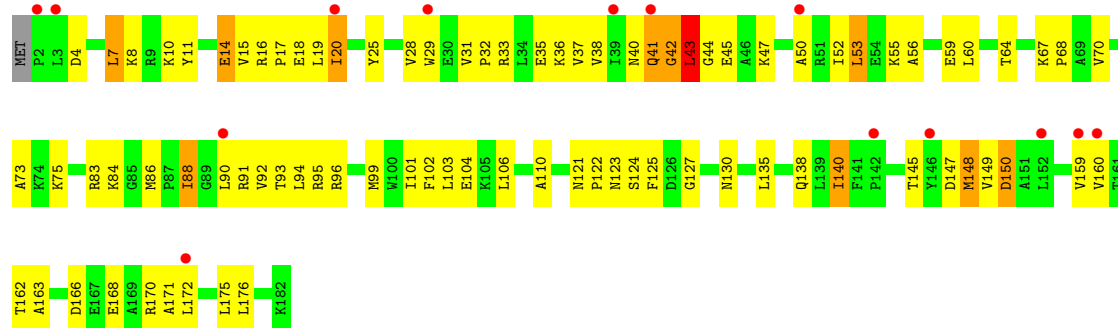
Chain 2F: .



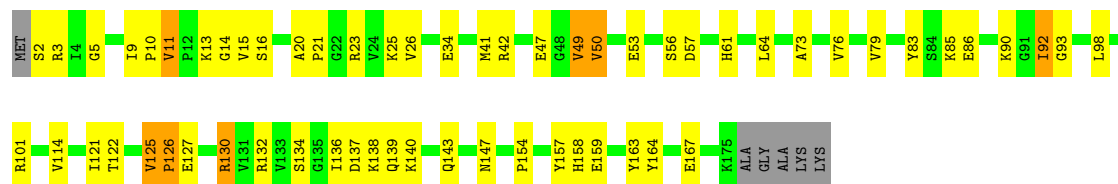
• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6



- Molecule 10: 50S ribosomal protein L14

Chain 1O: 78% 20%



- Molecule 10: 50S ribosomal protein L14

Chain 2O: 72% 27%



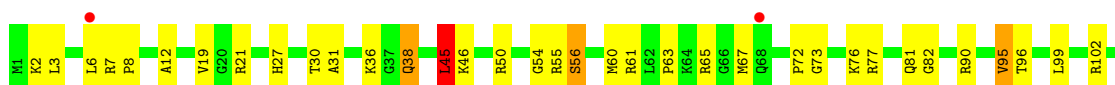
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 64% 31%



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 68% 28%



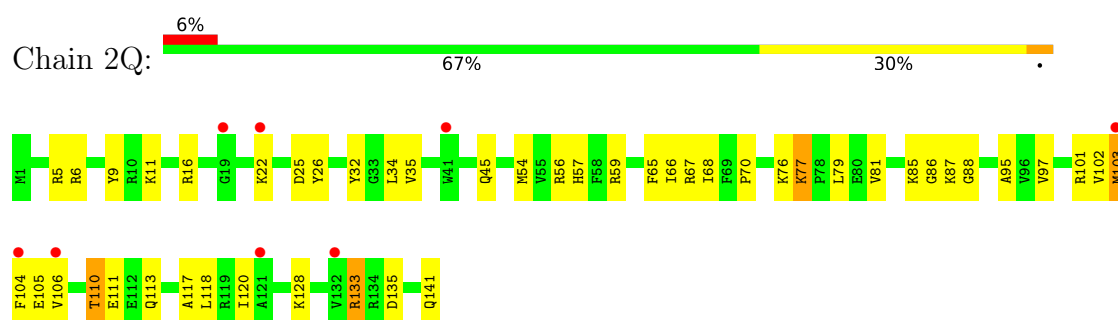
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 66% 33%

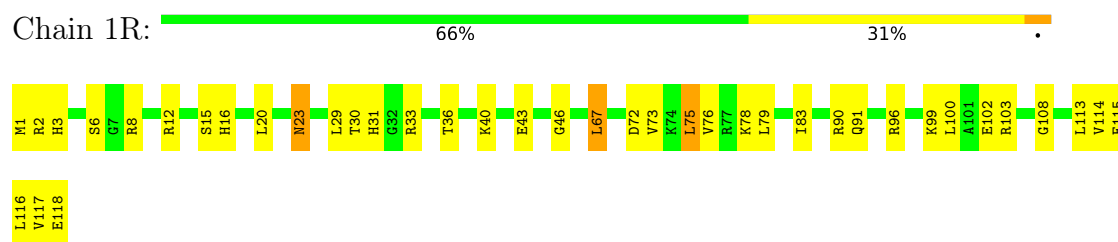


- Molecule 12: 50S ribosomal protein L16

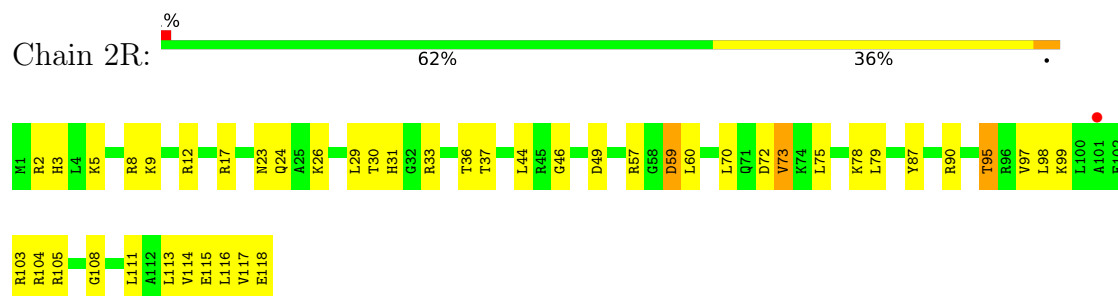




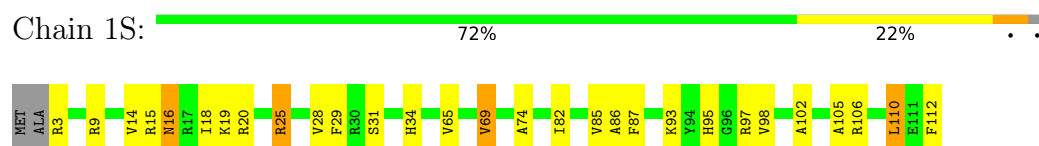
- Molecule 13: 50S ribosomal protein L17



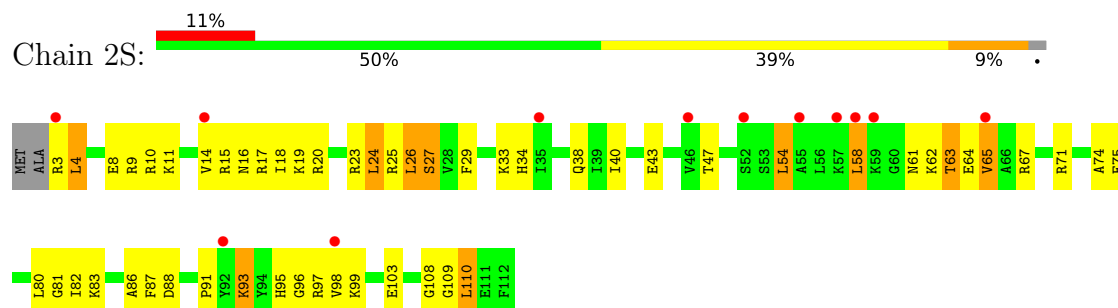
- Molecule 13: 50S ribosomal protein L17



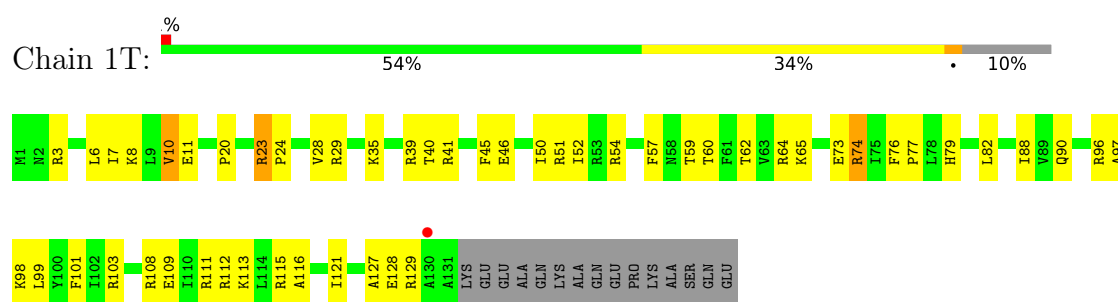
- Molecule 14: 50S ribosomal protein L18



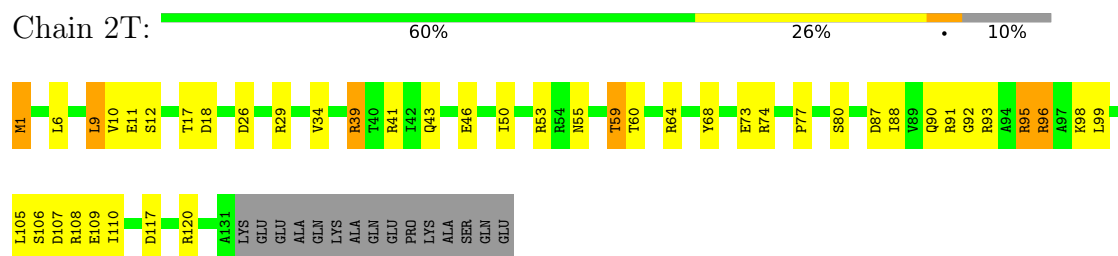
- Molecule 14: 50S ribosomal protein L18



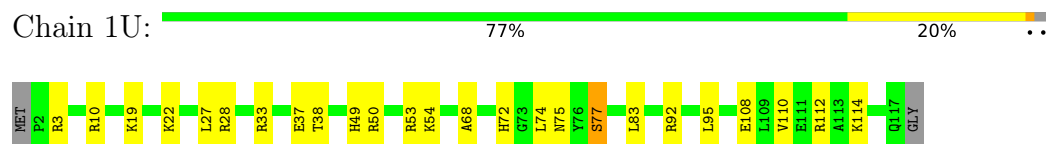
- Molecule 15: 50S ribosomal protein L19



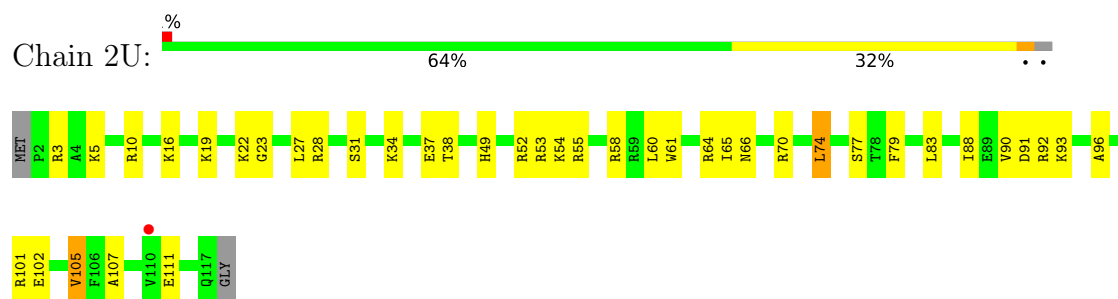
- Molecule 15: 50S ribosomal protein L19



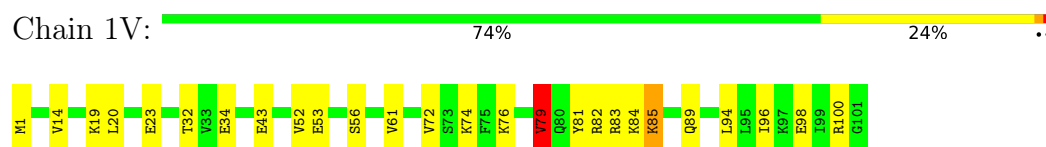
- Molecule 16: 50S ribosomal protein L20



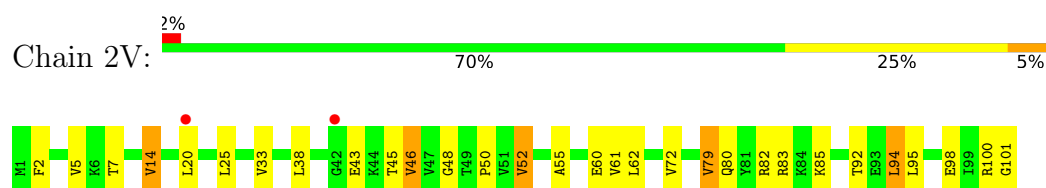
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



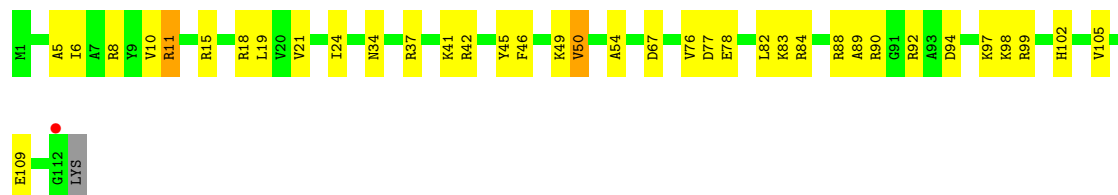
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  73% 23% ..



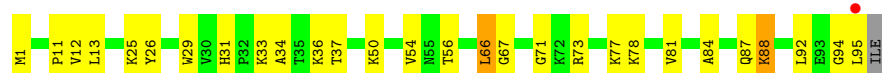
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  66% 31% ..



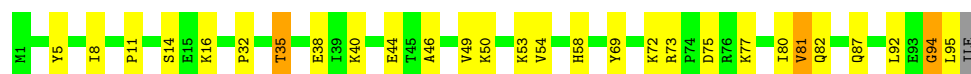
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  70% 27% ..



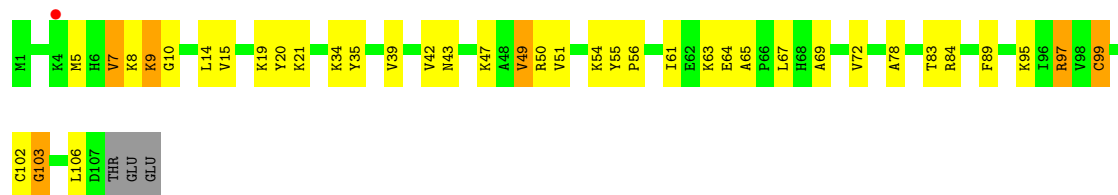
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  70% 26% ..



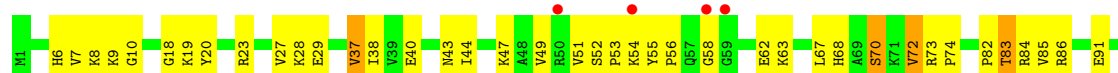
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  62% 30% 5% .



- Molecule 20: 50S ribosomal protein L24

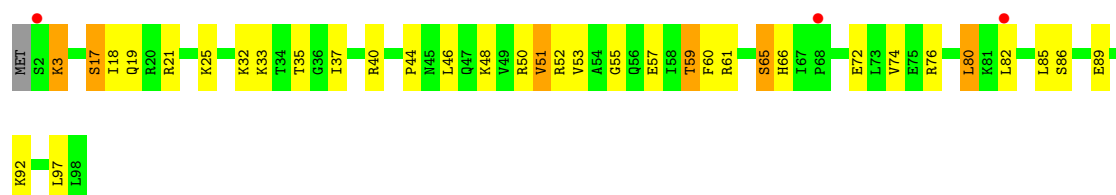
Chain 2Y:  58% 35% ..







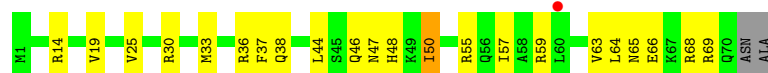
- Molecule 23: 50S ribosomal protein L28



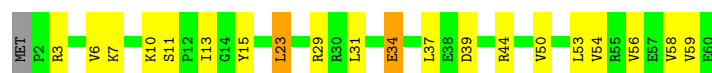
- Molecule 24: 50S ribosomal protein L29



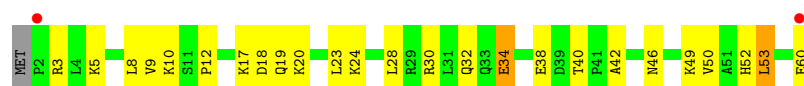
- Molecule 24: 50S ribosomal protein L29



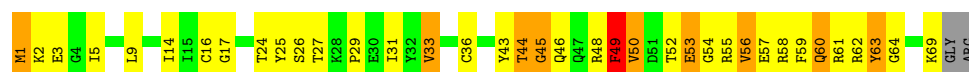
- Molecule 25: 50S ribosomal protein L30



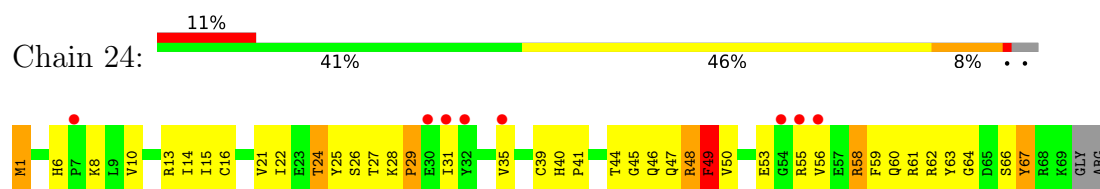
- Molecule 25: 50S ribosomal protein L30



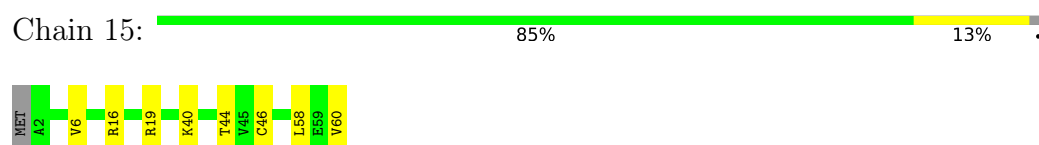
- Molecule 26: 50S ribosomal protein L31



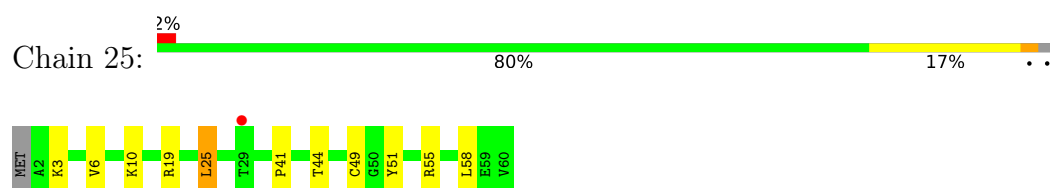
- Molecule 26: 50S ribosomal protein L31



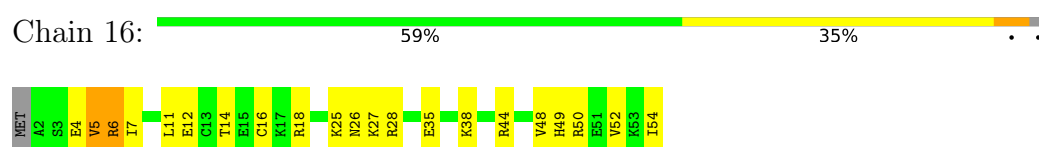
- Molecule 27: 50S ribosomal protein L32



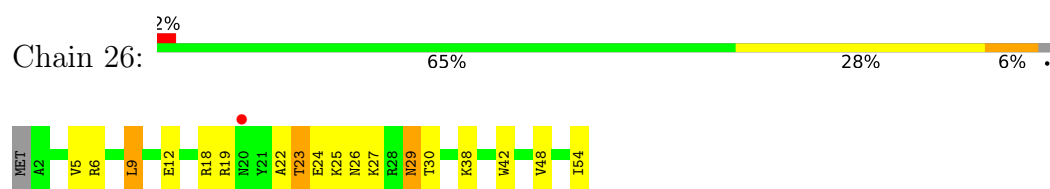
- Molecule 27: 50S ribosomal protein L32



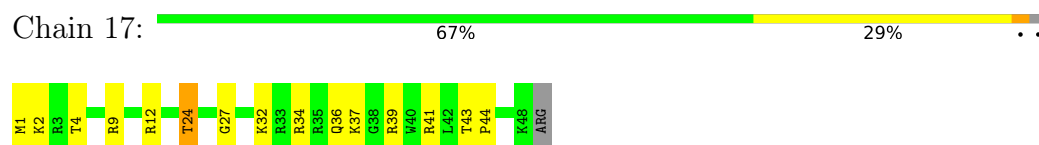
- Molecule 28: 50S ribosomal protein L33



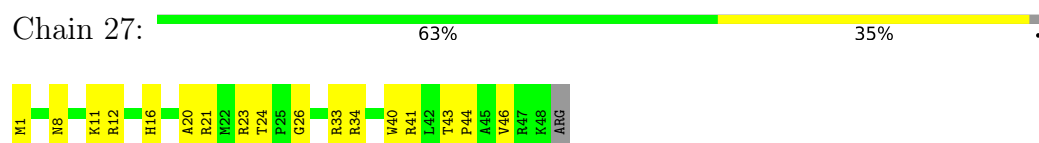
- Molecule 28: 50S ribosomal protein L33



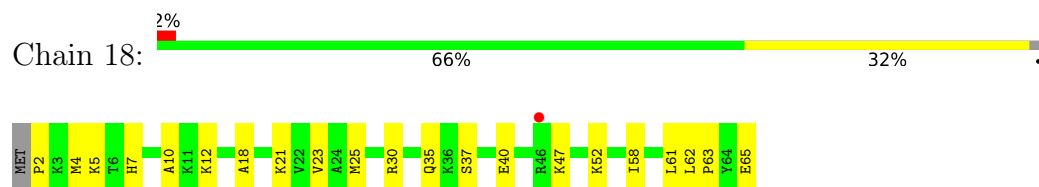
- Molecule 29: 50S ribosomal protein L34



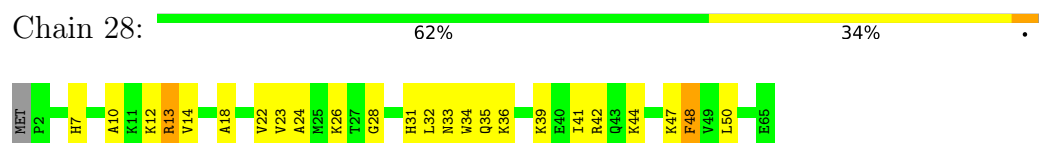
- Molecule 29: 50S ribosomal protein L34



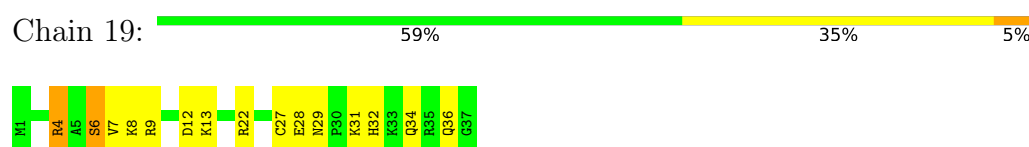
- Molecule 30: 50S ribosomal protein L35



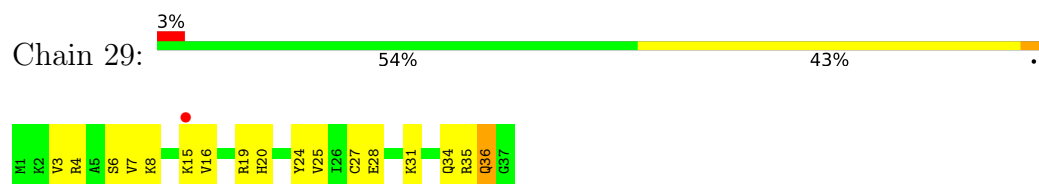
- Molecule 30: 50S ribosomal protein L35



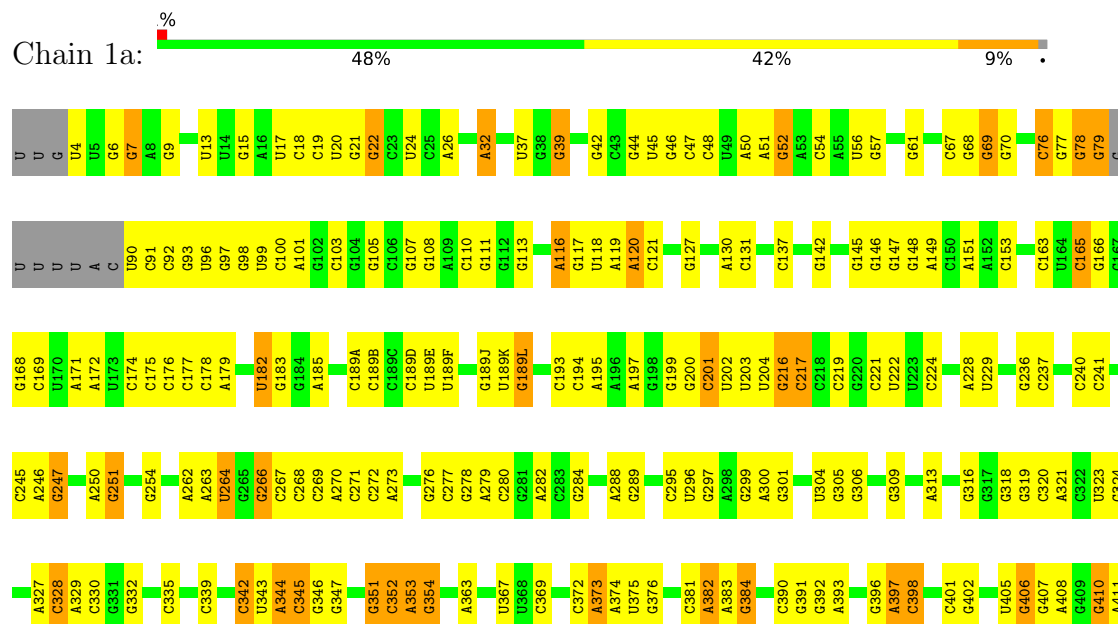
- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36

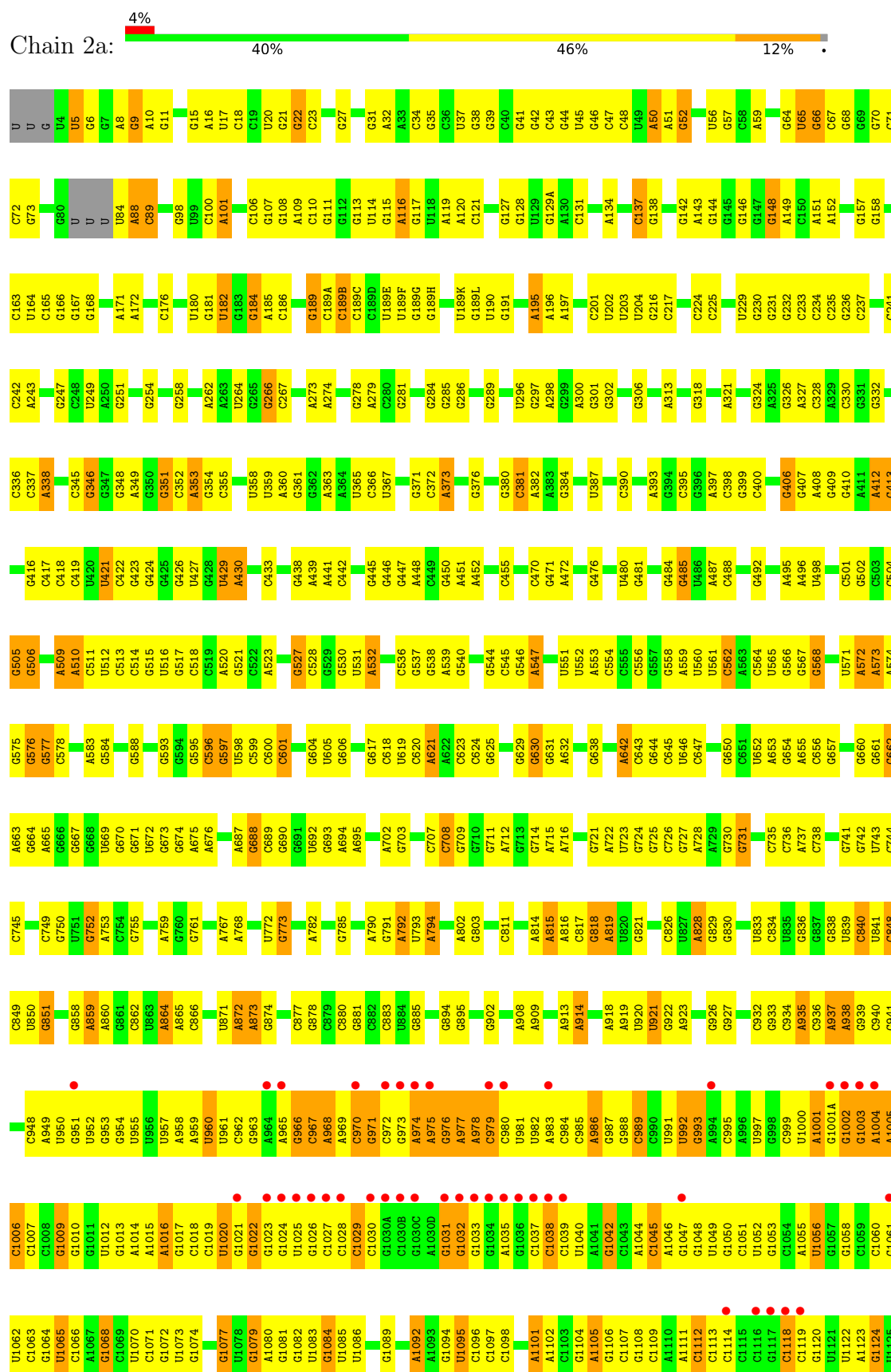


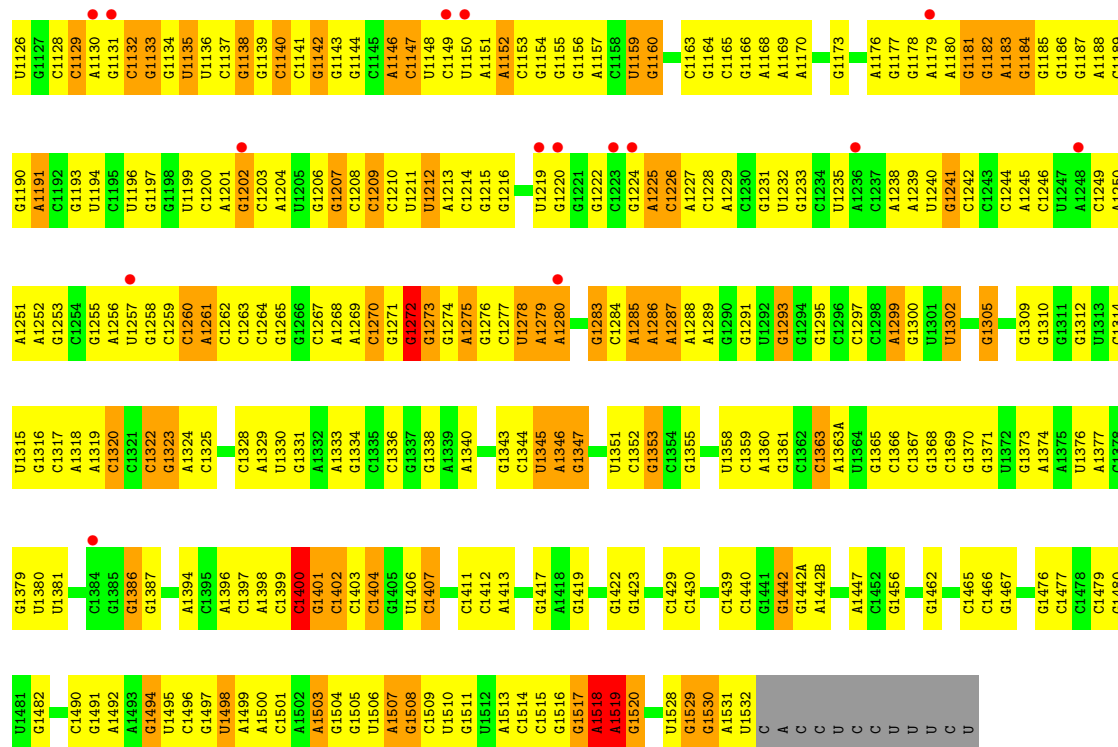
- Molecule 32: 16S Ribosomal RNA



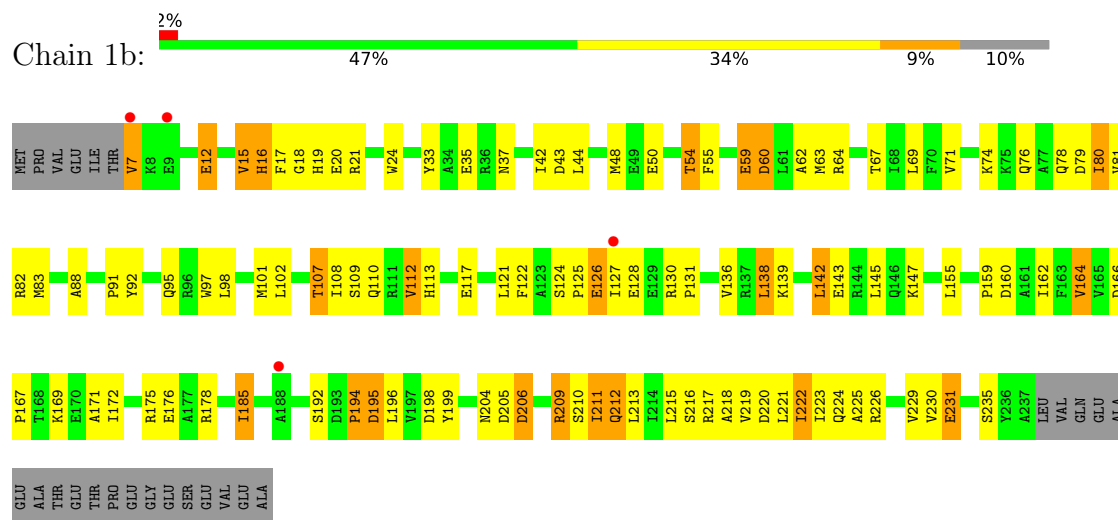
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U1510	U1414	G1266	C1189	G1104	G1030B	U961	G858	G755	A676	U580	C508	C418
U1511	G1418	G1337	U1194	C1107	G1030C	G963	G864	G760	U677	U581	A509	
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C1513	G1422	A1269	U1196	C1109	G1032	A965	A865	C762	C680	G584	C511	C423
C1514	G1423	G1270	G1197	C1118	G1033	G966	C868	A767	U679	G593	U516	C424
C1515	G1424	G1271	C1198	C1119	G1034	G967	C869	A768	G683	C596	G517	G425
G1516	U1345	G1272	U1199	C1120	A1035	C968	U870	G769	G688	U598	C518	G426
G1517	U1346	A1275	C1200	G1121	G1036	A969	U871	A770	A687	G597	C519	U427
A1518	G1347	G1276	A1201	U1122	C1037	C970	A872	G771	C689	U599	A520	U428
A1519	U1348	C1277	C1202	A1123	C1038	G971	A873	A772	G690	C600	G524	U429
U1522	A1433	U1278	G1207	G1124	C1039	C972	A874	A773	G691	C601	C525	A430
G1529	A1434	A1279	C1208	U1125	A1040	C973	G877	A781	U680	A602	G526	A431
G1530	U1435	A1280	C1209	U1126	A1041	A974	C878	A782	C692	A607	G527	A432
A1531	G1353	C1284	U1212	C1127	A1044	G976	G881	U789	A694	A607	G534	U434
C1532	G1354	A1285	U1213	C1128	G1048	A977	G885	A790	A696	A614	G535	C436
C1533	G1355	A1286	C1214	G1131	C1051	A978	G886	G791	A697	A614	C536	U437
A	G1442	A1287	G1215	C1132	U1052	C979	G887	A792	C701	C618	G540	A438
C	G1442A	A1288	G1216	G1133	G1053	C980	G888	U793	C701	C618	A532	A439
C	G1445	A1289	G1217	G1134	G1054	U981	G889	A794	G710	U619	A533	A441
U	U1446	G1290	C1218	U1135	A1055	U982	G890	A795	G710	A622	A534	C442
C	A1447	U1291	U1219	U1136	A1056	A983	G891	A796	G710	A622	A535	C443
C	A1452	U1292	U1220	C1137	U1057	A986	G902	G799	G713	G623	C536	C444
U	G1456	G1293	G1221	G1138	G1058	U992	G903	U801	G714	G624	C545	C445
U	G1457	C1298	G1222	G1139	G1059	U993	G904	U802	G715	G625	G546	C446
U	G1458	C1299	G1223	G1140	G1060	A994	G905	U803	G716	G626	A547	C447
C	G1461	G1300	G1224	G1141	G1061	C995	A915	G811	G719	G627	C548	A448
U	G1462	U1302	A1225	G1142	U1062	U996	G916	C812	A722	G628	G549	A452
U	G1463	C1303	A1226	G1143	G1063	G997	G917	A815	A723	G629	C550	A453
C	G1464	G1304	A1227	G1144	C1063	C998	A918	A816	G724	G630	C551	C454
C	C1465	G1305	G1233	C1145	G1068	C999	A918	C817	G725	G631	C552	C455
U	U1376	G1306	G1234	C1147	C1069	U1000	U921	G818	G726	G632	C553	C456
U	A1377	G1309	U1235	U1150	U1070	U1001	G922	U819	G727	G633	C554	C457
U	U1381	G1312	A1236	A1151	C1071	G1001A	G923	U820	A728	G634	C555	C458
U	C1382	U1313	C1237	A1152	G1077	G1002	G924	U821	A729	A640	C556	G460
U	G1385	C1314	A1238	G1153	U1078	G1003	G925	C822	A730	U641	C557	A461
U	G1386	U1240	U1240	G1154	G1079	G1004	G926	C823	G730	A642	G558	C470
U	G1390	A1245	A1245	A1157	A1080	A1005	G927	C824	G731	A642	C559	C471
U	U1391	C1246	C1246	C1158	G1081	C1006	C934	C825	G734	U646	U560	A472
U	G1392	A1318	U1247	U1159	G1082	A1015	C935	C826	A737	C647	U561	G473
U	C1397	C1320	G1250	G1160	U1085	A1016	C936	U827	C738	U652	C562	G476
U	A1398	C1321	A1250	C1163	U1086	G1017	A937	C829	C739	A653	C563	A477
U	C1399	G1322	A1251	C1172	U1086	U1020	A938	G836	G741	G660	U565	C483
U	C1400	G1323	A1252	G1173	U1091	G1021	G939	G837	G742	G661	G566	G484
U	A1498	C1324	G1253	G1173	A1092	G1022	G942	U838	U743	G662	G567	C485
U	A1500	C1325	C1254	A1179	A1093	G1023	U943	U839	C744	A663	G568	U486
U	C1501	G1326	G1255	A1180	G1094	G1024	G944	C840	G745	G664	G569	A487
U	A1502	C1327	A1256	A1180	U1095	U1025	G945	U841	C746	G665	A572	A495
U	C1403	U1257	U1257	A1183	G1099	G1026	A946	C848	C749	G666	A573	A496
U	C1404	U1257	U1257	G1184	U1099	G1027	G947	C849	G750	G667	A574	U498
U	C1407	C1260	C1260	G1185	C1100	C1028	C948	U850	G751	G668	G575	A499
U	C1411	C1263	C1263	G1186	A1101	C1029		G851	G752	G673	G576	C501

• Molecule 32: 16S Ribosomal RNA

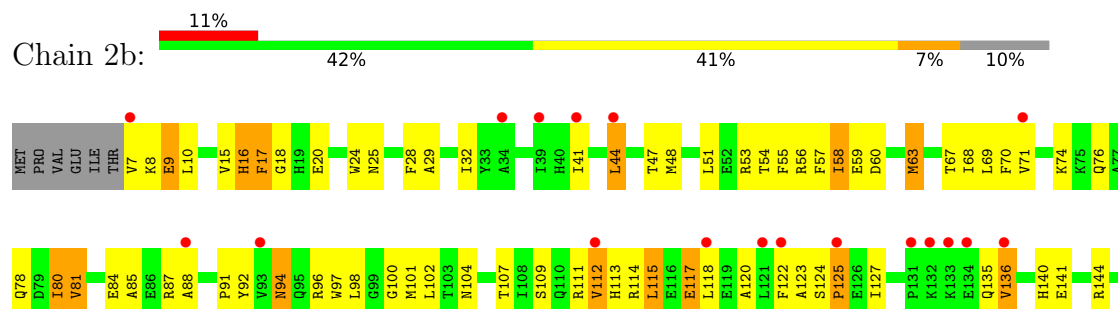


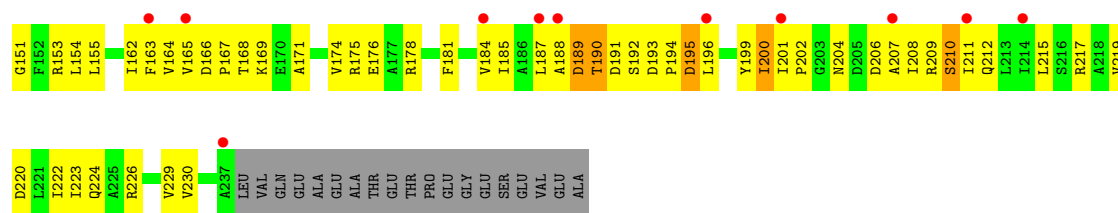


• Molecule 33: 30S ribosomal protein S2

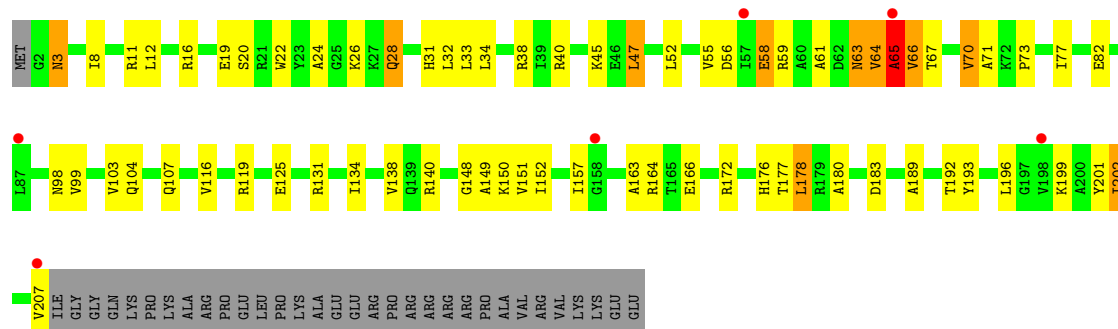


• Molecule 33: 30S ribosomal protein S2

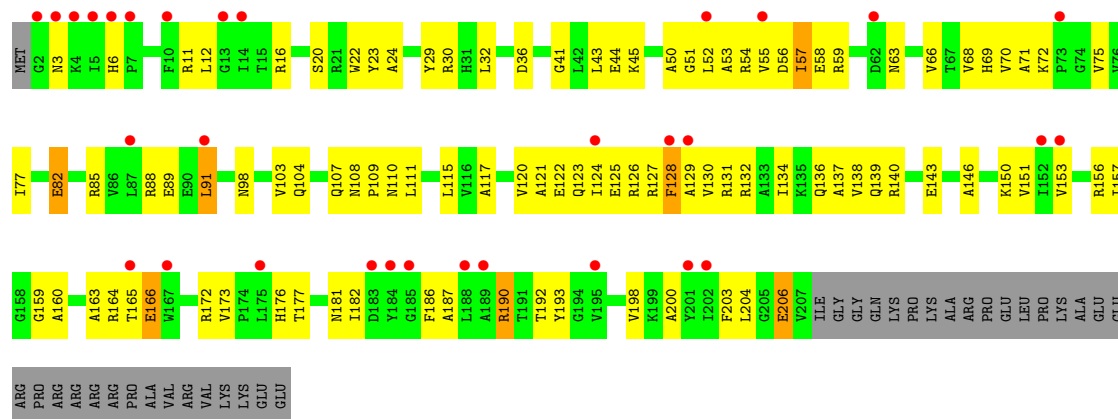




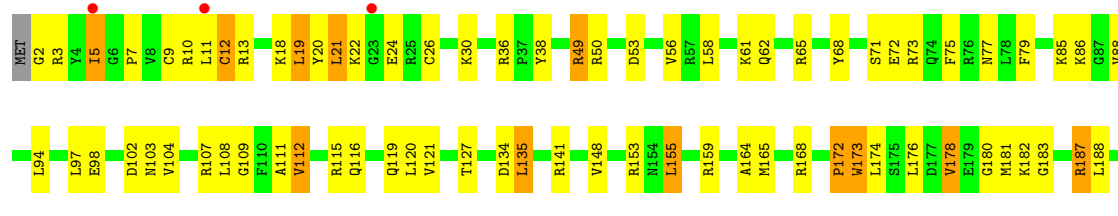
• Molecule 34: 30S ribosomal protein S3

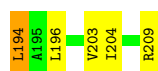


• Molecule 34: 30S ribosomal protein S3

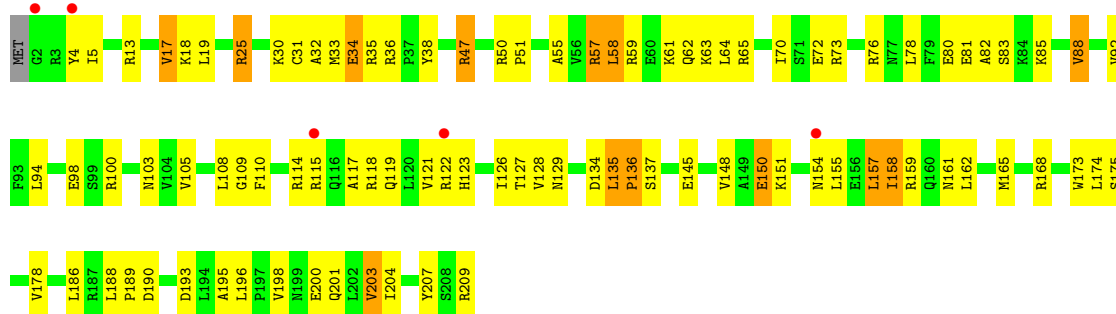


• Molecule 35: 30S ribosomal protein S4

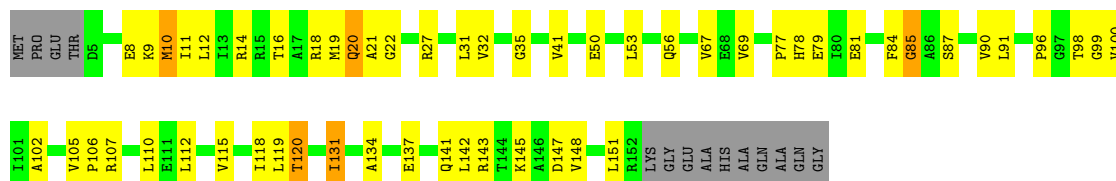




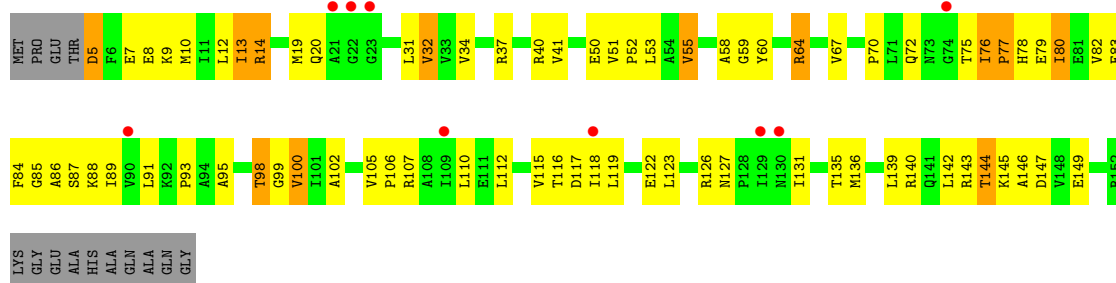
• Molecule 35: 30S ribosomal protein S4



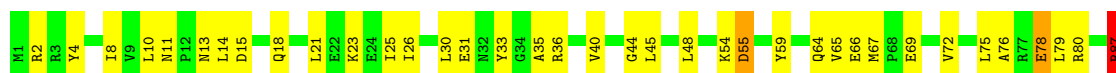
• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5



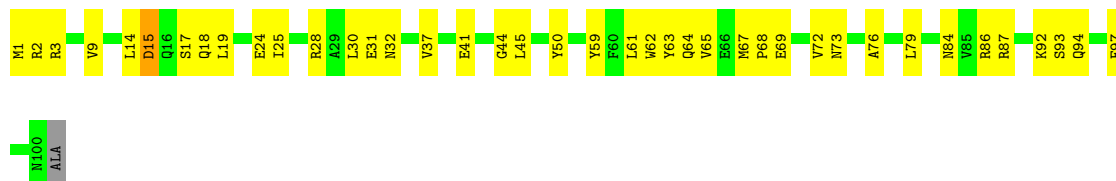
• Molecule 37: 30S ribosomal protein S6





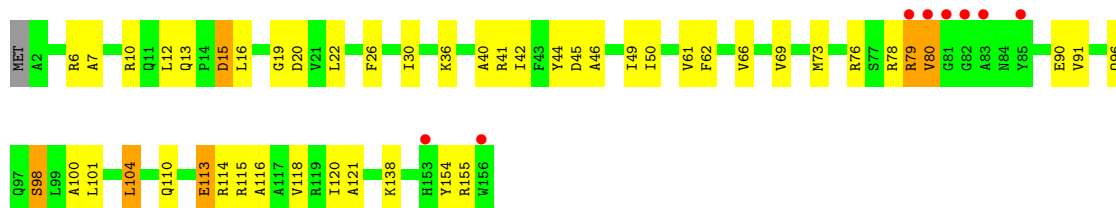
• Molecule 37: 30S ribosomal protein S6

Chain 2f: 59% 39% ..



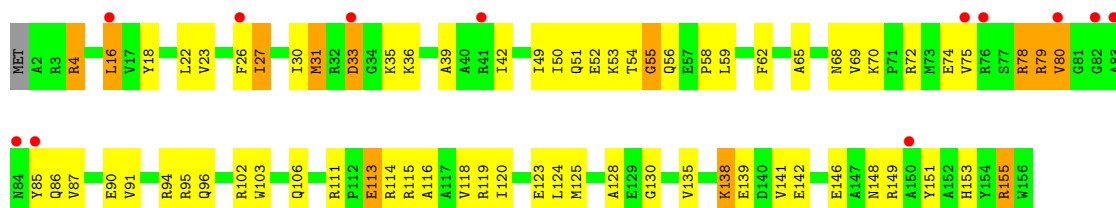
• Molecule 38: 30S ribosomal protein S7

Chain 1g: 5% 69% 27% ..



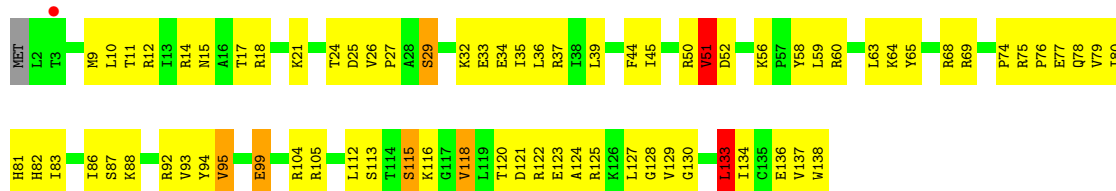
• Molecule 38: 30S ribosomal protein S7

Chain 2g: 8% 54% 37% 8% .



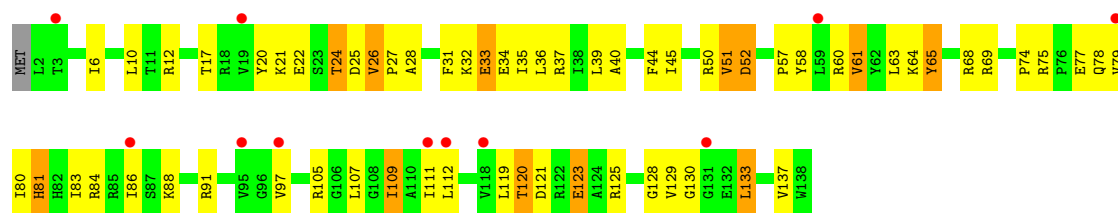
• Molecule 39: 30S ribosomal protein S8

Chain 1h: % 45% 49% ..

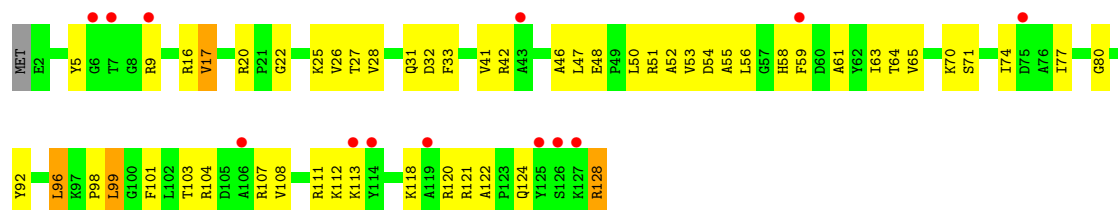


• Molecule 39: 30S ribosomal protein S8

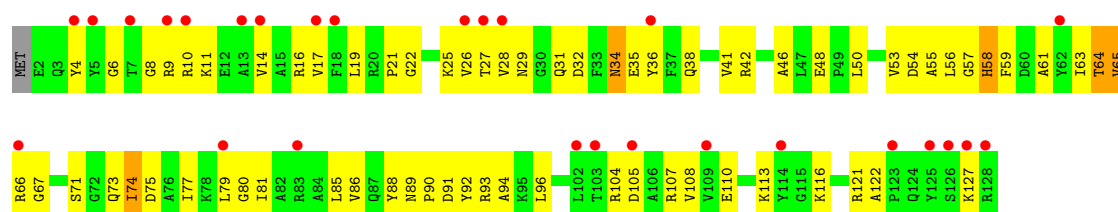
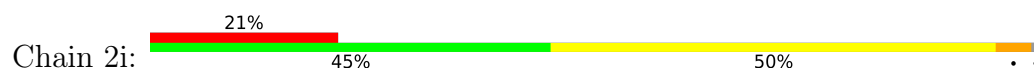
Chain 2h: 8% 54% 37% 9% .



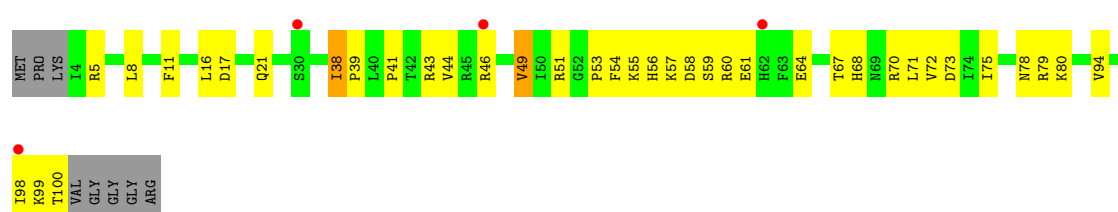
• Molecule 40: 30S ribosomal protein S9



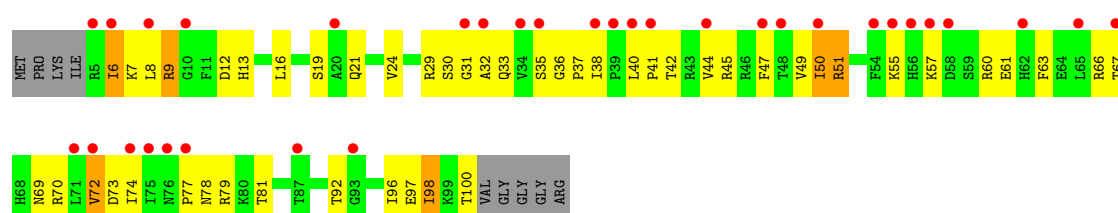
• Molecule 40: 30S ribosomal protein S9



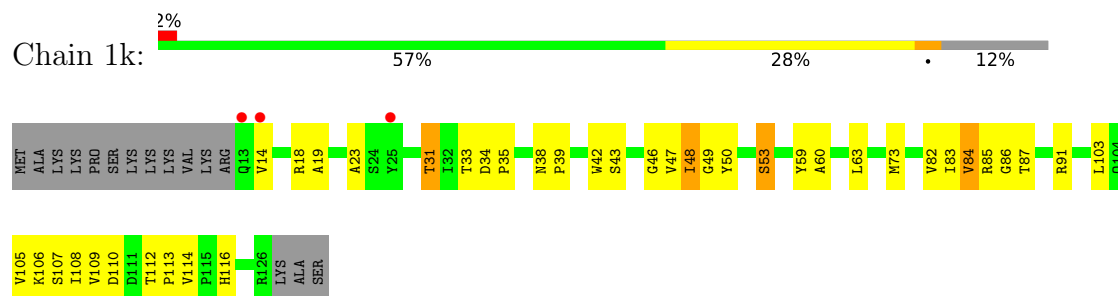
• Molecule 41: 30S ribosomal protein S10



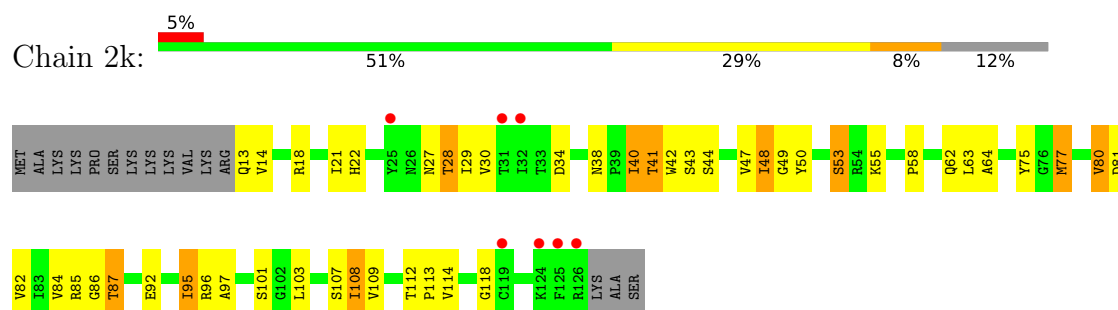
• Molecule 41: 30S ribosomal protein S10



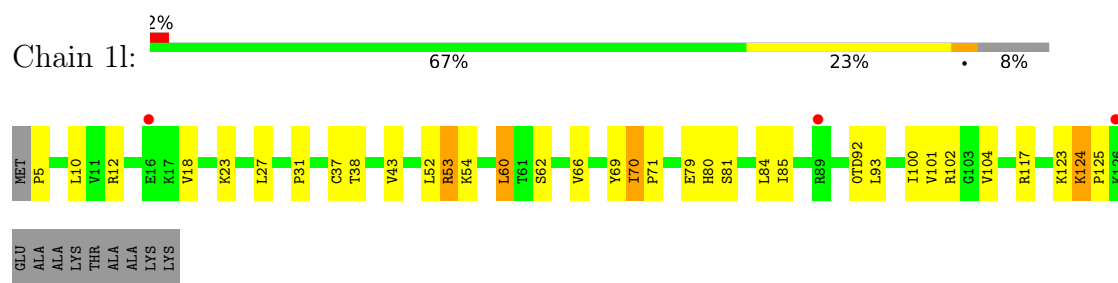
- Molecule 42: 30S ribosomal protein S11



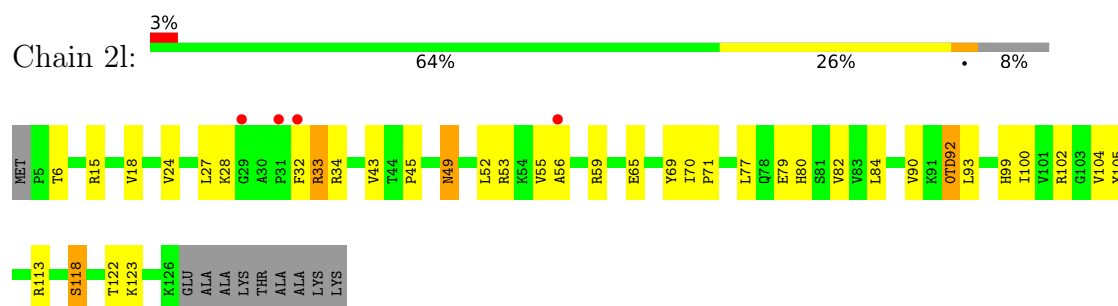
- Molecule 42: 30S ribosomal protein S11



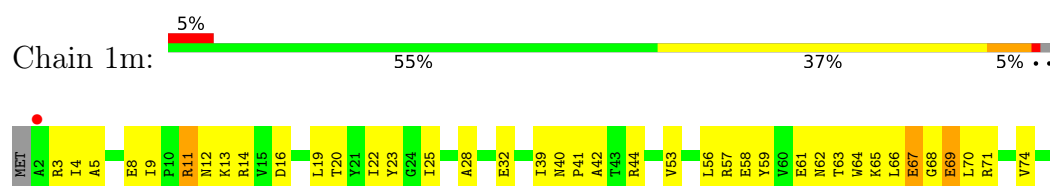
- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

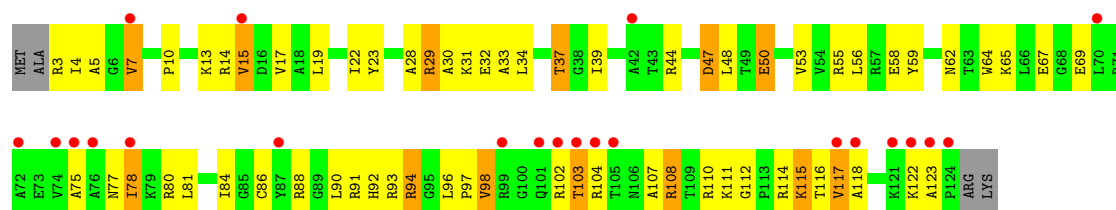


- Molecule 44: 30S ribosomal protein S13

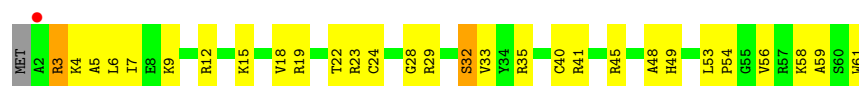




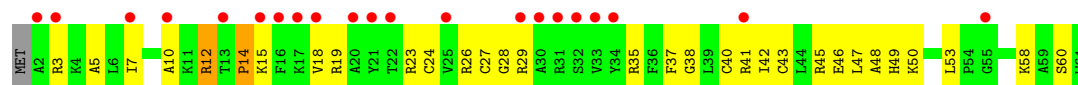
- Molecule 44: 30S ribosomal protein S13



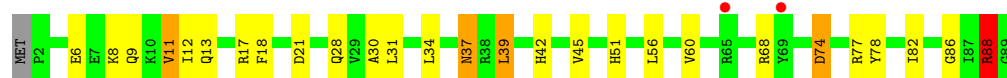
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

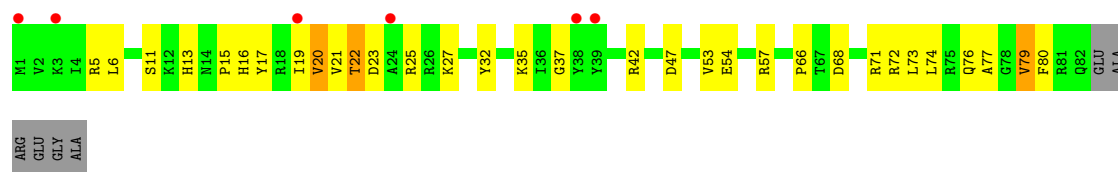


- Molecule 46: 30S ribosomal protein S15

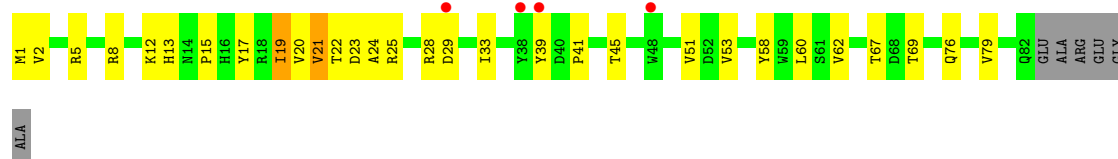


- Molecule 47: 30S ribosomal protein S16





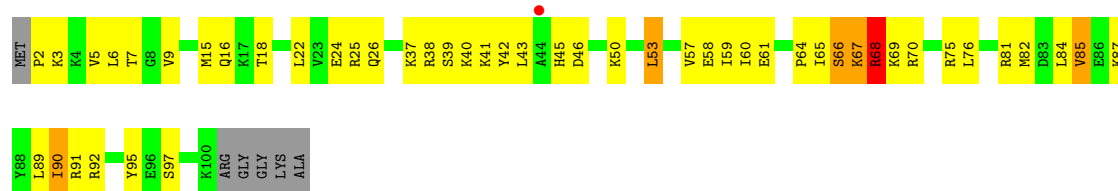
- Molecule 47: 30S ribosomal protein S16



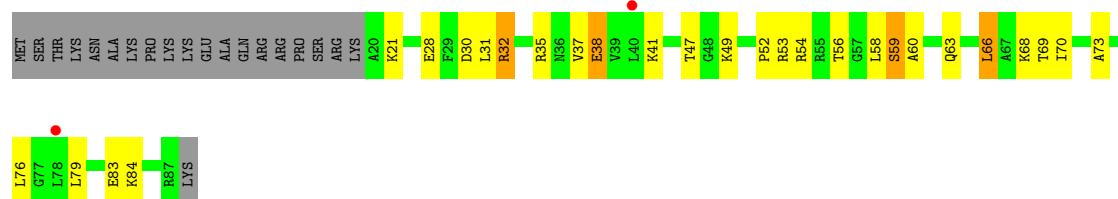
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

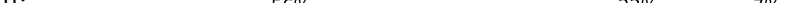
LYS	MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG LYS A20 R35 R36 V37 E38 K41 L44 S45 E46 P52 R53 R54 R55 T56 G57 L58 E62 Q63 R64 T65 L66 T69 R72 A73 R74 G77 L78 L79 K84 L85 V86 R87

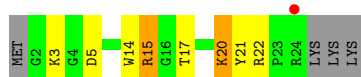
- Chain 1s:  49% 35% 11%

- Chain 2s:
-
- | Amino Acid | Percentage |
|------------|------------|
| MET | 14% |
| P2 | 34% |
| R3 | 41% |
| S4 | 14% |
| L5 | 11% |
| K6 | |
| K7 | |
| G8 | |
| V9 | |
| F10 | |
| V11 | |
| D12 | |
| D13 | |
| H14 | |
| L15 | |
| L16 | |
| E17 | |
| K18 | |
| V19 | |
| L20 | |
| E21 | |
| L22 | |
| N23 | |
| E27 | |
| K28 | |
| R29 | |
| L30 | |
| I31 | |
| K32 | |
| T33 | |
| W34 | |
| S35 | |
| R36 | |
| R37 | |
| S38 | |
| T39 | |
| I40 | |
| V41 | |
| P42 | |
| E43 | |
| M44 | |
| V45 | |
| T48 | |
| I49 | |
| A50 | |
| V51 | |
| H57 | |
| V60 | |
| I62 | |
| T63 | |
| E64 | |
| V67 | |
| G68 | |
| H69 | |

- Chain 1t:
-
- 50% 37% 6% 9%
- MET ALA GLN V88 LYS LYS PRO LYS R8 N9 L10 S11 A12 L13 K14 R17 Q18 R22 R23 L24 S31 L36 K39 A40 L43 A44 Q45 E46 G47 K48 E51 I55 M56 R57 E60 G69 S70 T71 L72 H73 K74 N75 A76 A77 R80 K81 S82 R83 L84 W85

- Chain 2t:
-
- | Amino Acid | Percentage |
|------------|------------|
| R8 | 7% |
| N9 | |
| L10 | |
| S11 | |
| K14 | |
| R15 | |
| H16 | |
| R17 | |
| Q18 | |
| S19 | |
| L24 | |
| K29 | |
| K30 | |
| S31 | |
| A40 | |
| E45 | |
| G47 | |
| K48 | |
| K54 | |
| I55 | |
| M56 | |
| A66 | |
| A67 | |
| K68 | |
| G69 | |
| T71 | |
| T72 | |
| L73 | |
| H74 | |
| K74 | |
| A77 | |
| A78 | |
| M85 | |
| E93 | |
| G103 | |

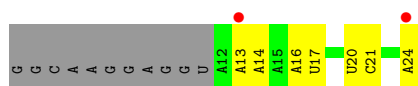
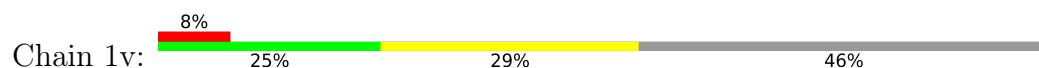
- Chain 1u: 



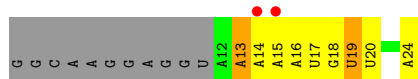
- Molecule 52: 30S ribosomal protein Thx



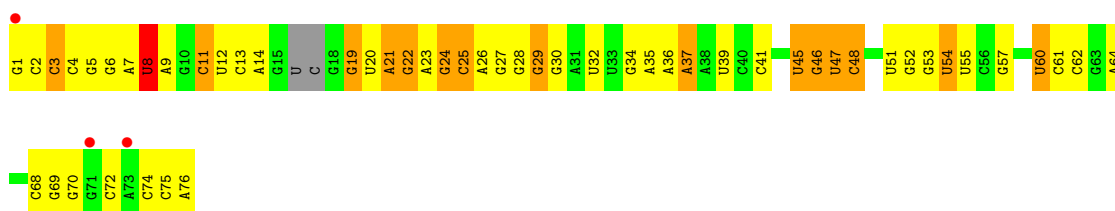
- Molecule 53: MF-mRNA



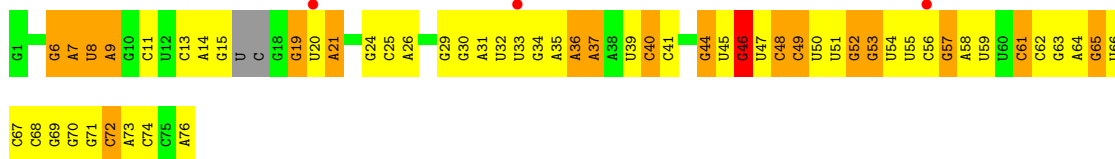
- Molecule 53: MF-mRNA



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

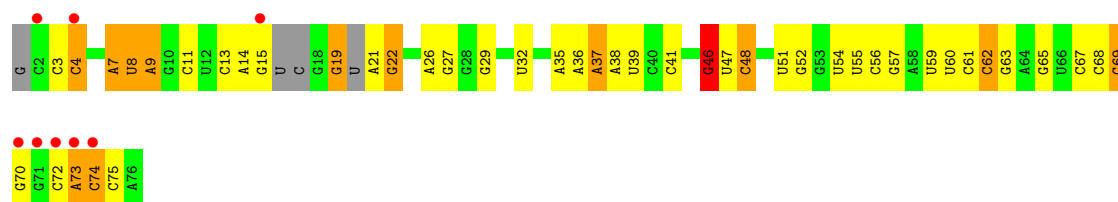


- Molecule 54: A-site and E-site Deacylated tRNAphe

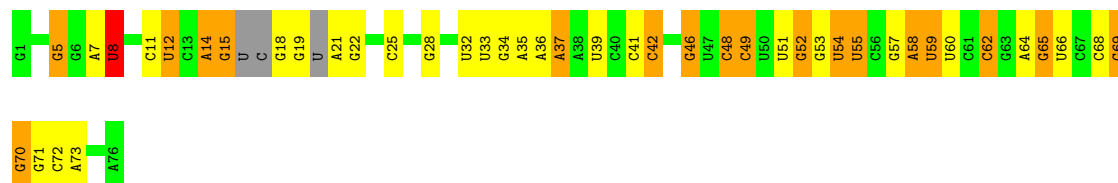


- Molecule 54: A-site and E-site Deacylated tRNAphe

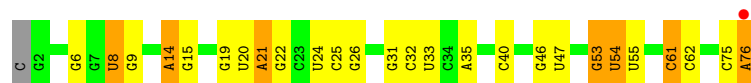




- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



- Molecule 55: P-site Deacylated tRNA^{met}



- Molecule 55: P-site Deacylated tRNA^{met}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.47Å 447.66Å 619.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.26 – 2.80 124.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (124.26-2.80) 98.6 (124.26-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.284 0.229 , 0.282	Depositor DCC
R_{free} test set	69396 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299897	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: OMU, MG, 4OC, M2G, 4SU, G7M, 2MA, OMG, MIA, 0TD, PSU, SF4, 5MC, 2MG, UR3, 5MU, MA6, K, OMC, A1AIX, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.30	0/69011	0.48	0/107720
1	2A	0.23	0/67295	0.41	1/105042 (0.0%)
2	1B	0.25	0/2882	0.43	0/4494
2	2B	0.20	0/2879	0.38	0/4487
3	1D	0.29	0/2186	0.53	0/2944
3	2D	0.23	0/2186	0.48	1/2944 (0.0%)
4	1E	0.28	0/1592	0.54	1/2149 (0.0%)
4	2E	0.23	0/1592	0.47	0/2149
5	1F	0.29	0/1622	0.49	0/2196
5	2F	0.22	0/1618	0.48	2/2191 (0.1%)
6	1G	0.24	0/1448	0.51	1/1957 (0.1%)
6	2G	0.20	0/1453	0.46	0/1963
7	1H	0.23	0/1356	0.45	0/1834
7	2H	0.20	0/1356	0.43	0/1834
8	1I	0.20	0/1112	0.41	0/1514
8	2I	0.19	0/1079	0.44	0/1475
9	1N	0.26	0/1144	0.48	0/1543
9	2N	0.20	0/1144	0.42	0/1543
10	1O	0.28	0/943	0.51	0/1269
10	2O	0.21	0/943	0.47	0/1269
11	1P	0.29	0/1152	0.58	0/1533
11	2P	0.22	0/1152	0.49	0/1533
12	1Q	0.31	0/1143	0.52	0/1527
12	2Q	0.22	0/1143	0.43	0/1527
13	1R	0.30	0/982	0.52	0/1312
13	2R	0.24	0/982	0.45	0/1312
14	1S	0.26	0/883	0.50	0/1176
14	2S	0.20	0/880	0.48	0/1172
15	1T	0.26	0/1105	0.53	0/1477
15	2T	0.22	0/1097	0.47	0/1468
16	1U	0.31	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.38	0/1301
17	1V	0.28	0/782	0.47	0/1049
17	2V	0.21	0/782	0.46	0/1049
18	1W	0.31	0/897	0.50	0/1205
18	2W	0.24	0/897	0.45	0/1205
19	1X	0.28	0/764	0.54	0/1025
19	2X	0.21	0/764	0.52	2/1025 (0.2%)
20	1Y	0.24	0/819	0.48	0/1095
20	2Y	0.23	0/819	0.47	1/1095 (0.1%)
21	1Z	0.24	0/1267	0.47	0/1717
21	2Z	0.23	0/1299	0.47	0/1763
22	10	0.26	0/662	0.48	0/881
22	20	0.22	0/662	0.43	0/881
23	11	0.30	0/762	0.49	0/1014
23	21	0.23	0/762	0.43	0/1014
24	12	0.24	0/590	0.46	0/781
24	22	0.20	0/590	0.39	0/781
25	13	0.28	0/474	0.47	0/635
25	23	0.21	0/469	0.44	0/630
26	14	0.26	0/565	0.52	0/761
26	24	0.25	0/545	0.52	0/737
27	15	0.30	0/469	0.56	0/635
27	25	0.28	0/469	0.47	0/635
28	16	0.27	0/460	0.47	0/613
28	26	0.21	0/456	0.44	0/608
29	17	0.34	0/426	0.55	0/561
29	27	0.25	0/426	0.55	0/561
30	18	0.30	0/525	0.53	0/691
30	28	0.22	0/525	0.44	0/691
31	19	0.26	0/310	0.47	0/407
31	29	0.20	0/310	0.41	0/407
32	1a	0.21	0/35795	0.39	0/55864
32	2a	0.20	0/35886	0.38	2/56005 (0.0%)
33	1b	0.24	0/1881	0.53	0/2542
33	2b	0.26	0/1860	0.55	2/2518 (0.1%)
34	1c	0.24	0/1572	0.50	2/2126 (0.1%)
34	2c	0.23	0/1566	0.53	2/2119 (0.1%)
35	1d	0.22	0/1685	0.46	0/2262
35	2d	0.20	0/1704	0.44	0/2284
36	1e	0.24	0/1145	0.45	0/1543
36	2e	0.19	0/1149	0.46	0/1548
37	1f	0.21	0/823	0.44	0/1115
37	2f	0.20	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.21	0/1250	0.49	0/1679
38	2g	0.22	0/1254	0.48	0/1683
39	1h	0.23	0/1108	0.45	0/1494
39	2h	0.22	0/1108	0.46	0/1494
40	1i	0.22	0/1002	0.48	0/1346
40	2i	0.25	0/997	0.52	0/1343
41	1j	0.24	0/722	0.51	0/982
41	2j	0.28	0/727	0.45	0/988
42	1k	0.18	0/844	0.44	0/1145
42	2k	0.20	0/848	0.46	0/1149
43	1l	0.23	0/937	0.43	0/1260
43	2l	0.20	0/937	0.45	0/1260
44	1m	0.22	0/969	0.47	0/1302
44	2m	0.24	0/961	0.48	0/1291
45	1n	0.21	0/501	0.45	0/664
45	2n	0.20	0/501	0.42	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.20	0/697	0.44	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.21	0/836	0.48	0/1117
48	2q	0.21	0/836	0.47	0/1117
49	1r	0.24	0/560	0.56	1/746 (0.1%)
49	2r	0.18	0/560	0.45	0/746
50	1s	0.19	0/667	0.45	0/900
50	2s	0.27	0/661	0.61	0/893
51	1t	0.21	0/730	0.47	0/965
51	2t	0.21	0/729	0.44	0/965
52	1u	0.24	0/203	0.44	0/266
52	2u	0.20	0/203	0.50	0/266
53	1v	0.24	0/310	0.39	0/480
53	2v	0.22	0/310	0.36	0/480
54	1w	0.31	2/1606 (0.1%)	0.45	0/2497
54	1y	0.30	1/1606 (0.1%)	0.43	0/2497
54	2w	0.32	2/1556 (0.1%)	0.42	0/2418
54	2y	0.31	2/1583 (0.1%)	0.41	0/2459
55	1x	0.27	0/1725	0.43	0/2689
55	2x	0.26	1/1725 (0.1%)	0.41	0/2689
All	All	0.25	8/316696 (0.0%)	0.44	18/474135 (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
29	27	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	5.57	1.61	1.56
54	2y	46	G7M	O3'-P	5.50	1.61	1.56
54	2w	46	G7M	O3'-P	5.46	1.61	1.56
55	2x	8	4SU	O3'-P	5.36	1.61	1.56
54	2w	8	4SU	O3'-P	5.26	1.61	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	1r	32	ARG	N-CA-C	-8.13	105.35	114.62
34	2c	126	ARG	N-CA-C	-6.71	105.08	113.20
34	2c	75	VAL	N-CA-C	-5.94	105.97	112.80
34	1c	65	ALA	CA-C-N	5.88	132.56	121.97
34	1c	65	ALA	C-N-CA	5.88	132.56	121.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	27	46	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31194	891	0
1	2A	60322	0	30424	985	1
2	1B	2577	0	1305	30	0
2	2B	2575	0	1303	62	0
3	1D	2136	0	2218	63	0
3	2D	2136	0	2218	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	48	0
4	2E	1559	0	1618	50	0
5	1F	1587	0	1628	46	0
5	2F	1583	0	1621	51	0
6	1G	1423	0	1436	50	0
6	2G	1428	0	1438	70	0
7	1H	1330	0	1407	34	0
7	2H	1330	0	1407	36	0
8	1I	1097	0	1140	27	0
8	2I	1064	0	1082	46	0
9	1N	1117	0	1184	23	0
9	2N	1117	0	1184	39	0
10	1O	933	0	996	18	0
10	2O	933	0	996	22	0
11	1P	1135	0	1212	48	0
11	2P	1135	0	1212	34	0
12	1Q	1122	0	1178	29	0
12	2Q	1122	0	1179	33	0
13	1R	968	0	1033	26	0
13	2R	968	0	1033	35	0
14	1S	873	0	927	21	0
14	2S	870	0	923	43	0
15	1T	1091	0	1151	36	0
15	2T	1083	0	1136	34	0
16	1U	959	0	1019	20	0
16	2U	959	0	1019	30	0
17	1V	771	0	830	14	0
17	2V	771	0	830	16	0
18	1W	886	0	940	19	0
18	2W	886	0	940	21	0
19	1X	750	0	814	22	0
19	2X	750	0	814	21	0
20	1Y	806	0	881	24	0
20	2Y	806	0	881	27	0
21	1Z	1240	0	1240	42	0
21	2Z	1271	0	1273	55	0
22	10	653	0	674	10	0
22	20	653	0	674	27	0
23	11	755	0	826	18	0
23	21	755	0	826	31	0
24	12	588	0	643	16	0
24	22	588	0	643	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	9	0
25	23	464	0	514	16	0
26	14	552	0	533	30	0
26	24	532	0	503	29	0
27	15	455	0	465	4	0
27	25	455	0	465	8	0
28	16	453	0	473	12	0
28	26	449	0	469	14	0
29	17	418	0	467	12	0
29	27	418	0	467	11	0
30	18	517	0	582	22	0
30	28	517	0	582	22	0
31	19	307	0	335	10	0
31	29	307	0	335	13	0
32	1a	32246	0	16294	544	0
32	2a	32327	0	16338	656	1
33	1b	1846	0	1867	75	0
33	2b	1825	0	1828	89	0
34	1c	1548	0	1535	48	0
34	2c	1542	0	1517	71	0
35	1d	1655	0	1672	66	0
35	2d	1674	0	1714	73	0
36	1e	1129	0	1185	46	0
36	2e	1133	0	1191	57	0
37	1f	810	0	804	26	0
37	2f	816	0	808	23	0
38	1g	1231	0	1238	29	0
38	2g	1235	0	1249	48	0
39	1h	1088	0	1126	51	0
39	2h	1088	0	1126	47	0
40	1i	983	0	986	40	0
40	2i	978	0	966	56	0
41	1j	709	0	650	31	0
41	2j	714	0	672	34	0
42	1k	829	0	825	23	0
42	2k	833	0	836	27	0
43	1l	932	0	979	21	0
43	2l	932	0	980	23	0
44	1m	958	0	1002	31	0
44	2m	950	0	988	56	0
45	1n	492	0	529	25	0
45	2n	492	0	529	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	19	0
46	2o	728	0	760	18	0
47	1p	681	0	697	23	0
47	2p	677	0	686	22	0
48	1q	823	0	891	27	0
48	2q	823	0	891	30	0
49	1r	555	0	618	16	0
49	2r	555	0	618	14	0
50	1s	652	0	662	31	0
50	2s	646	0	644	39	0
51	1t	728	0	798	28	0
51	2t	727	0	796	14	0
52	1u	199	0	208	7	0
52	2u	199	0	208	15	0
53	1v	277	0	140	3	0
53	2v	277	0	140	8	0
54	1w	1592	0	818	32	0
54	1y	1585	0	803	42	0
54	2w	1544	0	785	29	0
54	2y	1565	0	794	30	0
55	1x	1625	0	829	19	0
55	2x	1625	0	829	20	0
56	10	7	0	0	0	0
56	11	6	0	0	0	0
56	12	1	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	5	0	0	0	0
56	16	2	0	0	0	0
56	17	6	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1083	0	0	0	0
56	1B	38	0	0	0	0
56	1D	11	0	0	0	0
56	1E	12	0	0	0	0
56	1F	13	0	0	0	0
56	1G	4	0	0	0	0
56	1H	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	3	0	0	0	0
56	1P	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1Q	6	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	3	0	0	0	0
56	1U	8	0	0	0	0
56	1V	8	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	3	0	0	0	0
56	1a	226	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	1	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	2	0	0	0	0
56	1t	1	0	0	0	0
56	1w	7	0	0	0	0
56	1x	12	0	0	0	0
56	1y	1	0	0	0	0
56	20	2	0	0	0	0
56	21	3	0	0	0	0
56	23	2	0	0	0	0
56	25	2	0	0	0	0
56	27	4	0	0	0	0
56	28	6	0	0	0	0
56	2A	849	0	0	0	0
56	2B	20	0	0	0	0
56	2D	5	0	0	0	0
56	2E	7	0	0	0	0
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	1	0	0	0	0
56	2R	1	0	0	0	0
56	2T	4	0	0	0	0
56	2U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2V	2	0	0	0	0
56	2X	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	246	0	0	0	0
56	2d	1	0	0	0	0
56	2e	2	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	1	0	0	0	0
56	2l	4	0	0	0	0
56	2q	3	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	1	0	0	0	0
56	2x	6	0	0	0	0
56	2y	4	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	43	0	0	1	0
58	2A	43	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	3	0
60	2d	8	0	0	2	0
61	10	9	0	0	1	0
61	11	6	0	0	0	0
61	12	3	0	0	0	0
61	13	4	0	0	0	0
61	15	6	0	0	0	0
61	16	2	0	0	0	0
61	17	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	18	8	0	0	0	0
61	1A	1901	0	0	148	0
61	1B	57	0	0	1	0
61	1D	27	0	0	1	0
61	1E	19	0	0	2	0
61	1F	15	0	0	3	0
61	1G	3	0	0	0	0
61	1N	3	0	0	0	0
61	1O	4	0	0	0	0
61	1P	21	0	0	1	0
61	1Q	8	0	0	0	0
61	1R	12	0	0	0	0
61	1S	3	0	0	0	0
61	1T	7	0	0	0	0
61	1U	11	0	0	0	0
61	1V	5	0	0	0	0
61	1W	10	0	0	2	0
61	1X	4	0	0	0	0
61	1Y	2	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	364	0	0	34	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1e	2	0	0	0	0
61	1i	1	0	0	0	0
61	1l	7	0	0	0	0
61	1o	1	0	0	1	0
61	1q	2	0	0	0	0
61	1u	1	0	0	1	0
61	1v	5	0	0	0	0
61	1w	7	0	0	1	0
61	1x	10	0	0	0	0
61	1y	1	0	0	0	0
61	20	6	0	0	0	0
61	21	7	0	0	2	0
61	23	1	0	0	0	0
61	26	1	0	0	1	0
61	27	2	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	1097	0	0	113	0
61	2B	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2D	19	0	0	1	0
61	2E	13	0	0	0	0
61	2F	13	0	0	0	0
61	2I	1	0	0	0	0
61	2N	1	0	0	0	0
61	2O	2	0	0	0	0
61	2P	11	0	0	1	0
61	2Q	1	0	0	0	0
61	2R	5	0	0	0	0
61	2T	3	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	1	0	0	0	0
61	2X	2	0	0	1	0
61	2Y	2	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	260	0	0	22	0
61	2c	1	0	0	0	0
61	2d	3	0	0	0	0
61	2e	2	0	0	0	0
61	2j	2	0	0	0	0
61	2l	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	2	0	0	1	0
61	2t	2	0	0	0	0
61	2v	2	0	0	0	0
61	2w	2	0	0	1	0
61	2x	3	0	0	0	0
61	2y	2	0	0	0	0
All	All	299897	0	196685	5623	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5623 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.25	1.34
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.27	0.96
54:1y:49:C:H42	54:1y:65:G:H1	1.13	0.95
1:1A:2499:C:OP1	61:1A:6106:HOH:O	1.83	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:N3	1:1A:1086:A:N6	2.08	0.95

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:279:C:O2'	32:2a:84:U:O2'[3_754]	2.09	0.11

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%)	249 (91%)	24 (9%)	0	100	100
3	2D	273/276 (99%)	247 (90%)	26 (10%)	0	100	100
4	1E	202/206 (98%)	184 (91%)	16 (8%)	2 (1%)	12	38
4	2E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	8	28
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	55
5	2F	201/210 (96%)	180 (90%)	20 (10%)	1 (0%)	24	55
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	11	36
6	2G	179/182 (98%)	162 (90%)	14 (8%)	3 (2%)	7	25
7	1H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	7	25
7	2H	172/180 (96%)	151 (88%)	19 (11%)	2 (1%)	10	34
8	1I	144/148 (97%)	121 (84%)	22 (15%)	1 (1%)	18	47
8	2I	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	5	20
9	1N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	47
9	2N	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	5	19
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	2O	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	16	44
11	1P	147/150 (98%)	126 (86%)	17 (12%)	4 (3%)	4	15
11	2P	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	4	15
12	1Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	18	47
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
14	1S	108/112 (96%)	96 (89%)	12 (11%)	0	100	100
14	2S	108/112 (96%)	95 (88%)	10 (9%)	3 (3%)	4	14
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	44
16	1U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	38
17	2V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	12
18	1W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	36
19	2X	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6	22
20	2Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	38
21	1Z	148/206 (72%)	126 (85%)	20 (14%)	2 (1%)	9	30
21	2Z	156/206 (76%)	116 (74%)	37 (24%)	3 (2%)	6	22
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	34
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	36
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	36
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	2
26	24	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	3
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
30	28	62/65 (95%)	57 (92%)	5 (8%)	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%)	181 (79%)	41 (18%)	7 (3%)	3	12
33	2b	229/256 (90%)	176 (77%)	47 (20%)	6 (3%)	4	15
34	1c	204/239 (85%)	178 (87%)	23 (11%)	3 (2%)	8	28
34	2c	204/239 (85%)	161 (79%)	41 (20%)	2 (1%)	12	38
35	1d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	6	22
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	24	55
36	1e	146/162 (90%)	126 (86%)	19 (13%)	1 (1%)	18	47
36	2e	146/162 (90%)	124 (85%)	20 (14%)	2 (1%)	9	30
37	1f	98/101 (97%)	89 (91%)	8 (8%)	1 (1%)	12	38
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	18	47
38	2g	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	4	15
39	1h	135/138 (98%)	117 (87%)	15 (11%)	3 (2%)	5	19
39	2h	135/138 (98%)	119 (88%)	16 (12%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	15 (12%)	2 (2%)	7	27
40	2i	125/128 (98%)	98 (78%)	24 (19%)	3 (2%)	4	17
41	1j	95/105 (90%)	79 (83%)	13 (14%)	3 (3%)	3	11
41	2j	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	2
42	1k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	2k	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	14	41
43	1l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
43	2l	119/132 (90%)	105 (88%)	13 (11%)	1 (1%)	16	44
44	1m	121/126 (96%)	102 (84%)	17 (14%)	2 (2%)	7	25
44	2m	120/126 (95%)	99 (82%)	17 (14%)	4 (3%)	3	11
45	1n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	11
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	34
46	2o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10	34
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	12	38
48	2q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	5	20
49	1r	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	4	16
50	2s	81/93 (87%)	63 (78%)	17 (21%)	1 (1%)	10	34
51	1t	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	5	20
51	2t	94/106 (89%)	85 (90%)	8 (8%)	1 (1%)	11	36
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0	1
All	All	11370/12128 (94%)	10088 (89%)	1142 (10%)	140 (1%)	10	34

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
11	1P	36	LYS
11	1P	38	GLN
21	1Z	53	ILE

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%)	206 (96%)	9 (4%)	26	61
3	2D	215/218 (99%)	191 (89%)	24 (11%)	6	19
4	1E	164/166 (99%)	145 (88%)	19 (12%)	5	18
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	55
5	1F	160/166 (96%)	138 (86%)	22 (14%)	3	12
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	23
6	1G	143/156 (92%)	127 (89%)	16 (11%)	6	19
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	15
7	1H	144/148 (97%)	135 (94%)	9 (6%)	16	45
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	17
8	1I	113/124 (91%)	89 (79%)	24 (21%)	1	4
8	2I	105/124 (85%)	82 (78%)	23 (22%)	1	3
9	1N	118/119 (99%)	112 (95%)	6 (5%)	21	54
9	2N	118/119 (99%)	103 (87%)	15 (13%)	4	15
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	72
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	72
11	1P	115/116 (99%)	102 (89%)	13 (11%)	5	19
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	26
12	1Q	111/111 (100%)	99 (89%)	12 (11%)	6	21
12	2Q	111/111 (100%)	99 (89%)	12 (11%)	6	21
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	29
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	54
14	1S	86/88 (98%)	80 (93%)	6 (7%)	14	40
14	2S	85/88 (97%)	67 (79%)	18 (21%)	1	4
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	40
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	70
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	37
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7	24
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	12
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	42
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	29
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	75
19	2X	77/78 (99%)	73 (95%)	4 (5%)	21	53
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	14
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	22
21	1Z	135/179 (75%)	115 (85%)	20 (15%)	3	10
21	2Z	137/179 (76%)	113 (82%)	24 (18%)	2	7
22	10	65/67 (97%)	60 (92%)	5 (8%)	12	36
22	20	65/67 (97%)	60 (92%)	5 (8%)	12	36
23	11	80/83 (96%)	73 (91%)	7 (9%)	9	29
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	37
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	58
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	27
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	13
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	47
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	4
26	24	53/63 (84%)	44 (83%)	9 (17%)	2	7
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	47
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	34
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	13
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	34
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	38
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	38
30	18	54/55 (98%)	53 (98%)	1 (2%)	50	81
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	50
31	19	34/34 (100%)	30 (88%)	4 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	29
33	1b	192/220 (87%)	162 (84%)	30 (16%)	2	9
33	2b	187/220 (85%)	149 (80%)	38 (20%)	1	4
34	1c	142/188 (76%)	125 (88%)	17 (12%)	5	17
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	14
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	19
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4	15
36	1e	113/123 (92%)	104 (92%)	9 (8%)	11	34
36	2e	114/123 (93%)	99 (87%)	15 (13%)	4	14
37	1f	84/90 (93%)	71 (84%)	13 (16%)	2	9
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	39
38	1g	119/127 (94%)	103 (87%)	16 (13%)	4	13
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	18
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	26
39	2h	114/119 (96%)	97 (85%)	17 (15%)	3	10
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3	11
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	23
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	10
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	11
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	16
42	2k	83/99 (84%)	66 (80%)	17 (20%)	1	4
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8	27
43	2l	96/108 (89%)	83 (86%)	13 (14%)	4	13
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4	14
44	2m	92/101 (91%)	75 (82%)	17 (18%)	1	6
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	11
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	46
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	36
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	44
47	1p	69/74 (93%)	63 (91%)	6 (9%)	9	30
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	84 (89%)	10 (11%)	6	22
48	2q	94/97 (97%)	80 (85%)	14 (15%)	3	10
49	1r	59/77 (77%)	50 (85%)	9 (15%)	3	10
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	13
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	49
50	2s	67/80 (84%)	51 (76%)	16 (24%)	1	3
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	14
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	31
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	20
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50
All	All	9303/10064 (92%)	8276 (89%)	1027 (11%)	6	20

5 of 1027 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	2k	53	SER
44	2m	39	ILE
42	2k	48	ILE
41	1j	38	ILE
40	1i	58	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	119	GLN
36	2e	20	GLN
41	2j	21	GLN
36	1e	141	GLN
36	1e	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	491 (17%)	22 (0%)
1	2A	2791/2915 (95%)	527 (18%)	22 (0%)
2	1B	119/121 (98%)	9 (7%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1497/1521 (98%)	279 (18%)	0
32	2a	1501/1521 (98%)	361 (24%)	0
53	1v	12/24 (50%)	4 (33%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	72/76 (94%)	27 (37%)	0
54	1y	72/76 (94%)	27 (37%)	0
54	2w	69/76 (90%)	21 (30%)	0
54	2y	70/76 (92%)	24 (34%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9347/9620 (97%)	1823 (19%)	44 (0%)

5 of 1823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	61	G

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	856	C
1	2A	1530	C
1	2A	1026	U
1	2A	1460	A
1	2A	1913	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	1x	55	55	18,21,22	1.40	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.12	9 (27%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	1.95	4 (19%)
1	5MC	2A	1962	1,56	19,22,23	1.62	3 (15%)	26,32,35	1.16	2 (7%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.79	3 (11%)
32	G7M	2a	527	32,56	23,26,27	1.47	4 (17%)	34,39,42	1.67	5 (14%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	1.92	4 (19%)
54	PSU	2y	55	54	18,21,22	1.37	3 (16%)	21,30,33	2.00	4 (19%)
1	2MA	2A	2503	1	22,25,26	1.45	5 (22%)	32,37,40	2.20	9 (28%)
55	4SU	1x	8	55	18,21,22	2.12	4 (22%)	25,30,33	1.49	5 (20%)
1	OMU	1A	2552	1,56	19,22,23	1.29	2 (10%)	25,31,34	1.89	4 (16%)
54	5MU	1w	54	54	19,22,23	1.37	4 (21%)	27,32,35	1.93	7 (25%)
1	5MU	2A	1915	1	19,22,23	1.47	6 (31%)	27,32,35	2.08	5 (18%)
32	5MC	1a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.18	3 (11%)
32	4OC	2a	1402	32,56	20,23,24	0.79	0	25,32,35	1.00	1 (4%)
32	5MC	1a	1407	32	19,22,23	1.57	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.47	2 (11%)	21,30,33	2.05	3 (14%)
1	OMG	1A	2251	55,1,56	23,26,27	1.21	3 (13%)	32,38,41	2.16	8 (25%)
1	PSU	2A	1917	1	18,21,22	1.40	3 (16%)	21,30,33	2.07	3 (14%)
1	5MC	2A	1942	1	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
54	G7M	2y	46	54	23,26,27	1.60	3 (13%)	34,39,42	1.75	3 (8%)
54	PSU	2w	39	54	18,21,22	1.33	2 (11%)	21,30,33	1.89	3 (14%)
1	OMC	2A	1920	1	19,22,23	0.76	0	25,31,34	0.85	1 (4%)
55	4SU	2x	8	55	18,21,22	2.04	6 (33%)	25,30,33	1.57	6 (24%)
54	PSU	1w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.94	4 (19%)
54	4SU	2y	8	54	18,21,22	1.80	4 (22%)	25,30,33	2.46	6 (24%)
1	5MC	1A	1942	1	19,22,23	1.47	3 (15%)	26,32,35	1.23	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.45	0	33,38,41	2.09	9 (27%)
32	PSU	2a	516	32	18,21,22	1.34	2 (11%)	21,30,33	1.91	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.16	3 (11%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.12	6 (22%)
54	G7M	1w	46	54	23,26,27	1.52	3 (13%)	34,39,42	1.78	5 (14%)
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	21,30,33	1.97	4 (19%)
1	5MU	2A	1939	1	19,22,23	1.44	5 (26%)	27,32,35	2.25	6 (22%)
55	5MC	1x	32	55	19,22,23	1.64	3 (15%)	26,32,35	1.21	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	G7M	2w	46	54	23,26,27	1.44	4 (17%)	34,39,42	1.72	5 (14%)
32	5MC	2a	967	32	19,22,23	1.74	3 (15%)	26,32,35	1.12	3 (11%)
54	PSU	1w	32	54,56	18,21,22	1.36	2 (11%)	21,30,33	1.92	3 (14%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.11	2 (7%)
54	PSU	1y	55	54	18,21,22	1.41	2 (11%)	21,30,33	2.02	3 (14%)
55	5MU	1x	54	55	19,22,23	1.39	5 (26%)	27,32,35	1.98	8 (29%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.86	6 (18%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	1.97	3 (14%)
1	PSU	1A	2605	1,56	18,21,22	1.44	4 (22%)	21,30,33	2.08	4 (19%)
54	PSU	2y	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.83	3 (14%)
32	G7M	1a	527	32,56	23,26,27	1.54	4 (17%)	34,39,42	1.65	4 (11%)
1	5MU	1A	1939	1,56	19,22,23	1.53	6 (31%)	27,32,35	2.37	5 (18%)
54	MIA	1y	37	54	21,24,32	1.62	4 (19%)	30,35,47	2.11	7 (23%)
54	4SU	1w	8	54	18,21,22	1.83	5 (27%)	25,30,33	1.87	4 (16%)
32	PSU	1a	516	32	18,21,22	1.40	3 (16%)	21,30,33	1.96	4 (19%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	2.06	10 (30%)
54	MIA	2y	37	54	21,24,32	1.64	3 (14%)	30,35,47	2.00	8 (26%)
32	5MC	2a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.13	3 (11%)
43	0TD	1l	92	43	8,9,10	4.64	1 (12%)	6,11,13	5.39	2 (33%)
1	2MA	1A	2503	1,56	22,25,26	1.43	4 (18%)	32,37,40	2.35	9 (28%)
1	5MC	1A	1962	1,56	19,22,23	1.59	3 (15%)	26,32,35	1.13	3 (11%)
54	PSU	1y	32	54	18,21,22	1.37	3 (16%)	21,30,33	1.94	4 (19%)
54	PSU	1y	39	54	18,21,22	1.44	2 (11%)	21,30,33	1.70	3 (14%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.95	1 (4%)
55	5MC	2x	32	55	19,22,23	1.59	3 (15%)	26,32,35	1.30	3 (11%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	7.25	2 (33%)
54	PSU	1w	39	54	18,21,22	1.32	2 (11%)	21,30,33	1.88	3 (14%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
54	G7M	1y	46	54	23,26,27	1.68	3 (13%)	34,39,42	1.99	4 (11%)
32	UR3	2a	1498	32	19,22,23	1.05	1 (5%)	26,32,35	1.81	4 (15%)
32	5MC	1a	1400	32	19,22,23	1.55	3 (15%)	26,32,35	1.09	2 (7%)
54	MIA	1w	37	54	28,31,32	2.21	6 (21%)	38,44,47	2.72	13 (34%)
1	5MU	1A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.01	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.76	2 (10%)	26,32,35	1.26	4 (15%)
32	M2G	1a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.91	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	4SU	1y	8	54	18,21,22	1.79	5 (27%)	25,30,33	1.75	5 (20%)
32	2MG	1a	1207	32	23,26,27	1.26	2 (8%)	33,38,41	2.19	8 (24%)
54	4SU	2w	8	54	18,21,22	1.69	4 (22%)	25,30,33	2.02	5 (20%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.19	10 (30%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.16	6 (28%)
1	OMG	2A	2251	55,1,56	23,26,27	1.22	3 (13%)	32,38,41	1.98	7 (21%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.22	7 (21%)
54	5MU	2w	54	54	19,22,23	1.42	4 (21%)	27,32,35	1.82	6 (22%)
54	MIA	2w	37	54,53	24,27,32	2.16	5 (20%)	32,39,47	2.67	10 (31%)
54	PSU	2y	32	54	18,21,22	1.39	2 (11%)	21,30,33	2.01	4 (19%)
54	5MU	1y	54	54	19,22,23	1.39	4 (21%)	27,32,35	1.86	5 (18%)
54	5MU	2y	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.86	7 (25%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.02	1 (4%)
1	OMU	2A	2552	1,56	19,22,23	1.25	3 (15%)	25,31,34	1.82	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	1/9/29/30	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,56	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	0/7/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	4/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	3/7/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	2/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	2/7/25/26	0/3/3/3
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	3/7/25/34	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
54	MIA	2y	37	54	-	2/7/25/34	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	2MA	1A	2503	1,56	-	0/7/25/26	0/3/3/3
1	5MC	1A	1962	1,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
32	UR3	2a	1498	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	6/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1,56	-	1/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54,53	-	2/11/29/34	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2

The worst 5 of 244 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.72	1.69	1.82
43	2l	92	0TD	CB-SB	-12.23	1.69	1.82
54	2w	37	MIA	C2-S10	-7.15	1.69	1.75
54	1w	37	MIA	C13-C14	6.92	1.53	1.32
32	2a	967	5MC	C5-C4	6.44	1.49	1.44

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-17.47	70.96	102.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.65	79.62	102.36
54	2w	37	MIA	C5-C4-N3	-8.55	118.17	127.18
54	1w	37	MIA	C12-C13-C14	-8.12	112.44	127.01
54	1w	37	MIA	C5-C4-N3	-8.09	118.66	127.18

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
54	1w	37	MIA	C12-C13-C14-C16
1	2A	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

40 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1519	MA6	1	0
32	1a	1498	UR3	1	0
54	2y	55	PSU	5	0
1	2A	2503	2MA	2	0
55	1x	8	4SU	2	0
54	1w	54	5MU	1	0
1	2A	1915	5MU	1	0
32	2a	1402	4OC	2	0
1	2A	1942	5MC	1	0
54	2y	46	G7M	1	0
1	2A	1920	OMC	1	0
55	2x	8	4SU	1	0
54	2y	8	4SU	1	0
32	2a	1518	MA6	2	0
32	2a	1404	5MC	1	0
1	2A	1939	5MU	1	0
54	2w	46	G7M	1	0
32	2a	967	5MC	1	0
55	1x	54	5MU	1	0
32	2a	966	M2G	1	0
1	1A	1939	5MU	1	0
54	1y	37	MIA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	8	4SU	1	0
32	1a	1518	MA6	1	0
54	2y	37	MIA	1	0
32	2a	1407	5MC	1	0
1	1A	2503	2MA	1	0
43	2l	92	0TD	2	0
54	1y	46	G7M	4	0
32	2a	1498	UR3	1	0
54	1w	37	MIA	1	0
32	2a	1400	5MC	1	0
54	1y	8	4SU	2	0
54	2w	8	4SU	2	0
32	2a	1519	MA6	5	0
1	2A	2251	OMG	1	0
32	2a	1207	2MG	1	0
54	2w	37	MIA	1	0
54	2y	54	5MU	1	0
1	2A	2552	OMU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2741 ligands modelled in this entry, 2737 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	1d	302	35	0,12,12	-	-	-		
58	A1AIX	2A	3851	-	48,48,48	3.59	13 (27%)	61,70,70	1.78	12 (19%)
60	SF4	2d	302	35	0,12,12	-	-	-		
58	A1AIX	1A	4085	-	48,48,48	2.63	12 (25%)	61,70,70	1.60	12 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	1d	302	35	-	-	0/6/5/5
58	A1AIX	2A	3851	-	-	4/24/41/41	0/6/6/6
60	SF4	2d	302	35	-	-	0/6/5/5
58	A1AIX	1A	4085	-	-	2/24/41/41	0/6/6/6

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3851	A1AIX	OBL-NBK	18.11	1.54	1.22
58	1A	4085	A1AIX	OBL-NBK	8.89	1.38	1.22
58	2A	3851	A1AIX	CBE-CAA	-8.76	1.39	1.51
58	2A	3851	A1AIX	CAW-CAV	-8.21	1.37	1.51
58	1A	4085	A1AIX	CBE-CAA	-8.09	1.40	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3851	A1AIX	CAS-OAR-CAP	-6.38	108.16	117.51
58	2A	3851	A1AIX	CAX-CAW-CAV	-5.49	102.73	109.95
58	1A	4085	A1AIX	CAX-CAW-CAV	-4.38	104.18	109.95
58	1A	4085	A1AIX	CAS-OAR-CAP	-4.17	111.40	117.51
58	2A	3851	A1AIX	CAL-CAJ-NAI	-3.87	119.56	121.81

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4085	A1AIX	NBQ-CAB-CBC-OB
58	2A	3851	A1AIX	CAO-CAP-OAR-CAS
58	1A	4085	A1AIX	CAA-CAB-CBC-OB
58	2A	3851	A1AIX	CAN-CAP-OAR-CAS
58	2A	3851	A1AIX	NBQ-CAB-CBC-OB

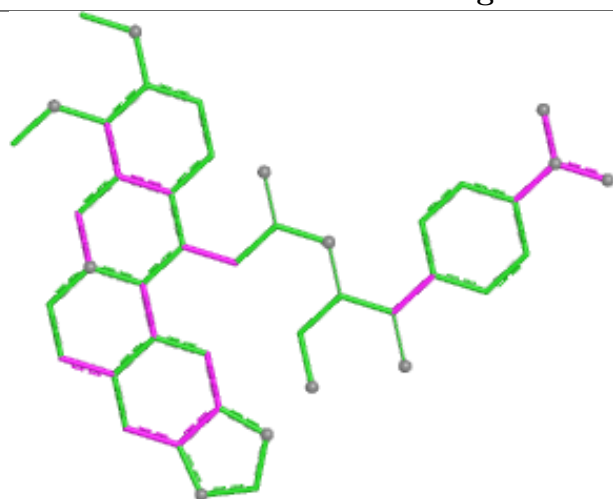
There are no ring outliers.

4 monomers are involved in 7 short contacts:

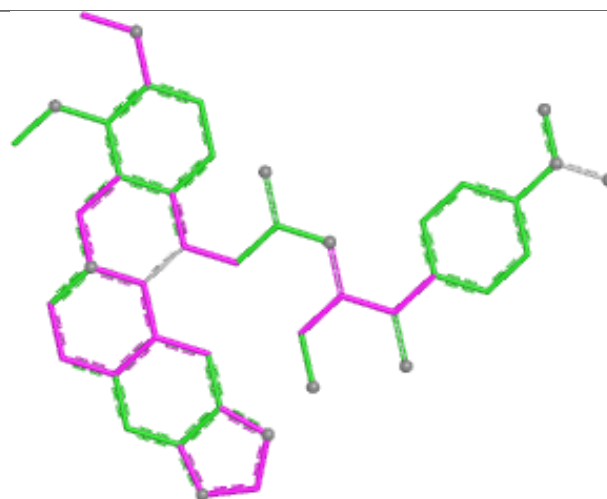
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	302	SF4	3	0
58	2A	3851	A1AIX	1	0
60	2d	302	SF4	2	0
58	1A	4085	A1AIX	1	0

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

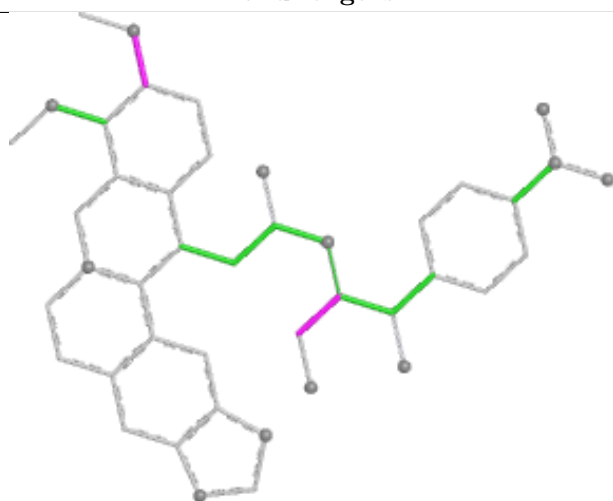
Ligand A1AIX 2A 3851



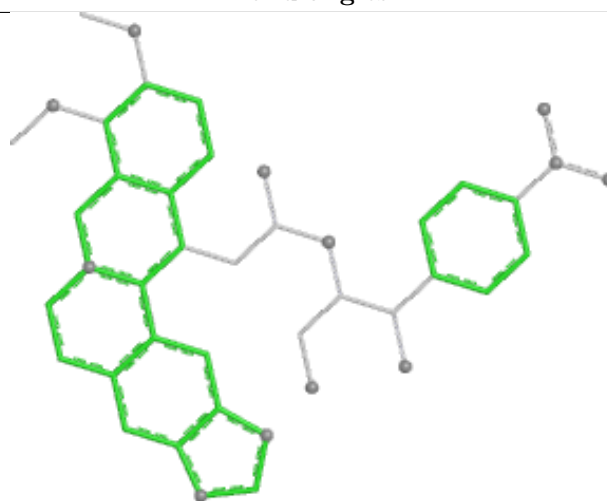
Bond lengths



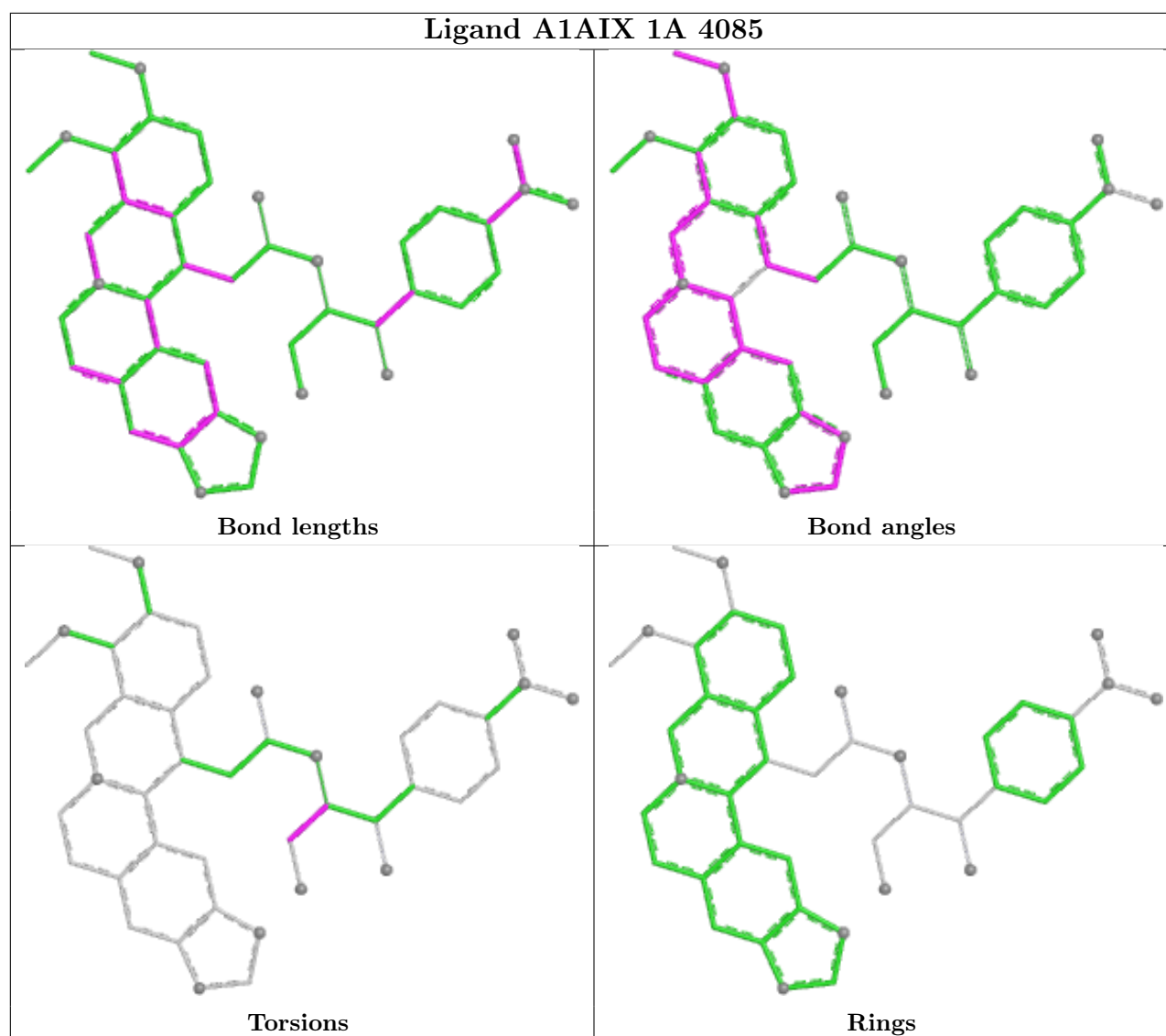
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.57	46 (1%) 70 61	16, 36, 96, 109	0
1	2A	2789/2915 (95%)	-0.12	42 (1%) 72 63	33, 60, 93, 107	0
2	1B	120/121 (99%)	-0.59	0 100 100	25, 45, 60, 87	0
2	2B	120/121 (99%)	0.60	1 (0%) 82 75	62, 82, 91, 100	0
3	1D	275/276 (99%)	-0.28	0 100 100	18, 36, 51, 70	0
3	2D	275/276 (99%)	0.21	1 (0%) 88 84	35, 54, 67, 78	0
4	1E	204/206 (99%)	-0.10	1 (0%) 87 82	19, 42, 61, 69	0
4	2E	204/206 (99%)	0.17	2 (0%) 79 72	35, 61, 72, 83	0
5	1F	203/210 (96%)	-0.21	0 100 100	19, 43, 68, 84	0
5	2F	203/210 (96%)	0.22	2 (0%) 79 72	34, 67, 78, 83	0
6	1G	181/182 (99%)	0.20	5 (2%) 55 45	36, 55, 70, 86	0
6	2G	181/182 (99%)	0.97	14 (7%) 19 14	71, 81, 87, 90	0
7	1H	174/180 (96%)	-0.13	0 100 100	34, 53, 67, 72	0
7	2H	174/180 (96%)	0.73	13 (7%) 20 15	67, 81, 90, 98	0
8	1I	146/148 (98%)	0.28	2 (1%) 73 64	45, 72, 80, 87	0
8	2I	146/148 (98%)	0.75	4 (2%) 56 46	58, 75, 83, 89	0
9	1N	140/140 (100%)	-0.17	1 (0%) 84 77	26, 39, 59, 72	0
9	2N	140/140 (100%)	0.53	6 (4%) 40 31	42, 67, 76, 82	0
10	1O	122/122 (100%)	-0.17	0 100 100	26, 41, 57, 63	0
10	2O	122/122 (100%)	0.19	0 100 100	47, 60, 69, 76	0
11	1P	149/150 (99%)	0.04	1 (0%) 84 77	21, 46, 69, 80	0
11	2P	149/150 (99%)	0.37	2 (1%) 75 66	40, 69, 81, 89	0
12	1Q	141/141 (100%)	-0.27	0 100 100	27, 40, 53, 73	0
12	2Q	141/141 (100%)	0.76	8 (5%) 29 22	49, 68, 78, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.28	0 100 100	26, 35, 51, 57	0
13	2R	118/118 (100%)	0.14	1 (0%) 82 75	41, 52, 64, 73	0
14	1S	110/112 (98%)	0.00	0 100 100	33, 46, 58, 66	0
14	2S	110/112 (98%)	1.08	12 (10%) 10 8	62, 74, 82, 87	0
15	1T	131/146 (89%)	0.02	1 (0%) 82 75	33, 47, 66, 75	0
15	2T	131/146 (89%)	0.28	0 100 100	49, 62, 75, 82	0
16	1U	116/118 (98%)	-0.30	0 100 100	20, 32, 49, 64	0
16	2U	116/118 (98%)	0.24	1 (0%) 81 74	44, 65, 76, 88	0
17	1V	101/101 (100%)	-0.35	0 100 100	20, 42, 57, 68	0
17	2V	101/101 (100%)	0.43	2 (1%) 65 56	48, 72, 80, 84	0
18	1W	112/113 (99%)	-0.37	0 100 100	23, 32, 52, 76	0
18	2W	112/113 (99%)	0.14	1 (0%) 81 74	38, 51, 68, 92	0
19	1X	95/96 (98%)	-0.38	1 (1%) 78 70	21, 36, 58, 82	0
19	2X	95/96 (98%)	0.35	0 100 100	44, 60, 69, 71	0
20	1Y	107/110 (97%)	0.22	1 (0%) 81 74	36, 51, 69, 77	0
20	2Y	107/110 (97%)	0.71	4 (3%) 45 36	62, 73, 82, 89	0
21	1Z	154/206 (74%)	0.41	7 (4%) 38 30	40, 58, 79, 85	0
21	2Z	160/206 (77%)	0.81	9 (5%) 30 23	68, 80, 87, 94	0
22	10	83/85 (97%)	-0.09	3 (3%) 46 37	27, 38, 61, 81	0
22	20	83/85 (97%)	0.75	5 (6%) 27 21	53, 64, 78, 84	0
23	11	97/98 (98%)	-0.04	1 (1%) 79 72	22, 43, 67, 70	0
23	21	97/98 (98%)	0.35	3 (3%) 51 41	41, 58, 75, 83	0
24	12	70/72 (97%)	-0.28	0 100 100	32, 48, 60, 71	0
24	22	70/72 (97%)	0.37	1 (1%) 73 64	58, 69, 76, 85	0
25	13	59/60 (98%)	-0.32	0 100 100	26, 35, 62, 70	0
25	23	59/60 (98%)	0.27	2 (3%) 48 39	51, 67, 81, 90	0
26	14	69/71 (97%)	0.27	0 100 100	46, 70, 86, 87	0
26	24	69/71 (97%)	0.94	8 (11%) 9 7	75, 87, 95, 104	0
27	15	59/60 (98%)	-0.34	0 100 100	20, 34, 53, 65	0
27	25	59/60 (98%)	0.15	1 (1%) 69 60	34, 53, 67, 77	0
28	16	53/54 (98%)	-0.43	0 100 100	29, 39, 51, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.53	1 (1%) 66 57	50, 62, 68, 75	0
29	17	48/49 (97%)	-0.39	0 100 100	22, 26, 50, 62	0
29	27	48/49 (97%)	-0.05	0 100 100	32, 42, 58, 68	0
30	18	64/65 (98%)	-0.31	1 (1%) 70 61	24, 33, 41, 49	0
30	28	64/65 (98%)	0.47	0 100 100	47, 56, 65, 72	0
31	19	37/37 (100%)	-0.25	0 100 100	31, 40, 53, 62	0
31	29	37/37 (100%)	0.96	1 (2%) 56 46	62, 71, 84, 90	0
32	1a	1488/1521 (97%)	-0.00	12 (0%) 82 75	34, 69, 93, 106	0
32	2a	1491/1521 (98%)	0.41	58 (3%) 43 34	59, 82, 98, 107	0
33	1b	231/256 (90%)	0.53	4 (1%) 69 60	61, 78, 85, 89	0
33	2b	231/256 (90%)	1.08	29 (12%) 8 6	73, 87, 92, 97	0
34	1c	206/239 (86%)	0.48	6 (2%) 53 43	62, 72, 82, 88	0
34	2c	206/239 (86%)	1.10	31 (15%) 5 4	74, 85, 92, 94	0
35	1d	208/209 (99%)	0.57	3 (1%) 73 64	58, 72, 80, 86	0
35	2d	208/209 (99%)	0.66	5 (2%) 59 49	65, 76, 84, 88	0
36	1e	148/162 (91%)	0.28	0 100 100	53, 65, 74, 86	0
36	2e	148/162 (91%)	0.65	9 (6%) 27 20	71, 81, 87, 90	0
37	1f	100/101 (99%)	0.16	1 (1%) 79 72	54, 67, 77, 82	0
37	2f	100/101 (99%)	0.20	0 100 100	66, 75, 82, 90	0
38	1g	155/156 (99%)	0.43	8 (5%) 33 25	55, 70, 82, 100	0
38	2g	155/156 (99%)	0.86	12 (7%) 19 14	70, 82, 89, 93	0
39	1h	137/138 (99%)	0.38	1 (0%) 84 77	52, 68, 74, 78	0
39	2h	137/138 (99%)	1.01	11 (8%) 18 13	71, 81, 86, 90	0
40	1i	127/128 (99%)	0.77	13 (10%) 12 9	51, 74, 83, 89	0
40	2i	127/128 (99%)	1.29	27 (21%) 2 2	78, 86, 92, 94	0
41	1j	97/105 (92%)	0.77	4 (4%) 41 33	57, 76, 85, 88	0
41	2j	96/105 (91%)	1.67	33 (34%) 1 1	73, 86, 92, 100	0
42	1k	114/129 (88%)	0.34	3 (2%) 57 47	47, 65, 76, 82	0
42	2k	114/129 (88%)	0.65	7 (6%) 27 20	68, 78, 84, 86	0
43	1l	121/132 (91%)	0.27	3 (2%) 58 48	48, 58, 68, 76	0
43	2l	121/132 (91%)	0.67	4 (3%) 49 39	60, 72, 81, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.40	6 (4%) 35 27	55, 68, 76, 81	0
44	2m	122/126 (96%)	1.32	22 (18%) 3 3	69, 83, 88, 92	0
45	1n	60/61 (98%)	0.65	1 (1%) 69 60	62, 68, 74, 76	0
45	2n	60/61 (98%)	1.84	21 (35%) 1 0	79, 87, 92, 94	0
46	1o	88/89 (98%)	0.50	2 (2%) 61 51	52, 64, 74, 82	0
46	2o	88/89 (98%)	0.42	3 (3%) 48 39	62, 77, 83, 85	0
47	1p	82/88 (93%)	1.08	6 (7%) 21 15	61, 73, 81, 86	0
47	2p	82/88 (93%)	0.83	4 (4%) 35 27	56, 70, 81, 82	0
48	1q	99/105 (94%)	0.73	1 (1%) 79 72	53, 66, 73, 76	0
48	2q	99/105 (94%)	0.45	1 (1%) 79 72	66, 74, 82, 87	0
49	1r	68/88 (77%)	0.24	2 (2%) 53 43	57, 68, 78, 83	0
49	2r	68/88 (77%)	0.29	0 100 100	68, 77, 82, 87	0
50	1s	83/93 (89%)	0.30	1 (1%) 76 68	60, 71, 80, 91	0
50	2s	83/93 (89%)	1.31	13 (15%) 5 4	78, 86, 92, 94	0
51	1t	96/106 (90%)	0.60	6 (6%) 26 19	60, 70, 78, 88	0
51	2t	96/106 (90%)	0.52	7 (7%) 21 15	57, 72, 82, 86	0
52	1u	23/27 (85%)	0.53	1 (4%) 40 31	59, 65, 71, 74	0
52	2u	23/27 (85%)	0.73	0 100 100	78, 81, 86, 91	0
53	1v	13/24 (54%)	0.79	2 (15%) 5 4	48, 68, 90, 99	0
53	2v	13/24 (54%)	1.20	2 (15%) 5 4	78, 89, 99, 99	0
54	1w	67/76 (88%)	0.63	3 (4%) 38 30	66, 94, 103, 107	0
54	1y	67/76 (88%)	0.80	3 (4%) 38 30	46, 96, 102, 104	0
54	2w	65/76 (85%)	0.97	8 (12%) 8 6	75, 98, 104, 107	0
54	2y	66/76 (86%)	0.80	0 100 100	63, 99, 104, 106	0
55	1x	72/77 (93%)	-0.03	1 (1%) 73 64	34, 60, 77, 89	0
55	2x	72/77 (93%)	0.37	0 100 100	60, 81, 92, 94	0
All	All	20875/21748 (95%)	0.16	618 (2%) 52 42	16, 65, 91, 109	0

The worst 5 of 618 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	6.3
45	2n	2	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	5.3
1	1A	2115	G	5.1
22	10	6	GLY	4.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	G7M	2y	46	24/25	0.45	0.15	94,102,109,118	0
54	G7M	1w	46	24/25	0.50	0.14	83,93,109,114	0
54	G7M	2w	46	24/25	0.56	0.12	85,95,104,116	0
54	PSU	2y	39	20/21	0.64	0.16	89,97,108,118	0
54	MIA	1y	37	22/30	0.65	0.16	79,88,96,113	0
54	PSU	2y	55	20/21	0.66	0.11	93,99,105,111	0
54	G7M	1y	46	24/25	0.67	0.13	91,101,105,120	0
54	4SU	2y	8	20/21	0.68	0.12	83,102,109,114	0
54	5MU	2w	54	21/22	0.68	0.13	78,90,94,98	0
54	4SU	1y	8	20/21	0.70	0.11	94,98,110,117	0
54	PSU	1y	55	20/21	0.70	0.13	87,96,109,113	0
54	PSU	2y	32	20/21	0.71	0.14	86,96,102,112	0
54	4SU	2w	8	20/21	0.72	0.12	87,101,105,107	0
54	PSU	2w	55	20/21	0.73	0.11	81,94,101,107	0
54	5MU	2y	54	21/22	0.75	0.11	88,98,104,112	0
54	4SU	1w	8	20/21	0.76	0.10	86,91,98,106	0
55	4SU	2x	8	20/21	0.76	0.13	79,87,104,106	0
54	PSU	1y	32	20/21	0.77	0.14	82,91,106,106	0
54	MIA	2y	37	22/30	0.77	0.12	81,92,105,113	0
54	5MU	1y	54	21/22	0.78	0.12	85,94,101,105	0
54	PSU	1w	55	20/21	0.78	0.10	78,90,93,96	0
54	PSU	1y	39	20/21	0.80	0.13	79,90,97,97	0
1	5MU	2A	1915	21/22	0.81	0.12	74,82,91,95	0
32	PSU	2a	516	20/21	0.82	0.12	82,87,94,99	0
54	MIA	2w	37	25/30	0.83	0.14	81,91,93,97	0
54	PSU	2w	39	20/21	0.84	0.13	79,89,93,93	0
54	PSU	2w	32	20/21	0.85	0.16	89,94,104,108	0
32	2MG	2a	1207	24/25	0.85	0.13	80,87,94,98	0
55	PSU	2x	55	20/21	0.87	0.09	72,78,91,94	0
55	5MU	2x	54	21/22	0.87	0.10	70,81,89,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	967	21/22	0.88	0.20	68,76,86,92	0
54	5MU	1w	54	21/22	0.88	0.08	72,79,87,93	0
32	4OC	2a	1402	22/23	0.88	0.15	66,75,79,80	0
32	M2G	2a	966	25/26	0.88	0.19	66,73,95,101	0
55	PSU	1x	55	20/21	0.89	0.09	55,61,68,74	0
54	PSU	1w	32	20/21	0.89	0.13	75,81,89,94	0
32	G7M	2a	527	24/25	0.89	0.12	65,73,80,82	0
1	5MU	1A	1915	21/22	0.90	0.10	54,63,67,75	0
32	5MC	2a	1400	21/22	0.90	0.17	76,82,87,90	0
55	5MC	2x	32	21/22	0.90	0.12	70,77,80,85	0
54	MIA	1w	37	29/30	0.90	0.13	58,71,76,76	0
55	5MU	1x	54	21/22	0.91	0.09	54,61,69,72	0
1	PSU	2A	1917	20/21	0.91	0.10	60,73,83,84	0
1	OMC	2A	1920	21/22	0.91	0.12	64,72,74,74	0
1	PSU	2A	1911	20/21	0.91	0.10	55,69,77,78	0
32	5MC	2a	1404	21/22	0.92	0.12	64,69,75,78	0
32	5MC	2a	1407	21/22	0.92	0.11	65,72,76,77	0
32	PSU	1a	516	20/21	0.92	0.09	61,68,73,79	0
43	0TD	1l	92	10/11	0.92	0.15	54,59,65,77	0
54	PSU	1w	39	20/21	0.93	0.09	68,78,83,84	0
32	UR3	2a	1498	21/22	0.93	0.12	57,67,72,83	0
43	0TD	2l	92	10/11	0.93	0.11	63,71,75,77	0
1	5MC	2A	1962	21/22	0.94	0.11	45,57,64,68	0
32	5MC	1a	1404	21/22	0.94	0.11	34,48,54,60	0
55	4SU	1x	8	20/21	0.94	0.10	56,61,73,73	0
55	5MC	1x	32	21/22	0.94	0.10	55,59,64,67	0
32	2MG	1a	1207	24/25	0.94	0.09	63,70,73,75	0
32	G7M	1a	527	24/25	0.95	0.10	46,53,60,64	0
32	M2G	1a	966	25/26	0.95	0.11	40,54,58,61	0
1	PSU	1A	1917	20/21	0.95	0.08	44,57,61,63	0
32	MA6	2a	1519	24/25	0.96	0.11	61,71,76,77	0
32	5MC	1a	1400	21/22	0.96	0.12	42,52,57,58	0
32	4OC	1a	1402	22/23	0.96	0.10	47,49,54,61	0
1	PSU	1A	1911	20/21	0.96	0.08	37,53,62,62	0
32	MA6	1a	1518	24/25	0.96	0.09	38,41,47,49	0
1	OMG	2A	2251	24/25	0.96	0.08	38,45,48,51	0
1	PSU	2A	2605	20/21	0.96	0.07	36,41,48,48	0
32	5MC	1a	967	21/22	0.96	0.10	48,57,64,69	0
1	5MC	1A	1942	21/22	0.96	0.09	32,39,43,52	0
32	MA6	2a	1518	24/25	0.96	0.10	60,69,74,75	0
32	UR3	1a	1498	21/22	0.97	0.07	38,41,46,48	0
1	2MA	2A	2503	23/24	0.97	0.09	35,39,42,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMU	2A	2552	21/22	0.97	0.06	37,42,51,53	0
1	OMU	1A	2552	21/22	0.97	0.07	21,26,34,41	0
1	5MU	2A	1939	21/22	0.97	0.08	33,41,45,48	0
1	5MC	2A	1942	21/22	0.97	0.10	39,59,62,70	0
32	MA6	1a	1519	24/25	0.97	0.07	36,43,49,51	0
1	2MA	1A	2503	23/24	0.98	0.06	18,24,28,29	0
1	5MU	1A	1939	21/22	0.98	0.06	25,29,36,42	0
1	PSU	1A	2605	20/21	0.98	0.07	25,31,36,39	0
1	OMC	1A	1920	21/22	0.98	0.08	35,49,55,58	0
1	5MC	1A	1962	21/22	0.98	0.08	33,40,44,52	0
32	5MC	1a	1407	21/22	0.98	0.08	30,46,50,53	0
1	OMG	1A	2251	24/25	0.98	0.06	12,27,34,36	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	1A	4032	1/1	0.48	0.33	70,70,70,70	0
56	MG	1a	1649	1/1	0.50	0.31	85,85,85,85	0
56	MG	1A	3673	1/1	0.56	0.26	66,66,66,66	0
56	MG	2A	3799	1/1	0.57	0.14	73,73,73,73	0
56	MG	2A	3735	1/1	0.63	0.22	73,73,73,73	0
56	MG	1B	230	1/1	0.64	0.23	76,76,76,76	0
56	MG	2A	3039	1/1	0.64	0.20	75,75,75,75	0
56	MG	2A	3369	1/1	0.65	0.16	65,65,65,65	0
56	MG	2a	3048	1/1	0.65	0.22	76,76,76,76	0
56	MG	2a	3035	1/1	0.66	0.29	75,75,75,75	0
56	MG	1A	4030	1/1	0.66	0.23	99,99,99,99	0
56	MG	2v	102	1/1	0.66	0.41	74,74,74,74	0
56	MG	2A	3090	1/1	0.67	0.14	77,77,77,77	0
56	MG	1A	3237	1/1	0.68	0.28	70,70,70,70	0
56	MG	2B	216	1/1	0.69	0.18	69,69,69,69	0
56	MG	2a	3128	1/1	0.69	0.29	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3373	1/1	0.69	0.26	62,62,62,62	0
56	MG	2A	3183	1/1	0.70	0.26	83,83,83,83	0
56	MG	2a	3112	1/1	0.70	0.15	62,62,62,62	0
56	MG	2A	3337	1/1	0.71	0.23	65,65,65,65	0
56	MG	2A	3297	1/1	0.71	0.13	76,76,76,76	0
56	MG	1Q	204	1/1	0.72	0.18	67,67,67,67	0
56	MG	2A	3332	1/1	0.72	0.16	66,66,66,66	0
56	MG	1a	1625	1/1	0.72	0.28	68,68,68,68	0
56	MG	2a	3212	1/1	0.72	0.19	84,84,84,84	0
56	MG	2a	3243	1/1	0.72	0.24	68,68,68,68	0
56	MG	1A	3847	1/1	0.72	0.16	63,63,63,63	0
56	MG	1B	234	1/1	0.73	0.20	79,79,79,79	0
56	MG	2a	3042	1/1	0.73	0.15	75,75,75,75	0
56	MG	2A	3597	1/1	0.73	0.18	71,71,71,71	0
56	MG	2A	3642	1/1	0.73	0.16	66,66,66,66	0
56	MG	2A	3083	1/1	0.73	0.24	64,64,64,64	0
56	MG	1A	3218	1/1	0.73	0.14	47,47,47,47	0
56	MG	2A	3145	1/1	0.73	0.27	71,71,71,71	0
56	MG	2B	220	1/1	0.73	0.23	77,77,77,77	0
56	MG	2a	3199	1/1	0.74	0.22	85,85,85,85	0
56	MG	2a	3208	1/1	0.74	0.12	60,60,60,60	0
56	MG	2a	3017	1/1	0.74	0.20	76,76,76,76	0
56	MG	2a	3223	1/1	0.74	0.16	82,82,82,82	0
56	MG	2a	3049	1/1	0.74	0.25	80,80,80,80	0
56	MG	2a	3135	1/1	0.74	0.28	76,76,76,76	0
56	MG	2A	3237	1/1	0.75	0.18	63,63,63,63	0
56	MG	2A	3634	1/1	0.75	0.27	66,66,66,66	0
56	MG	1a	1656	1/1	0.75	0.23	62,62,62,62	0
56	MG	2A	3729	1/1	0.75	0.15	87,87,87,87	0
56	MG	1w	105	1/1	0.75	0.11	78,78,78,78	0
56	MG	1A	3970	1/1	0.75	0.12	50,50,50,50	0
56	MG	2a	3239	1/1	0.75	0.23	69,69,69,69	0
56	MG	2a	3084	1/1	0.75	0.10	81,81,81,81	0
56	MG	2A	3044	1/1	0.75	0.17	69,69,69,69	0
56	MG	2a	3109	1/1	0.76	0.30	77,77,77,77	0
56	MG	1A	3092	1/1	0.76	0.16	59,59,59,59	0
56	MG	2A	3143	1/1	0.76	0.18	63,63,63,63	0
56	MG	1A	3383	1/1	0.76	0.37	68,68,68,68	0
56	MG	1a	1650	1/1	0.76	0.23	78,78,78,78	0
56	MG	2A	3204	1/1	0.76	0.34	66,66,66,66	0
56	MG	1A	3944	1/1	0.76	0.20	34,34,34,34	0
56	MG	2A	3282	1/1	0.76	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3286	1/1	0.76	0.14	67,67,67,67	0
56	MG	2a	3051	1/1	0.76	0.14	77,77,77,77	0
56	MG	2A	3296	1/1	0.76	0.13	72,72,72,72	0
56	MG	1a	1632	1/1	0.77	0.32	60,60,60,60	0
56	MG	1A	3848	1/1	0.77	0.13	51,51,51,51	0
56	MG	2a	3113	1/1	0.77	0.17	77,77,77,77	0
56	MG	2A	3641	1/1	0.77	0.16	66,66,66,66	0
56	MG	2a	3029	1/1	0.77	0.25	87,87,87,87	0
56	MG	2a	3166	1/1	0.77	0.15	52,52,52,52	0
56	MG	1A	3912	1/1	0.77	0.26	56,56,56,56	0
56	MG	1A	4043	1/1	0.77	0.15	66,66,66,66	0
56	MG	2A	3275	1/1	0.77	0.14	66,66,66,66	0
56	MG	1A	4055	1/1	0.77	0.21	53,53,53,53	0
56	MG	2A	3820	1/1	0.77	0.12	77,77,77,77	0
56	MG	2A	3826	1/1	0.77	0.19	54,54,54,54	0
56	MG	2a	3108	1/1	0.77	0.30	71,71,71,71	0
56	MG	1A	4056	1/1	0.78	0.21	69,69,69,69	0
56	MG	1A	3786	1/1	0.78	0.24	57,57,57,57	0
56	MG	1A	3783	1/1	0.78	0.16	61,61,61,61	0
56	MG	1a	1764	1/1	0.78	0.12	75,75,75,75	0
56	MG	2A	3603	1/1	0.78	0.13	61,61,61,61	0
56	MG	1a	1770	1/1	0.78	0.16	64,64,64,64	0
56	MG	2j	201	1/1	0.78	0.23	81,81,81,81	0
56	MG	2a	3194	1/1	0.78	0.21	71,71,71,71	0
56	MG	2A	3563	1/1	0.79	0.28	77,77,77,77	0
56	MG	1a	1655	1/1	0.79	0.23	63,63,63,63	0
56	MG	2A	3305	1/1	0.79	0.12	61,61,61,61	0
56	MG	2A	3609	1/1	0.79	0.22	66,66,66,66	0
56	MG	2A	3621	1/1	0.79	0.19	65,65,65,65	0
56	MG	2A	3836	1/1	0.79	0.14	61,61,61,61	0
56	MG	1a	1781	1/1	0.79	0.10	70,70,70,70	0
56	MG	1A	3471	1/1	0.79	0.11	56,56,56,56	0
56	MG	1A	3603	1/1	0.79	0.14	61,61,61,61	0
56	MG	2a	3020	1/1	0.79	0.21	69,69,69,69	0
56	MG	2v	101	1/1	0.79	0.15	78,78,78,78	0
56	MG	2A	3655	1/1	0.79	0.21	74,74,74,74	0
56	MG	2v	103	1/1	0.79	0.46	72,72,72,72	0
56	MG	2A	3397	1/1	0.80	0.15	63,63,63,63	0
56	MG	2a	3100	1/1	0.80	0.19	80,80,80,80	0
56	MG	2A	3731	1/1	0.80	0.10	84,84,84,84	0
56	MG	2A	3520	1/1	0.80	0.12	41,41,41,41	0
56	MG	2A	3781	1/1	0.80	0.14	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3085	1/1	0.80	0.12	76,76,76,76	0
56	MG	2A	3570	1/1	0.80	0.21	56,56,56,56	0
56	MG	2A	3582	1/1	0.80	0.16	33,33,33,33	0
56	MG	2a	3158	1/1	0.80	0.11	80,80,80,80	0
56	MG	1A	3388	1/1	0.80	0.22	46,46,46,46	0
56	MG	2a	3186	1/1	0.80	0.16	80,80,80,80	0
56	MG	2A	3846	1/1	0.80	0.18	68,68,68,68	0
56	MG	2a	3198	1/1	0.80	0.26	78,78,78,78	0
56	MG	1A	3988	1/1	0.80	0.12	33,33,33,33	0
56	MG	2a	3204	1/1	0.80	0.30	77,77,77,77	0
56	MG	1A	3274	1/1	0.80	0.25	44,44,44,44	0
56	MG	2A	3613	1/1	0.80	0.19	66,66,66,66	0
56	MG	2A	3153	1/1	0.80	0.21	62,62,62,62	0
56	MG	2a	3235	1/1	0.80	0.13	76,76,76,76	0
56	MG	2a	3238	1/1	0.80	0.15	74,74,74,74	0
56	MG	2A	3630	1/1	0.80	0.09	63,63,63,63	0
56	MG	1a	1666	1/1	0.80	0.28	69,69,69,69	0
56	MG	1a	1738	1/1	0.80	0.20	78,78,78,78	0
56	MG	1G	204	1/1	0.80	0.22	56,56,56,56	0
56	MG	2A	3266	1/1	0.80	0.21	65,65,65,65	0
56	MG	2A	3689	1/1	0.80	0.22	49,49,49,49	0
56	MG	2A	3311	1/1	0.81	0.27	57,57,57,57	0
56	MG	2A	3806	1/1	0.81	0.24	61,61,61,61	0
56	MG	2A	3253	1/1	0.81	0.10	48,48,48,48	0
56	MG	2a	3123	1/1	0.81	0.19	66,66,66,66	0
56	MG	2a	3127	1/1	0.81	0.24	66,66,66,66	0
56	MG	2A	3335	1/1	0.81	0.17	69,69,69,69	0
56	MG	2A	3095	1/1	0.81	0.24	60,60,60,60	0
56	MG	2a	3141	1/1	0.81	0.22	73,73,73,73	0
56	MG	2a	3157	1/1	0.81	0.14	80,80,80,80	0
56	MG	2A	3267	1/1	0.81	0.14	53,53,53,53	0
56	MG	2B	209	1/1	0.81	0.12	67,67,67,67	0
56	MG	2B	213	1/1	0.81	0.16	69,69,69,69	0
56	MG	2B	215	1/1	0.81	0.21	69,69,69,69	0
56	MG	2A	3376	1/1	0.81	0.20	65,65,65,65	0
56	MG	1A	3913	1/1	0.81	0.14	19,19,19,19	0
56	MG	1a	1763	1/1	0.81	0.15	76,76,76,76	0
56	MG	2A	3554	1/1	0.81	0.15	74,74,74,74	0
56	MG	2a	3211	1/1	0.81	0.12	73,73,73,73	0
56	MG	2A	3660	1/1	0.81	0.12	52,52,52,52	0
56	MG	2A	3687	1/1	0.81	0.19	73,73,73,73	0
56	MG	1A	3230	1/1	0.81	0.10	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	3713	1/1	0.81	0.19	60,60,60,60	0
56	MG	1A	3488	1/1	0.81	0.17	49,49,49,49	0
56	MG	1A	3792	1/1	0.81	0.13	56,56,56,56	0
56	MG	2a	3065	1/1	0.81	0.35	65,65,65,65	0
56	MG	2A	3593	1/1	0.81	0.14	48,48,48,48	0
56	MG	1a	1812	1/1	0.81	0.11	58,58,58,58	0
56	MG	2A	3788	1/1	0.81	0.14	54,54,54,54	0
56	MG	2A	3076	1/1	0.82	0.26	64,64,64,64	0
56	MG	1A	3683	1/1	0.82	0.19	66,66,66,66	0
56	MG	2A	3504	1/1	0.82	0.22	48,48,48,48	0
56	MG	2a	3203	1/1	0.82	0.17	71,71,71,71	0
56	MG	1a	1696	1/1	0.82	0.15	55,55,55,55	0
56	MG	2A	3550	1/1	0.82	0.11	46,46,46,46	0
56	MG	2a	3209	1/1	0.82	0.20	76,76,76,76	0
56	MG	2a	3115	1/1	0.82	0.19	74,74,74,74	0
56	MG	2a	3118	1/1	0.82	0.14	72,72,72,72	0
56	MG	2a	3214	1/1	0.82	0.28	75,75,75,75	0
56	MG	2A	3300	1/1	0.82	0.30	66,66,66,66	0
56	MG	1a	1703	1/1	0.82	0.23	69,69,69,69	0
56	MG	1Y	203	1/1	0.82	0.08	54,54,54,54	0
56	MG	2A	3821	1/1	0.82	0.18	60,60,60,60	0
56	MG	2A	3007	1/1	0.82	0.23	62,62,62,62	0
56	MG	1A	3187	1/1	0.82	0.15	70,70,70,70	0
56	MG	2l	202	1/1	0.82	0.23	70,70,70,70	0
56	MG	2A	3845	1/1	0.82	0.22	78,78,78,78	0
56	MG	1A	4076	1/1	0.82	0.10	31,31,31,31	0
56	MG	2A	3283	1/1	0.82	0.26	61,61,61,61	0
56	MG	1a	1813	1/1	0.83	0.21	56,56,56,56	0
56	MG	2a	3142	1/1	0.83	0.19	65,65,65,65	0
56	MG	2a	3147	1/1	0.83	0.10	92,92,92,92	0
56	MG	2a	3022	1/1	0.83	0.16	62,62,62,62	0
56	MG	1a	1745	1/1	0.83	0.22	70,70,70,70	0
56	MG	2A	3624	1/1	0.83	0.11	54,54,54,54	0
56	MG	2a	3039	1/1	0.83	0.33	76,76,76,76	0
56	MG	2A	3437	1/1	0.83	0.23	62,62,62,62	0
56	MG	1a	1748	1/1	0.83	0.13	65,65,65,65	0
56	MG	2A	3022	1/1	0.83	0.21	70,70,70,70	0
56	MG	1A	3411	1/1	0.83	0.13	55,55,55,55	0
56	MG	2a	3060	1/1	0.83	0.15	82,82,82,82	0
56	MG	2A	3198	1/1	0.83	0.28	69,69,69,69	0
56	MG	2A	3842	1/1	0.83	0.25	66,66,66,66	0
56	MG	2a	3089	1/1	0.83	0.14	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	2a	3096	1/1	0.83	0.17	78,78,78,78	0
56	MG	1B	235	1/1	0.83	0.12	61,61,61,61	0
56	MG	2a	3215	1/1	0.83	0.14	66,66,66,66	0
56	MG	2a	3222	1/1	0.83	0.09	83,83,83,83	0
56	MG	2A	3227	1/1	0.83	0.28	61,61,61,61	0
56	MG	2a	3231	1/1	0.83	0.16	70,70,70,70	0
56	MG	1A	3322	1/1	0.83	0.17	56,56,56,56	0
56	MG	2a	3236	1/1	0.83	0.09	60,60,60,60	0
56	MG	2A	3692	1/1	0.83	0.12	48,48,48,48	0
56	MG	2A	3249	1/1	0.83	0.15	70,70,70,70	0
56	MG	1a	1773	1/1	0.83	0.10	72,72,72,72	0
56	MG	1A	3171	1/1	0.83	0.23	66,66,66,66	0
56	MG	2a	3007	1/1	0.83	0.30	67,67,67,67	0
56	MG	2a	3009	1/1	0.83	0.28	69,69,69,69	0
56	MG	2a	3010	1/1	0.83	0.17	72,72,72,72	0
56	MG	1A	3982	1/1	0.83	0.09	30,30,30,30	0
56	MG	1a	1643	1/1	0.84	0.16	61,61,61,61	0
56	MG	1A	3777	1/1	0.84	0.13	38,38,38,38	0
56	MG	2B	205	1/1	0.84	0.20	71,71,71,71	0
56	MG	2a	3122	1/1	0.84	0.26	60,60,60,60	0
56	MG	1A	4061	1/1	0.84	0.24	60,60,60,60	0
56	MG	2B	212	1/1	0.84	0.12	64,64,64,64	0
56	MG	2A	3310	1/1	0.84	0.11	56,56,56,56	0
56	MG	1a	1782	1/1	0.84	0.13	57,57,57,57	0
56	MG	1A	3917	1/1	0.84	0.20	52,52,52,52	0
56	MG	2B	217	1/1	0.84	0.09	63,63,63,63	0
56	MG	2A	3196	1/1	0.84	0.16	58,58,58,58	0
56	MG	2a	3152	1/1	0.84	0.17	66,66,66,66	0
56	MG	27	104	1/1	0.84	0.18	60,60,60,60	0
56	MG	2a	3005	1/1	0.84	0.23	67,67,67,67	0
56	MG	1A	3550	1/1	0.84	0.34	42,42,42,42	0
56	MG	1A	3585	1/1	0.84	0.17	43,43,43,43	0
56	MG	1A	3465	1/1	0.84	0.14	65,65,65,65	0
56	MG	1A	3831	1/1	0.84	0.13	26,26,26,26	0
56	MG	2A	3411	1/1	0.84	0.13	53,53,53,53	0
56	MG	2A	3416	1/1	0.84	0.18	73,73,73,73	0
56	MG	2A	3426	1/1	0.84	0.34	55,55,55,55	0
56	MG	2A	3429	1/1	0.84	0.23	56,56,56,56	0
56	MG	2a	3037	1/1	0.84	0.32	70,70,70,70	0
56	MG	1a	1724	1/1	0.84	0.19	52,52,52,52	0
56	MG	1A	3624	1/1	0.84	0.11	44,44,44,44	0
56	MG	2A	3047	1/1	0.84	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	3741	1/1	0.84	0.09	44,44,44,44	0
56	MG	2A	3525	1/1	0.84	0.16	69,69,69,69	0
56	MG	2A	3539	1/1	0.84	0.13	60,60,60,60	0
56	MG	2A	3058	1/1	0.84	0.20	68,68,68,68	0
56	MG	2a	3234	1/1	0.84	0.14	73,73,73,73	0
56	MG	2a	3073	1/1	0.84	0.19	72,72,72,72	0
56	MG	2A	3271	1/1	0.84	0.17	57,57,57,57	0
56	MG	2a	3087	1/1	0.84	0.33	58,58,58,58	0
56	MG	1A	3083	1/1	0.84	0.15	44,44,44,44	0
56	MG	2a	3095	1/1	0.84	0.14	68,68,68,68	0
56	MG	2A	3082	1/1	0.84	0.11	61,61,61,61	0
56	MG	10	104	1/1	0.84	0.16	63,63,63,63	0
56	MG	2A	3835	1/1	0.84	0.12	70,70,70,70	0
56	MG	1A	3900	1/1	0.84	0.12	60,60,60,60	0
56	MG	1A	3371	1/1	0.84	0.12	58,58,58,58	0
56	MG	2x	106	1/1	0.84	0.29	70,70,70,70	0
56	MG	2y	102	1/1	0.84	0.16	81,81,81,81	0
56	MG	1A	3212	1/1	0.85	0.23	53,53,53,53	0
56	MG	1B	214	1/1	0.85	0.27	45,45,45,45	0
56	MG	1B	219	1/1	0.85	0.11	34,34,34,34	0
56	MG	1B	229	1/1	0.85	0.11	71,71,71,71	0
56	MG	2A	3573	1/1	0.85	0.12	51,51,51,51	0
56	MG	2A	3086	1/1	0.85	0.09	76,76,76,76	0
56	MG	1A	3564	1/1	0.85	0.20	48,48,48,48	0
56	MG	2A	3293	1/1	0.85	0.24	64,64,64,64	0
56	MG	1a	1659	1/1	0.85	0.15	66,66,66,66	0
56	MG	2A	3112	1/1	0.85	0.23	52,52,52,52	0
56	MG	1A	4018	1/1	0.85	0.17	83,83,83,83	0
56	MG	2a	3136	1/1	0.85	0.39	71,71,71,71	0
56	MG	1A	3088	1/1	0.85	0.12	42,42,42,42	0
56	MG	2F	305	1/1	0.85	0.18	61,61,61,61	0
56	MG	2A	3151	1/1	0.85	0.07	77,77,77,77	0
56	MG	1x	110	1/1	0.85	0.20	65,65,65,65	0
56	MG	2a	3154	1/1	0.85	0.16	75,75,75,75	0
56	MG	2a	3006	1/1	0.85	0.17	66,66,66,66	0
56	MG	2A	3175	1/1	0.85	0.10	50,50,50,50	0
56	MG	2A	3177	1/1	0.85	0.10	58,58,58,58	0
56	MG	2A	3001	1/1	0.85	0.28	47,47,47,47	0
56	MG	2A	3347	1/1	0.85	0.08	64,64,64,64	0
56	MG	2A	3360	1/1	0.85	0.23	43,43,43,43	0
56	MG	1A	3599	1/1	0.85	0.10	45,45,45,45	0
56	MG	1A	3201	1/1	0.85	0.17	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	3389	1/1	0.85	0.13	67,67,67,67	0
56	MG	2A	3706	1/1	0.85	0.11	48,48,48,48	0
56	MG	1A	3366	1/1	0.85	0.16	61,61,61,61	0
56	MG	2A	3221	1/1	0.85	0.09	68,68,68,68	0
56	MG	2a	3045	1/1	0.85	0.15	66,66,66,66	0
56	MG	1A	3963	1/1	0.85	0.11	72,72,72,72	0
56	MG	2A	3236	1/1	0.85	0.07	59,59,59,59	0
56	MG	1A	3540	1/1	0.85	0.30	55,55,55,55	0
56	MG	2a	3053	1/1	0.85	0.09	73,73,73,73	0
56	MG	2a	3059	1/1	0.85	0.19	65,65,65,65	0
56	MG	2A	3050	1/1	0.85	0.20	55,55,55,55	0
56	MG	2A	3452	1/1	0.85	0.27	78,78,78,78	0
56	MG	2a	3067	1/1	0.85	0.11	67,67,67,67	0
56	MG	2a	3070	1/1	0.85	0.27	59,59,59,59	0
56	MG	2A	3469	1/1	0.85	0.12	49,49,49,49	0
56	MG	2A	3250	1/1	0.85	0.20	74,74,74,74	0
56	MG	2A	3251	1/1	0.85	0.10	65,65,65,65	0
56	MG	2A	3052	1/1	0.85	0.18	64,64,64,64	0
56	MG	2A	3822	1/1	0.85	0.29	61,61,61,61	0
56	MG	1A	4072	1/1	0.85	0.18	62,62,62,62	0
56	MG	2a	3098	1/1	0.85	0.15	73,73,73,73	0
56	MG	2A	3548	1/1	0.85	0.11	55,55,55,55	0
56	MG	2a	3105	1/1	0.85	0.10	67,67,67,67	0
56	MG	2y	103	1/1	0.85	0.28	79,79,79,79	0
56	MG	1a	1727	1/1	0.86	0.14	59,59,59,59	0
56	MG	1A	3916	1/1	0.86	0.10	59,59,59,59	0
56	MG	1a	1616	1/1	0.86	0.20	66,66,66,66	0
56	MG	1A	3223	1/1	0.86	0.14	46,46,46,46	0
56	MG	1A	3329	1/1	0.86	0.08	40,40,40,40	0
56	MG	2A	3468	1/1	0.86	0.17	53,53,53,53	0
56	MG	1A	3948	1/1	0.86	0.14	77,77,77,77	0
56	MG	2A	3483	1/1	0.86	0.24	65,65,65,65	0
56	MG	1a	1645	1/1	0.86	0.15	54,54,54,54	0
56	MG	2a	3110	1/1	0.86	0.16	70,70,70,70	0
56	MG	2A	3254	1/1	0.86	0.18	58,58,58,58	0
56	MG	2A	3523	1/1	0.86	0.11	57,57,57,57	0
56	MG	2A	3255	1/1	0.86	0.24	60,60,60,60	0
56	MG	2A	3838	1/1	0.86	0.21	60,60,60,60	0
56	MG	2A	3265	1/1	0.86	0.19	59,59,59,59	0
56	MG	2A	3546	1/1	0.86	0.16	61,61,61,61	0
56	MG	1A	3394	1/1	0.86	0.18	55,55,55,55	0
56	MG	2A	3847	1/1	0.86	0.35	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	2a	3132	1/1	0.86	0.37	65,65,65,65	0
56	MG	2B	202	1/1	0.86	0.12	69,69,69,69	0
56	MG	1A	3263	1/1	0.86	0.31	67,67,67,67	0
56	MG	1A	3828	1/1	0.86	0.11	51,51,51,51	0
56	MG	2A	3555	1/1	0.86	0.09	55,55,55,55	0
56	MG	1A	3119	1/1	0.86	0.06	75,75,75,75	0
56	MG	1A	3302	1/1	0.86	0.08	47,47,47,47	0
56	MG	2A	3114	1/1	0.86	0.23	68,68,68,68	0
56	MG	2A	3133	1/1	0.86	0.15	68,68,68,68	0
56	MG	2A	3142	1/1	0.86	0.23	74,74,74,74	0
56	MG	2E	306	1/1	0.86	0.09	40,40,40,40	0
56	MG	2a	3183	1/1	0.86	0.18	76,76,76,76	0
56	MG	1w	104	1/1	0.86	0.10	82,82,82,82	0
56	MG	2a	3190	1/1	0.86	0.21	67,67,67,67	0
56	MG	1a	1660	1/1	0.86	0.11	54,54,54,54	0
56	MG	1x	102	1/1	0.86	0.26	60,60,60,60	0
56	MG	1x	104	1/1	0.86	0.31	66,66,66,66	0
56	MG	1A	3473	1/1	0.86	0.23	63,63,63,63	0
56	MG	1a	1675	1/1	0.86	0.28	55,55,55,55	0
56	MG	1A	3378	1/1	0.86	0.21	55,55,55,55	0
56	MG	2A	3188	1/1	0.86	0.15	50,50,50,50	0
56	MG	2A	3192	1/1	0.86	0.12	68,68,68,68	0
56	MG	2A	3339	1/1	0.86	0.18	65,65,65,65	0
56	MG	2A	3649	1/1	0.86	0.11	68,68,68,68	0
56	MG	2A	3346	1/1	0.86	0.07	65,65,65,65	0
56	MG	2a	3218	1/1	0.86	0.21	77,77,77,77	0
56	MG	2a	3220	1/1	0.86	0.13	71,71,71,71	0
56	MG	2a	3036	1/1	0.86	0.25	70,70,70,70	0
56	MG	1A	3533	1/1	0.86	0.16	56,56,56,56	0
56	MG	2a	3227	1/1	0.86	0.15	67,67,67,67	0
56	MG	2A	3674	1/1	0.86	0.14	80,80,80,80	0
56	MG	2a	3040	1/1	0.86	0.10	56,56,56,56	0
56	MG	2A	3677	1/1	0.86	0.11	59,59,59,59	0
56	MG	2A	3678	1/1	0.86	0.11	60,60,60,60	0
56	MG	2A	3028	1/1	0.86	0.29	59,59,59,59	0
56	MG	1a	1705	1/1	0.86	0.11	51,51,51,51	0
56	MG	2A	3211	1/1	0.86	0.15	57,57,57,57	0
56	MG	2A	3697	1/1	0.86	0.28	59,59,59,59	0
56	MG	2A	3698	1/1	0.86	0.11	75,75,75,75	0
56	MG	2A	3384	1/1	0.86	0.21	60,60,60,60	0
56	MG	2A	3214	1/1	0.86	0.11	68,68,68,68	0
56	MG	2A	3716	1/1	0.86	0.13	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3726	1/1	0.86	0.08	57,57,57,57	0
56	MG	2A	3215	1/1	0.86	0.28	73,73,73,73	0
56	MG	1A	3774	1/1	0.86	0.10	27,27,27,27	0
56	MG	1a	1689	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3276	1/1	0.87	0.11	52,52,52,52	0
56	MG	2A	3647	1/1	0.87	0.10	56,56,56,56	0
56	MG	1B	226	1/1	0.87	0.15	63,63,63,63	0
56	MG	2a	3063	1/1	0.87	0.20	65,65,65,65	0
56	MG	2A	3653	1/1	0.87	0.12	43,43,43,43	0
56	MG	1A	3663	1/1	0.87	0.18	63,63,63,63	0
56	MG	2a	3069	1/1	0.87	0.21	73,73,73,73	0
56	MG	2A	3075	1/1	0.87	0.15	55,55,55,55	0
56	MG	1A	3665	1/1	0.87	0.12	34,34,34,34	0
56	MG	2a	3082	1/1	0.87	0.25	63,63,63,63	0
56	MG	1a	1707	1/1	0.87	0.15	63,63,63,63	0
56	MG	1B	232	1/1	0.87	0.10	55,55,55,55	0
56	MG	1A	3419	1/1	0.87	0.17	65,65,65,65	0
56	MG	1A	3422	1/1	0.87	0.14	59,59,59,59	0
56	MG	2A	3306	1/1	0.87	0.18	68,68,68,68	0
56	MG	1a	1741	1/1	0.87	0.15	78,78,78,78	0
56	MG	1D	311	1/1	0.87	0.10	28,28,28,28	0
56	MG	2A	3111	1/1	0.87	0.19	67,67,67,67	0
56	MG	2a	3106	1/1	0.87	0.16	74,74,74,74	0
56	MG	2A	3710	1/1	0.87	0.18	68,68,68,68	0
56	MG	1A	3727	1/1	0.87	0.10	17,17,17,17	0
56	MG	1a	1757	1/1	0.87	0.18	64,64,64,64	0
56	MG	1A	3732	1/1	0.87	0.10	65,65,65,65	0
56	MG	2A	3135	1/1	0.87	0.18	53,53,53,53	0
56	MG	1A	3545	1/1	0.87	0.21	55,55,55,55	0
56	MG	2a	3116	1/1	0.87	0.09	79,79,79,79	0
56	MG	1A	3301	1/1	0.87	0.10	42,42,42,42	0
56	MG	2a	3120	1/1	0.87	0.23	60,60,60,60	0
56	MG	2A	3364	1/1	0.87	0.23	56,56,56,56	0
56	MG	2A	3759	1/1	0.87	0.15	49,49,49,49	0
56	MG	1A	3268	1/1	0.87	0.35	62,62,62,62	0
56	MG	1a	1777	1/1	0.87	0.11	50,50,50,50	0
56	MG	2A	3380	1/1	0.87	0.17	63,63,63,63	0
56	MG	1a	1619	1/1	0.87	0.21	47,47,47,47	0
56	MG	2A	3813	1/1	0.87	0.25	63,63,63,63	0
56	MG	1A	3566	1/1	0.87	0.09	40,40,40,40	0
56	MG	1a	1810	1/1	0.87	0.23	58,58,58,58	0
56	MG	1A	3571	1/1	0.87	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3186	1/1	0.87	0.11	47,47,47,47	0
56	MG	2A	3424	1/1	0.87	0.10	51,51,51,51	0
56	MG	1A	3798	1/1	0.87	0.13	65,65,65,65	0
56	MG	1a	1818	1/1	0.87	0.18	60,60,60,60	0
56	MG	1a	1823	1/1	0.87	0.24	53,53,53,53	0
56	MG	2a	3180	1/1	0.87	0.19	57,57,57,57	0
56	MG	2A	3197	1/1	0.87	0.26	62,62,62,62	0
56	MG	2A	3463	1/1	0.87	0.19	57,57,57,57	0
56	MG	2a	3187	1/1	0.87	0.24	70,70,70,70	0
56	MG	1a	1824	1/1	0.87	0.18	52,52,52,52	0
56	MG	2a	3193	1/1	0.87	0.12	65,65,65,65	0
56	MG	1a	1826	1/1	0.87	0.18	49,49,49,49	0
56	MG	2A	3480	1/1	0.87	0.14	57,57,57,57	0
56	MG	2B	208	1/1	0.87	0.13	64,64,64,64	0
56	MG	1b	301	1/1	0.87	0.17	76,76,76,76	0
56	MG	2A	3213	1/1	0.87	0.12	61,61,61,61	0
56	MG	2A	3516	1/1	0.87	0.22	58,58,58,58	0
56	MG	1k	201	1/1	0.87	0.22	55,55,55,55	0
56	MG	1A	3335	1/1	0.87	0.26	49,49,49,49	0
56	MG	2A	3217	1/1	0.87	0.26	56,56,56,56	0
56	MG	2A	3218	1/1	0.87	0.37	63,63,63,63	0
56	MG	2A	3543	1/1	0.87	0.10	65,65,65,65	0
56	MG	2A	3544	1/1	0.87	0.12	35,35,35,35	0
56	MG	1A	3830	1/1	0.87	0.18	60,60,60,60	0
56	MG	1A	3342	1/1	0.87	0.09	44,44,44,44	0
56	MG	1A	3525	1/1	0.87	0.17	62,62,62,62	0
56	MG	1x	107	1/1	0.87	0.25	60,60,60,60	0
56	MG	2A	3240	1/1	0.87	0.17	57,57,57,57	0
56	MG	2A	3247	1/1	0.87	0.13	51,51,51,51	0
56	MG	1A	3532	1/1	0.87	0.26	60,60,60,60	0
56	MG	1A	3894	1/1	0.87	0.09	59,59,59,59	0
56	MG	1A	3635	1/1	0.87	0.16	27,27,27,27	0
56	MG	2A	3584	1/1	0.87	0.11	47,47,47,47	0
56	MG	1a	1662	1/1	0.87	0.25	73,73,73,73	0
56	MG	2d	301	1/1	0.87	0.23	58,58,58,58	0
56	MG	2e	202	1/1	0.87	0.20	57,57,57,57	0
56	MG	2g	201	1/1	0.87	0.12	74,74,74,74	0
56	MG	2A	3023	1/1	0.87	0.11	52,52,52,52	0
56	MG	2l	201	1/1	0.87	0.17	72,72,72,72	0
56	MG	1a	1665	1/1	0.87	0.22	64,64,64,64	0
56	MG	1A	3657	1/1	0.87	0.20	49,49,49,49	0
56	MG	2A	3041	1/1	0.87	0.13	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	1671	1/1	0.87	0.22	65,65,65,65	0
56	MG	2w	101	1/1	0.87	0.26	74,74,74,74	0
56	MG	2A	3268	1/1	0.87	0.13	72,72,72,72	0
56	MG	2A	3269	1/1	0.87	0.07	69,69,69,69	0
56	MG	1B	222	1/1	0.87	0.13	68,68,68,68	0
56	MG	2a	3068	1/1	0.88	0.17	41,41,41,41	0
56	MG	2A	3078	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3425	1/1	0.88	0.27	44,44,44,44	0
56	MG	1A	3620	1/1	0.88	0.08	25,25,25,25	0
56	MG	1A	3935	1/1	0.88	0.08	25,25,25,25	0
56	MG	2A	3430	1/1	0.88	0.10	49,49,49,49	0
56	MG	2a	3086	1/1	0.88	0.17	50,50,50,50	0
56	MG	1a	1785	1/1	0.88	0.14	68,68,68,68	0
56	MG	1a	1801	1/1	0.88	0.12	80,80,80,80	0
56	MG	2A	3458	1/1	0.88	0.12	51,51,51,51	0
56	MG	2A	3461	1/1	0.88	0.15	69,69,69,69	0
56	MG	1A	3356	1/1	0.88	0.17	40,40,40,40	0
56	MG	1A	3286	1/1	0.88	0.10	51,51,51,51	0
56	MG	2A	3099	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3796	1/1	0.88	0.12	50,50,50,50	0
56	MG	2A	3472	1/1	0.88	0.11	57,57,57,57	0
56	MG	1A	3552	1/1	0.88	0.17	45,45,45,45	0
56	MG	2A	3811	1/1	0.88	0.11	49,49,49,49	0
56	MG	1A	3295	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3819	1/1	0.88	0.12	74,74,74,74	0
56	MG	1A	3806	1/1	0.88	0.22	47,47,47,47	0
56	MG	2A	3514	1/1	0.88	0.09	34,34,34,34	0
56	MG	2A	3132	1/1	0.88	0.16	63,63,63,63	0
56	MG	1a	1673	1/1	0.88	0.12	66,66,66,66	0
56	MG	2A	3831	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3521	1/1	0.88	0.14	45,45,45,45	0
56	MG	1A	3814	1/1	0.88	0.15	63,63,63,63	0
56	MG	1A	4012	1/1	0.88	0.12	26,26,26,26	0
56	MG	2A	3536	1/1	0.88	0.22	59,59,59,59	0
56	MG	2A	3280	1/1	0.88	0.15	55,55,55,55	0
56	MG	1O	202	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3513	1/1	0.88	0.14	36,36,36,36	0
56	MG	1V	207	1/1	0.88	0.09	48,48,48,48	0
56	MG	2a	3145	1/1	0.88	0.11	91,91,91,91	0
56	MG	1A	3666	1/1	0.88	0.12	46,46,46,46	0
56	MG	2B	207	1/1	0.88	0.07	65,65,65,65	0
56	MG	1a	1711	1/1	0.88	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1722	1/1	0.88	0.29	58,58,58,58	0
56	MG	1A	3070	1/1	0.88	0.22	52,52,52,52	0
56	MG	2A	3302	1/1	0.88	0.09	64,64,64,64	0
56	MG	2a	3168	1/1	0.88	0.12	73,73,73,73	0
56	MG	1A	4033	1/1	0.88	0.12	81,81,81,81	0
56	MG	2a	3181	1/1	0.88	0.20	68,68,68,68	0
56	MG	2A	3004	1/1	0.88	0.21	61,61,61,61	0
56	MG	1a	1617	1/1	0.88	0.11	64,64,64,64	0
56	MG	2A	3194	1/1	0.88	0.26	72,72,72,72	0
56	MG	2a	3189	1/1	0.88	0.13	91,91,91,91	0
56	MG	2E	302	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3314	1/1	0.88	0.09	65,65,65,65	0
56	MG	2E	307	1/1	0.88	0.09	59,59,59,59	0
56	MG	1A	3679	1/1	0.88	0.13	46,46,46,46	0
56	MG	2F	307	1/1	0.88	0.10	56,56,56,56	0
56	MG	2a	3200	1/1	0.88	0.10	70,70,70,70	0
56	MG	2N	201	1/1	0.88	0.11	69,69,69,69	0
56	MG	2R	201	1/1	0.88	0.13	58,58,58,58	0
56	MG	2a	3205	1/1	0.88	0.25	62,62,62,62	0
56	MG	1a	1622	1/1	0.88	0.14	65,65,65,65	0
56	MG	1A	3102	1/1	0.88	0.09	30,30,30,30	0
56	MG	1a	1755	1/1	0.88	0.08	58,58,58,58	0
56	MG	2A	3615	1/1	0.88	0.35	55,55,55,55	0
56	MG	1A	3865	1/1	0.88	0.18	60,60,60,60	0
56	MG	1A	3723	1/1	0.88	0.11	41,41,41,41	0
56	MG	2a	3012	1/1	0.88	0.31	76,76,76,76	0
56	MG	2a	3219	1/1	0.88	0.25	63,63,63,63	0
56	MG	2a	3013	1/1	0.88	0.23	63,63,63,63	0
56	MG	2A	3352	1/1	0.88	0.12	60,60,60,60	0
56	MG	2a	3018	1/1	0.88	0.19	60,60,60,60	0
56	MG	2A	3357	1/1	0.88	0.21	49,49,49,49	0
56	MG	2A	3640	1/1	0.88	0.16	68,68,68,68	0
56	MG	2A	3358	1/1	0.88	0.22	57,57,57,57	0
56	MG	1A	3724	1/1	0.88	0.11	56,56,56,56	0
56	MG	1a	1768	1/1	0.88	0.13	67,67,67,67	0
56	MG	2a	3237	1/1	0.88	0.14	63,63,63,63	0
56	MG	1A	3598	1/1	0.88	0.11	40,40,40,40	0
56	MG	2A	3057	1/1	0.88	0.19	52,52,52,52	0
56	MG	2A	3378	1/1	0.88	0.15	46,46,46,46	0
56	MG	1a	1771	1/1	0.88	0.10	54,54,54,54	0
56	MG	2e	201	1/1	0.88	0.08	75,75,75,75	0
56	MG	2A	3383	1/1	0.88	0.23	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	3047	1/1	0.88	0.16	73,73,73,73	0
56	MG	2A	3222	1/1	0.88	0.08	46,46,46,46	0
56	MG	2A	3064	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	3427	1/1	0.88	0.24	36,36,36,36	0
56	MG	2t	201	1/1	0.88	0.24	60,60,60,60	0
56	MG	2A	3410	1/1	0.88	0.23	43,43,43,43	0
56	MG	2A	3690	1/1	0.88	0.12	70,70,70,70	0
56	MG	1A	3354	1/1	0.88	0.18	63,63,63,63	0
56	MG	2A	3695	1/1	0.88	0.09	41,41,41,41	0
56	MG	2a	3064	1/1	0.88	0.09	61,61,61,61	0
56	MG	2A	3077	1/1	0.88	0.05	50,50,50,50	0
56	MG	2A	3417	1/1	0.88	0.13	52,52,52,52	0
57	K	2A	3399	1/1	0.88	0.11	73,73,73,73	0
56	MG	1A	3451	1/1	0.89	0.08	46,46,46,46	0
56	MG	1A	3872	1/1	0.89	0.10	31,31,31,31	0
56	MG	1A	3561	1/1	0.89	0.19	62,62,62,62	0
56	MG	2A	3003	1/1	0.89	0.28	60,60,60,60	0
56	MG	1A	3185	1/1	0.89	0.12	34,34,34,34	0
56	MG	2A	3408	1/1	0.89	0.25	55,55,55,55	0
56	MG	2a	3071	1/1	0.89	0.15	60,60,60,60	0
56	MG	1a	1695	1/1	0.89	0.22	59,59,59,59	0
56	MG	2a	3078	1/1	0.89	0.19	64,64,64,64	0
56	MG	1A	3469	1/1	0.89	0.17	42,42,42,42	0
56	MG	1A	3328	1/1	0.89	0.39	42,42,42,42	0
56	MG	1A	3581	1/1	0.89	0.12	50,50,50,50	0
56	MG	1A	3747	1/1	0.89	0.18	78,78,78,78	0
56	MG	2A	3734	1/1	0.89	0.18	60,60,60,60	0
56	MG	2a	3094	1/1	0.89	0.16	69,69,69,69	0
56	MG	1a	1708	1/1	0.89	0.20	50,50,50,50	0
56	MG	2A	3740	1/1	0.89	0.16	70,70,70,70	0
56	MG	1A	3770	1/1	0.89	0.07	43,43,43,43	0
56	MG	1a	1717	1/1	0.89	0.32	60,60,60,60	0
56	MG	2A	3232	1/1	0.89	0.09	48,48,48,48	0
56	MG	2A	3233	1/1	0.89	0.10	49,49,49,49	0
56	MG	2A	3793	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3942	1/1	0.89	0.08	22,22,22,22	0
56	MG	2A	3455	1/1	0.89	0.14	59,59,59,59	0
56	MG	1A	3279	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3587	1/1	0.89	0.12	57,57,57,57	0
56	MG	2a	3114	1/1	0.89	0.13	78,78,78,78	0
56	MG	1A	3962	1/1	0.89	0.09	56,56,56,56	0
56	MG	2A	3817	1/1	0.89	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3063	1/1	0.89	0.09	48,48,48,48	0
56	MG	1A	3379	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3068	1/1	0.89	0.34	65,65,65,65	0
56	MG	2A	3072	1/1	0.89	0.13	60,60,60,60	0
56	MG	2a	3124	1/1	0.89	0.23	68,68,68,68	0
56	MG	2A	3824	1/1	0.89	0.09	59,59,59,59	0
56	MG	1Q	205	1/1	0.89	0.12	57,57,57,57	0
56	MG	2A	3495	1/1	0.89	0.10	42,42,42,42	0
56	MG	1S	202	1/1	0.89	0.11	44,44,44,44	0
56	MG	1A	3491	1/1	0.89	0.16	54,54,54,54	0
56	MG	1A	3508	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3840	1/1	0.89	0.14	60,60,60,60	0
56	MG	1Z	302	1/1	0.89	0.07	47,47,47,47	0
56	MG	1A	3509	1/1	0.89	0.25	51,51,51,51	0
56	MG	17	105	1/1	0.89	0.14	58,58,58,58	0
56	MG	2A	3270	1/1	0.89	0.11	63,63,63,63	0
56	MG	1a	1608	1/1	0.89	0.16	53,53,53,53	0
56	MG	2B	203	1/1	0.89	0.13	73,73,73,73	0
56	MG	2B	204	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	3990	1/1	0.89	0.07	41,41,41,41	0
56	MG	1A	3057	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3096	1/1	0.89	0.19	51,51,51,51	0
56	MG	1A	3241	1/1	0.89	0.13	42,42,42,42	0
56	MG	2B	210	1/1	0.89	0.11	50,50,50,50	0
56	MG	2B	211	1/1	0.89	0.19	72,72,72,72	0
56	MG	2a	3188	1/1	0.89	0.17	81,81,81,81	0
56	MG	1a	1620	1/1	0.89	0.29	68,68,68,68	0
56	MG	2A	3284	1/1	0.89	0.34	57,57,57,57	0
56	MG	2B	214	1/1	0.89	0.09	67,67,67,67	0
56	MG	1A	4019	1/1	0.89	0.10	49,49,49,49	0
56	MG	2A	3291	1/1	0.89	0.11	55,55,55,55	0
56	MG	1A	4025	1/1	0.89	0.22	32,32,32,32	0
56	MG	1A	4027	1/1	0.89	0.22	45,45,45,45	0
56	MG	2a	3201	1/1	0.89	0.15	74,74,74,74	0
56	MG	1a	1635	1/1	0.89	0.25	51,51,51,51	0
56	MG	2A	3578	1/1	0.89	0.21	66,66,66,66	0
56	MG	1A	3346	1/1	0.89	0.08	49,49,49,49	0
56	MG	1A	3023	1/1	0.89	0.07	37,37,37,37	0
56	MG	2A	3585	1/1	0.89	0.12	49,49,49,49	0
56	MG	2A	3591	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3227	1/1	0.89	0.13	44,44,44,44	0
56	MG	2A	3144	1/1	0.89	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	28	105	1/1	0.89	0.15	65,65,65,65	0
56	MG	2A	3602	1/1	0.89	0.14	69,69,69,69	0
56	MG	2A	3307	1/1	0.89	0.14	59,59,59,59	0
56	MG	2A	3608	1/1	0.89	0.10	49,49,49,49	0
56	MG	1A	3838	1/1	0.89	0.10	16,16,16,16	0
56	MG	2A	3147	1/1	0.89	0.14	49,49,49,49	0
56	MG	1a	1652	1/1	0.89	0.16	46,46,46,46	0
56	MG	2A	3324	1/1	0.89	0.27	69,69,69,69	0
56	MG	2a	3016	1/1	0.89	0.12	50,50,50,50	0
56	MG	1A	3321	1/1	0.89	0.14	48,48,48,48	0
56	MG	2A	3163	1/1	0.89	0.11	50,50,50,50	0
56	MG	2a	3019	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3633	1/1	0.89	0.09	51,51,51,51	0
56	MG	2A	3165	1/1	0.89	0.27	65,65,65,65	0
56	MG	2A	3167	1/1	0.89	0.30	65,65,65,65	0
56	MG	2A	3170	1/1	0.89	0.18	68,68,68,68	0
56	MG	2A	3171	1/1	0.89	0.21	65,65,65,65	0
56	MG	2A	3349	1/1	0.89	0.10	45,45,45,45	0
56	MG	2A	3172	1/1	0.89	0.15	65,65,65,65	0
56	MG	2A	3355	1/1	0.89	0.19	63,63,63,63	0
56	MG	2a	3041	1/1	0.89	0.17	74,74,74,74	0
56	MG	1A	3367	1/1	0.89	0.13	56,56,56,56	0
56	MG	2q	202	1/1	0.89	0.14	76,76,76,76	0
56	MG	2q	203	1/1	0.89	0.10	62,62,62,62	0
56	MG	1e	3101	1/1	0.89	0.08	69,69,69,69	0
56	MG	2A	3664	1/1	0.89	0.10	36,36,36,36	0
56	MG	2A	3669	1/1	0.89	0.24	63,63,63,63	0
56	MG	1A	4058	1/1	0.89	0.16	60,60,60,60	0
56	MG	1A	3858	1/1	0.89	0.28	29,29,29,29	0
56	MG	1A	4063	1/1	0.89	0.16	68,68,68,68	0
56	MG	2A	3373	1/1	0.89	0.12	65,65,65,65	0
56	MG	1A	4069	1/1	0.89	0.11	43,43,43,43	0
56	MG	1A	3863	1/1	0.89	0.18	26,26,26,26	0
56	MG	1A	3920	1/1	0.90	0.14	52,52,52,52	0
56	MG	1A	3922	1/1	0.90	0.09	56,56,56,56	0
56	MG	1A	3930	1/1	0.90	0.14	25,25,25,25	0
56	MG	2A	3149	1/1	0.90	0.07	59,59,59,59	0
56	MG	2A	3663	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3447	1/1	0.90	0.09	49,49,49,49	0
56	MG	1A	3312	1/1	0.90	0.20	40,40,40,40	0
56	MG	2A	3350	1/1	0.90	0.09	53,53,53,53	0
56	MG	2a	3054	1/1	0.90	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3754	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3562	1/1	0.90	0.19	40,40,40,40	0
56	MG	2A	3166	1/1	0.90	0.16	60,60,60,60	0
56	MG	1a	1783	1/1	0.90	0.09	59,59,59,59	0
56	MG	1l	101	1/1	0.90	0.22	40,40,40,40	0
56	MG	1A	3463	1/1	0.90	0.12	54,54,54,54	0
56	MG	2A	3367	1/1	0.90	0.29	62,62,62,62	0
56	MG	18	102	1/1	0.90	0.13	30,30,30,30	0
56	MG	2A	3371	1/1	0.90	0.26	56,56,56,56	0
56	MG	1A	3002	1/1	0.90	0.12	44,44,44,44	0
56	MG	1A	3781	1/1	0.90	0.10	51,51,51,51	0
56	MG	1A	3971	1/1	0.90	0.15	61,61,61,61	0
56	MG	2a	3081	1/1	0.90	0.19	79,79,79,79	0
56	MG	1a	1618	1/1	0.90	0.24	49,49,49,49	0
56	MG	2A	3720	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	3468	1/1	0.90	0.14	41,41,41,41	0
56	MG	2A	3191	1/1	0.90	0.16	39,39,39,39	0
56	MG	1A	3784	1/1	0.90	0.10	29,29,29,29	0
56	MG	1A	3785	1/1	0.90	0.08	34,34,34,34	0
56	MG	2A	3404	1/1	0.90	0.06	61,61,61,61	0
56	MG	1A	3999	1/1	0.90	0.11	49,49,49,49	0
56	MG	1a	1626	1/1	0.90	0.22	61,61,61,61	0
56	MG	2A	3742	1/1	0.90	0.09	59,59,59,59	0
56	MG	2a	3103	1/1	0.90	0.16	68,68,68,68	0
56	MG	2a	3104	1/1	0.90	0.19	60,60,60,60	0
56	MG	1a	1629	1/1	0.90	0.10	53,53,53,53	0
56	MG	1A	3107	1/1	0.90	0.21	46,46,46,46	0
56	MG	2A	3206	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	3372	1/1	0.90	0.10	48,48,48,48	0
56	MG	2A	3795	1/1	0.90	0.15	69,69,69,69	0
56	MG	2a	3111	1/1	0.90	0.10	74,74,74,74	0
56	MG	1A	3797	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3327	1/1	0.90	0.20	51,51,51,51	0
56	MG	2A	3803	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3805	1/1	0.90	0.10	58,58,58,58	0
56	MG	1x	109	1/1	0.90	0.17	72,72,72,72	0
56	MG	1A	3799	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	4029	1/1	0.90	0.12	58,58,58,58	0
56	MG	1A	3486	1/1	0.90	0.10	58,58,58,58	0
56	MG	1a	1653	1/1	0.90	0.08	64,64,64,64	0
56	MG	2A	3457	1/1	0.90	0.09	65,65,65,65	0
56	MG	1a	1654	1/1	0.90	0.15	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	3228	1/1	0.90	0.13	66,66,66,66	0
56	MG	2A	3231	1/1	0.90	0.19	62,62,62,62	0
56	MG	2A	3825	1/1	0.90	0.29	65,65,65,65	0
56	MG	2A	3019	1/1	0.90	0.10	55,55,55,55	0
56	MG	2a	3138	1/1	0.90	0.28	76,76,76,76	0
56	MG	2A	3830	1/1	0.90	0.20	58,58,58,58	0
56	MG	1A	3808	1/1	0.90	0.25	34,34,34,34	0
56	MG	2A	3832	1/1	0.90	0.15	58,58,58,58	0
56	MG	1A	3113	1/1	0.90	0.16	56,56,56,56	0
56	MG	1A	3815	1/1	0.90	0.11	36,36,36,36	0
56	MG	1A	3823	1/1	0.90	0.37	45,45,45,45	0
56	MG	2A	3245	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	3601	1/1	0.90	0.11	22,22,22,22	0
56	MG	1A	3047	1/1	0.90	0.20	31,31,31,31	0
56	MG	2A	3515	1/1	0.90	0.10	40,40,40,40	0
56	MG	2A	3046	1/1	0.90	0.20	69,69,69,69	0
56	MG	1A	3503	1/1	0.90	0.18	57,57,57,57	0
56	MG	1A	3332	1/1	0.90	0.30	44,44,44,44	0
56	MG	1A	3384	1/1	0.90	0.35	67,67,67,67	0
56	MG	1A	4071	1/1	0.90	0.12	65,65,65,65	0
56	MG	2A	3532	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3258	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1682	1/1	0.90	0.27	57,57,57,57	0
56	MG	1A	3512	1/1	0.90	0.16	60,60,60,60	0
56	MG	1a	1692	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3545	1/1	0.90	0.20	62,62,62,62	0
56	MG	1a	1694	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3135	1/1	0.90	0.39	30,30,30,30	0
56	MG	1A	4078	1/1	0.90	0.13	52,52,52,52	0
56	MG	2a	3202	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3553	1/1	0.90	0.08	63,63,63,63	0
56	MG	1A	3521	1/1	0.90	0.14	40,40,40,40	0
56	MG	2A	3273	1/1	0.90	0.15	64,64,64,64	0
56	MG	2a	3206	1/1	0.90	0.17	56,56,56,56	0
56	MG	2D	302	1/1	0.90	0.09	42,42,42,42	0
56	MG	2A	3562	1/1	0.90	0.14	39,39,39,39	0
56	MG	1A	3338	1/1	0.90	0.21	42,42,42,42	0
56	MG	1A	3866	1/1	0.90	0.08	35,35,35,35	0
56	MG	2F	302	1/1	0.90	0.16	42,42,42,42	0
56	MG	1A	3672	1/1	0.90	0.09	69,69,69,69	0
56	MG	1A	3878	1/1	0.90	0.15	41,41,41,41	0
56	MG	1a	1715	1/1	0.90	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2O	201	1/1	0.90	0.10	58,58,58,58	0
56	MG	1A	3527	1/1	0.90	0.09	50,50,50,50	0
56	MG	20	102	1/1	0.90	0.11	52,52,52,52	0
56	MG	2a	3224	1/1	0.90	0.09	52,52,52,52	0
56	MG	1a	1718	1/1	0.90	0.14	54,54,54,54	0
56	MG	28	101	1/1	0.90	0.22	66,66,66,66	0
56	MG	2a	3233	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3091	1/1	0.90	0.12	56,56,56,56	0
56	MG	1A	3403	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3295	1/1	0.90	0.13	80,80,80,80	0
56	MG	1A	3907	1/1	0.90	0.08	22,22,22,22	0
56	MG	2a	3008	1/1	0.90	0.17	62,62,62,62	0
56	MG	1A	3225	1/1	0.90	0.11	56,56,56,56	0
56	MG	2A	3298	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3100	1/1	0.90	0.16	39,39,39,39	0
56	MG	1A	3091	1/1	0.90	0.13	44,44,44,44	0
56	MG	1E	308	1/1	0.90	0.17	55,55,55,55	0
56	MG	2f	201	1/1	0.90	0.11	66,66,66,66	0
56	MG	1F	311	1/1	0.90	0.18	42,42,42,42	0
56	MG	2A	3120	1/1	0.90	0.18	55,55,55,55	0
56	MG	1F	312	1/1	0.90	0.11	54,54,54,54	0
56	MG	2A	3632	1/1	0.90	0.21	57,57,57,57	0
56	MG	2l	203	1/1	0.90	0.09	72,72,72,72	0
56	MG	2q	201	1/1	0.90	0.07	61,61,61,61	0
56	MG	2a	3021	1/1	0.90	0.16	56,56,56,56	0
56	MG	1A	3179	1/1	0.90	0.14	50,50,50,50	0
56	MG	2a	3028	1/1	0.90	0.12	79,79,79,79	0
56	MG	1N	204	1/1	0.90	0.11	50,50,50,50	0
56	MG	2a	3032	1/1	0.90	0.23	60,60,60,60	0
56	MG	2a	3033	1/1	0.90	0.15	59,59,59,59	0
56	MG	2A	3638	1/1	0.90	0.18	62,62,62,62	0
56	MG	2A	3315	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3077	1/1	0.90	0.11	36,36,36,36	0
56	MG	2A	3330	1/1	0.90	0.23	53,53,53,53	0
56	MG	1P	207	1/1	0.90	0.14	37,37,37,37	0
56	MG	1A	3933	1/1	0.91	0.09	23,23,23,23	0
56	MG	1A	3418	1/1	0.91	0.15	56,56,56,56	0
56	MG	2A	3285	1/1	0.91	0.07	64,64,64,64	0
56	MG	1A	3126	1/1	0.91	0.14	42,42,42,42	0
56	MG	2A	3290	1/1	0.91	0.12	47,47,47,47	0
56	MG	1a	1714	1/1	0.91	0.25	63,63,63,63	0
56	MG	1A	3005	1/1	0.91	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	3305	1/1	0.91	0.10	29,29,29,29	0
56	MG	2A	3606	1/1	0.91	0.10	36,36,36,36	0
56	MG	2A	3607	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	3954	1/1	0.91	0.10	31,31,31,31	0
56	MG	2a	3030	1/1	0.91	0.22	46,46,46,46	0
56	MG	1a	1720	1/1	0.91	0.32	58,58,58,58	0
56	MG	1A	3522	1/1	0.91	0.14	32,32,32,32	0
56	MG	2a	3034	1/1	0.91	0.17	74,74,74,74	0
56	MG	2A	3102	1/1	0.91	0.23	41,41,41,41	0
56	MG	2A	3618	1/1	0.91	0.15	61,61,61,61	0
56	MG	2A	3619	1/1	0.91	0.09	47,47,47,47	0
56	MG	1A	3523	1/1	0.91	0.21	54,54,54,54	0
56	MG	2A	3622	1/1	0.91	0.07	40,40,40,40	0
56	MG	1A	3966	1/1	0.91	0.07	71,71,71,71	0
56	MG	2A	3113	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3968	1/1	0.91	0.07	55,55,55,55	0
56	MG	2a	3046	1/1	0.91	0.11	60,60,60,60	0
56	MG	2A	3308	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3438	1/1	0.91	0.11	62,62,62,62	0
56	MG	2A	3129	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3131	1/1	0.91	0.24	59,59,59,59	0
56	MG	1S	203	1/1	0.91	0.15	57,57,57,57	0
56	MG	2A	3316	1/1	0.91	0.08	46,46,46,46	0
56	MG	1A	3639	1/1	0.91	0.09	56,56,56,56	0
56	MG	2A	3325	1/1	0.91	0.15	65,65,65,65	0
56	MG	1a	1753	1/1	0.91	0.08	69,69,69,69	0
56	MG	2A	3140	1/1	0.91	0.08	57,57,57,57	0
56	MG	1W	203	1/1	0.91	0.21	64,64,64,64	0
56	MG	1A	3310	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3986	1/1	0.91	0.10	30,30,30,30	0
56	MG	2A	3340	1/1	0.91	0.45	74,74,74,74	0
56	MG	2A	3341	1/1	0.91	0.10	53,53,53,53	0
56	MG	10	101	1/1	0.91	0.06	25,25,25,25	0
56	MG	1A	3658	1/1	0.91	0.08	27,27,27,27	0
56	MG	2a	3077	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3680	1/1	0.91	0.09	75,75,75,75	0
56	MG	1A	3811	1/1	0.91	0.07	50,50,50,50	0
56	MG	1A	3528	1/1	0.91	0.07	53,53,53,53	0
56	MG	1A	4000	1/1	0.91	0.12	46,46,46,46	0
56	MG	2A	3157	1/1	0.91	0.17	65,65,65,65	0
56	MG	2A	3356	1/1	0.91	0.17	41,41,41,41	0
56	MG	2a	3088	1/1	0.91	0.08	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	19	101	1/1	0.91	0.11	53,53,53,53	0
56	MG	1a	1606	1/1	0.91	0.08	66,66,66,66	0
56	MG	2A	3701	1/1	0.91	0.15	63,63,63,63	0
56	MG	2A	3702	1/1	0.91	0.18	58,58,58,58	0
56	MG	1a	1607	1/1	0.91	0.13	36,36,36,36	0
56	MG	2a	3099	1/1	0.91	0.11	69,69,69,69	0
56	MG	1A	4011	1/1	0.91	0.13	44,44,44,44	0
56	MG	1A	3530	1/1	0.91	0.16	59,59,59,59	0
56	MG	1a	1786	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3717	1/1	0.91	0.12	57,57,57,57	0
56	MG	1a	1792	1/1	0.91	0.07	69,69,69,69	0
56	MG	2A	3174	1/1	0.91	0.22	55,55,55,55	0
56	MG	1a	1795	1/1	0.91	0.07	78,78,78,78	0
56	MG	1A	3146	1/1	0.91	0.21	57,57,57,57	0
56	MG	1A	3825	1/1	0.91	0.36	21,21,21,21	0
56	MG	2A	3381	1/1	0.91	0.15	44,44,44,44	0
56	MG	1A	3316	1/1	0.91	0.09	35,35,35,35	0
56	MG	1A	3538	1/1	0.91	0.15	41,41,41,41	0
56	MG	2A	3385	1/1	0.91	0.26	53,53,53,53	0
56	MG	2A	3745	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3750	1/1	0.91	0.10	69,69,69,69	0
56	MG	2A	3189	1/1	0.91	0.25	60,60,60,60	0
56	MG	2A	3760	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3773	1/1	0.91	0.09	47,47,47,47	0
56	MG	2A	3391	1/1	0.91	0.18	55,55,55,55	0
56	MG	1a	1815	1/1	0.91	0.15	73,73,73,73	0
56	MG	2A	3403	1/1	0.91	0.08	57,57,57,57	0
56	MG	2a	3130	1/1	0.91	0.22	60,60,60,60	0
56	MG	1A	3677	1/1	0.91	0.09	33,33,33,33	0
56	MG	2a	3133	1/1	0.91	0.11	67,67,67,67	0
56	MG	1a	1624	1/1	0.91	0.29	56,56,56,56	0
56	MG	2A	3409	1/1	0.91	0.14	46,46,46,46	0
56	MG	2A	3801	1/1	0.91	0.12	44,44,44,44	0
56	MG	1A	3464	1/1	0.91	0.06	51,51,51,51	0
56	MG	2A	3804	1/1	0.91	0.07	55,55,55,55	0
56	MG	2a	3143	1/1	0.91	0.10	70,70,70,70	0
56	MG	1A	4031	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3840	1/1	0.91	0.07	33,33,33,33	0
56	MG	1A	3153	1/1	0.91	0.19	57,57,57,57	0
56	MG	2A	3205	1/1	0.91	0.08	48,48,48,48	0
56	MG	2A	3814	1/1	0.91	0.10	51,51,51,51	0
56	MG	1a	1634	1/1	0.91	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3159	1/1	0.91	0.13	69,69,69,69	0
56	MG	1n	102	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3212	1/1	0.91	0.15	49,49,49,49	0
56	MG	1w	101	1/1	0.91	0.08	66,66,66,66	0
56	MG	2A	3431	1/1	0.91	0.13	50,50,50,50	0
56	MG	1A	4036	1/1	0.91	0.12	46,46,46,46	0
56	MG	1a	1640	1/1	0.91	0.08	71,71,71,71	0
56	MG	2A	3454	1/1	0.91	0.12	54,54,54,54	0
56	MG	2A	3829	1/1	0.91	0.05	67,67,67,67	0
56	MG	1A	3691	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	4047	1/1	0.91	0.12	40,40,40,40	0
56	MG	2a	3191	1/1	0.91	0.15	67,67,67,67	0
56	MG	1a	1648	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3460	1/1	0.91	0.16	54,54,54,54	0
56	MG	1A	3702	1/1	0.91	0.09	23,23,23,23	0
56	MG	1A	3707	1/1	0.91	0.08	64,64,64,64	0
56	MG	2A	3839	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3464	1/1	0.91	0.15	38,38,38,38	0
56	MG	1x	112	1/1	0.91	0.27	57,57,57,57	0
56	MG	2A	3843	1/1	0.91	0.15	46,46,46,46	0
56	MG	1A	3001	1/1	0.91	0.08	40,40,40,40	0
56	MG	1A	3390	1/1	0.91	0.27	47,47,47,47	0
56	MG	2A	3474	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3392	1/1	0.91	0.12	47,47,47,47	0
56	MG	1A	3874	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3490	1/1	0.91	0.08	39,39,39,39	0
56	MG	2A	3014	1/1	0.91	0.07	45,45,45,45	0
56	MG	2B	206	1/1	0.91	0.13	70,70,70,70	0
56	MG	2A	3498	1/1	0.91	0.07	51,51,51,51	0
56	MG	1A	3358	1/1	0.91	0.17	47,47,47,47	0
56	MG	1A	3742	1/1	0.91	0.07	33,33,33,33	0
56	MG	1A	3399	1/1	0.91	0.12	58,58,58,58	0
56	MG	2a	3221	1/1	0.91	0.24	62,62,62,62	0
56	MG	1A	4077	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3519	1/1	0.91	0.14	64,64,64,64	0
56	MG	1a	1664	1/1	0.91	0.18	43,43,43,43	0
56	MG	1A	3905	1/1	0.91	0.07	42,42,42,42	0
56	MG	1A	4079	1/1	0.91	0.17	41,41,41,41	0
56	MG	1A	4082	1/1	0.91	0.29	57,57,57,57	0
56	MG	1A	3487	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3756	1/1	0.91	0.07	57,57,57,57	0
56	MG	2A	3261	1/1	0.91	0.18	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	2E	301	1/1	0.91	0.09	47,47,47,47	0
56	MG	2A	3262	1/1	0.91	0.09	60,60,60,60	0
56	MG	2E	303	1/1	0.91	0.14	47,47,47,47	0
56	MG	2a	3241	1/1	0.91	0.19	64,64,64,64	0
56	MG	1a	1676	1/1	0.91	0.25	52,52,52,52	0
56	MG	1a	1677	1/1	0.91	0.31	51,51,51,51	0
56	MG	1A	3757	1/1	0.91	0.06	40,40,40,40	0
56	MG	1a	1683	1/1	0.91	0.29	59,59,59,59	0
56	MG	1A	3764	1/1	0.91	0.09	34,34,34,34	0
56	MG	1A	3401	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3214	1/1	0.91	0.14	42,42,42,42	0
56	MG	1A	3405	1/1	0.91	0.13	40,40,40,40	0
56	MG	2V	201	1/1	0.91	0.14	54,54,54,54	0
56	MG	2A	3557	1/1	0.91	0.09	44,44,44,44	0
56	MG	2l	204	1/1	0.91	0.14	55,55,55,55	0
56	MG	23	101	1/1	0.91	0.08	42,42,42,42	0
56	MG	25	102	1/1	0.91	0.26	61,61,61,61	0
56	MG	1A	3928	1/1	0.91	0.10	67,67,67,67	0
56	MG	1A	3238	1/1	0.91	0.07	42,42,42,42	0
56	MG	28	102	1/1	0.91	0.20	56,56,56,56	0
56	MG	2A	3565	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3279	1/1	0.91	0.14	54,54,54,54	0
56	MG	1a	1704	1/1	0.91	0.20	49,49,49,49	0
56	MG	2x	102	1/1	0.91	0.29	59,59,59,59	0
56	MG	2x	103	1/1	0.91	0.12	66,66,66,66	0
56	MG	2A	3574	1/1	0.91	0.07	43,43,43,43	0
56	MG	1D	310	1/1	0.91	0.12	46,46,46,46	0
56	MG	2A	3580	1/1	0.91	0.17	44,44,44,44	0
56	MG	2A	3581	1/1	0.91	0.09	34,34,34,34	0
56	MG	2A	3600	1/1	0.92	0.22	55,55,55,55	0
56	MG	1a	1687	1/1	0.92	0.19	55,55,55,55	0
56	MG	1A	3040	1/1	0.92	0.31	35,35,35,35	0
56	MG	2a	3011	1/1	0.92	0.27	73,73,73,73	0
56	MG	1a	1690	1/1	0.92	0.14	57,57,57,57	0
56	MG	1a	1691	1/1	0.92	0.11	42,42,42,42	0
56	MG	2a	3015	1/1	0.92	0.12	77,77,77,77	0
56	MG	1A	3406	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	3157	1/1	0.92	0.32	33,33,33,33	0
56	MG	1A	3412	1/1	0.92	0.06	50,50,50,50	0
56	MG	1B	238	1/1	0.92	0.17	48,48,48,48	0
56	MG	1D	301	1/1	0.92	0.08	43,43,43,43	0
56	MG	1D	308	1/1	0.92	0.10	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	3620	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	3026	1/1	0.92	0.09	51,51,51,51	0
56	MG	2A	3097	1/1	0.92	0.11	70,70,70,70	0
56	MG	1A	3537	1/1	0.92	0.15	36,36,36,36	0
56	MG	1A	3414	1/1	0.92	0.11	35,35,35,35	0
56	MG	2a	3031	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3312	1/1	0.92	0.16	58,58,58,58	0
56	MG	2A	3631	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3755	1/1	0.92	0.08	33,33,33,33	0
56	MG	2A	3105	1/1	0.92	0.24	46,46,46,46	0
56	MG	2A	3106	1/1	0.92	0.21	49,49,49,49	0
56	MG	2A	3637	1/1	0.92	0.12	51,51,51,51	0
56	MG	2A	3317	1/1	0.92	0.21	43,43,43,43	0
56	MG	2A	3318	1/1	0.92	0.17	49,49,49,49	0
56	MG	1E	311	1/1	0.92	0.11	50,50,50,50	0
56	MG	1F	310	1/1	0.92	0.21	36,36,36,36	0
56	MG	2a	3043	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	3239	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3164	1/1	0.92	0.19	40,40,40,40	0
56	MG	2A	3652	1/1	0.92	0.14	37,37,37,37	0
56	MG	2A	3117	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3420	1/1	0.92	0.07	59,59,59,59	0
56	MG	2A	3659	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3122	1/1	0.92	0.11	57,57,57,57	0
56	MG	1N	201	1/1	0.92	0.24	50,50,50,50	0
56	MG	2a	3056	1/1	0.92	0.12	77,77,77,77	0
56	MG	2A	3130	1/1	0.92	0.08	47,47,47,47	0
56	MG	2A	3344	1/1	0.92	0.15	66,66,66,66	0
56	MG	2a	3062	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3673	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	3333	1/1	0.92	0.15	43,43,43,43	0
56	MG	1A	3773	1/1	0.92	0.07	34,34,34,34	0
56	MG	2A	3348	1/1	0.92	0.06	58,58,58,58	0
56	MG	1O	203	1/1	0.92	0.13	60,60,60,60	0
56	MG	1A	3423	1/1	0.92	0.16	73,73,73,73	0
56	MG	1A	3776	1/1	0.92	0.07	29,29,29,29	0
56	MG	1A	3242	1/1	0.92	0.18	37,37,37,37	0
56	MG	1A	3780	1/1	0.92	0.11	54,54,54,54	0
56	MG	2A	3693	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3430	1/1	0.92	0.10	62,62,62,62	0
56	MG	2a	3079	1/1	0.92	0.18	72,72,72,72	0
56	MG	2a	3080	1/1	0.92	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3696	1/1	0.92	0.16	58,58,58,58	0
56	MG	1V	205	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3969	1/1	0.92	0.09	63,63,63,63	0
56	MG	1A	3782	1/1	0.92	0.10	50,50,50,50	0
56	MG	1Y	201	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3703	1/1	0.92	0.09	50,50,50,50	0
56	MG	1A	3433	1/1	0.92	0.19	51,51,51,51	0
56	MG	2a	3090	1/1	0.92	0.16	67,67,67,67	0
56	MG	2a	3091	1/1	0.92	0.23	59,59,59,59	0
56	MG	2a	3092	1/1	0.92	0.15	59,59,59,59	0
56	MG	2a	3093	1/1	0.92	0.09	44,44,44,44	0
56	MG	2A	3707	1/1	0.92	0.06	51,51,51,51	0
56	MG	1A	3977	1/1	0.92	0.12	60,60,60,60	0
56	MG	2A	3711	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3372	1/1	0.92	0.26	54,54,54,54	0
56	MG	2A	3714	1/1	0.92	0.11	76,76,76,76	0
56	MG	1A	3980	1/1	0.92	0.09	55,55,55,55	0
56	MG	10	103	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3719	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3568	1/1	0.92	0.11	29,29,29,29	0
56	MG	1A	3041	1/1	0.92	0.08	40,40,40,40	0
56	MG	2a	3107	1/1	0.92	0.16	62,62,62,62	0
56	MG	2A	3168	1/1	0.92	0.16	49,49,49,49	0
56	MG	12	101	1/1	0.92	0.09	40,40,40,40	0
56	MG	15	105	1/1	0.92	0.08	54,54,54,54	0
56	MG	1A	3267	1/1	0.92	0.17	45,45,45,45	0
56	MG	2A	3737	1/1	0.92	0.10	70,70,70,70	0
56	MG	2A	3387	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3583	1/1	0.92	0.13	40,40,40,40	0
56	MG	1A	3017	1/1	0.92	0.13	38,38,38,38	0
56	MG	2A	3393	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	3272	1/1	0.92	0.30	52,52,52,52	0
56	MG	2A	3402	1/1	0.92	0.12	44,44,44,44	0
56	MG	2a	3121	1/1	0.92	0.23	49,49,49,49	0
56	MG	2A	3180	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3769	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3772	1/1	0.92	0.09	56,56,56,56	0
56	MG	2a	3125	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	4001	1/1	0.92	0.11	40,40,40,40	0
56	MG	2A	3406	1/1	0.92	0.10	60,60,60,60	0
56	MG	2A	3784	1/1	0.92	0.10	49,49,49,49	0
56	MG	1a	1804	1/1	0.92	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3051	1/1	0.92	0.12	41,41,41,41	0
56	MG	1a	1811	1/1	0.92	0.26	80,80,80,80	0
56	MG	1a	1609	1/1	0.92	0.16	55,55,55,55	0
56	MG	1a	1611	1/1	0.92	0.11	50,50,50,50	0
56	MG	1a	1615	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3802	1/1	0.92	0.13	46,46,46,46	0
56	MG	1A	3054	1/1	0.92	0.11	45,45,45,45	0
56	MG	1a	1822	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3285	1/1	0.92	0.18	35,35,35,35	0
56	MG	1A	3193	1/1	0.92	0.06	49,49,49,49	0
56	MG	2A	3810	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	3604	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3618	1/1	0.92	0.17	38,38,38,38	0
56	MG	1A	3294	1/1	0.92	0.13	42,42,42,42	0
56	MG	2a	3160	1/1	0.92	0.07	69,69,69,69	0
56	MG	2A	3815	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3816	1/1	0.92	0.11	45,45,45,45	0
56	MG	2a	3173	1/1	0.92	0.11	72,72,72,72	0
56	MG	2a	3177	1/1	0.92	0.09	74,74,74,74	0
56	MG	2A	3444	1/1	0.92	0.30	57,57,57,57	0
56	MG	1A	3106	1/1	0.92	0.14	38,38,38,38	0
56	MG	1n	101	1/1	0.92	0.38	60,60,60,60	0
56	MG	1A	3632	1/1	0.92	0.09	25,25,25,25	0
56	MG	1A	3475	1/1	0.92	0.21	45,45,45,45	0
56	MG	1A	3296	1/1	0.92	0.20	53,53,53,53	0
56	MG	1A	3834	1/1	0.92	0.09	31,31,31,31	0
56	MG	2A	3219	1/1	0.92	0.20	63,63,63,63	0
56	MG	1A	4038	1/1	0.92	0.07	64,64,64,64	0
56	MG	1A	4039	1/1	0.92	0.11	65,65,65,65	0
56	MG	2A	3223	1/1	0.92	0.04	52,52,52,52	0
56	MG	2a	3197	1/1	0.92	0.13	66,66,66,66	0
56	MG	2A	3224	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	3298	1/1	0.92	0.06	30,30,30,30	0
56	MG	1x	108	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3837	1/1	0.92	0.17	35,35,35,35	0
56	MG	1A	3055	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	3843	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3022	1/1	0.92	0.16	26,26,26,26	0
56	MG	2A	3235	1/1	0.92	0.20	72,72,72,72	0
56	MG	1y	101	1/1	0.92	0.10	62,62,62,62	0
56	MG	2a	3207	1/1	0.92	0.17	66,66,66,66	0
56	MG	1A	3496	1/1	0.92	0.17	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	3506	1/1	0.92	0.08	36,36,36,36	0
56	MG	1A	3854	1/1	0.92	0.08	37,37,37,37	0
56	MG	2A	3850	1/1	0.92	0.12	81,81,81,81	0
56	MG	1A	3010	1/1	0.92	0.14	39,39,39,39	0
56	MG	1A	3072	1/1	0.92	0.23	32,32,32,32	0
56	MG	2a	3217	1/1	0.92	0.11	75,75,75,75	0
56	MG	2A	3518	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3013	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3311	1/1	0.92	0.11	36,36,36,36	0
56	MG	2A	3016	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3252	1/1	0.92	0.20	61,61,61,61	0
56	MG	2A	3017	1/1	0.92	0.16	50,50,50,50	0
56	MG	2A	3528	1/1	0.92	0.09	45,45,45,45	0
56	MG	1A	3391	1/1	0.92	0.05	45,45,45,45	0
56	MG	2A	3535	1/1	0.92	0.06	62,62,62,62	0
56	MG	1A	3032	1/1	0.92	0.09	38,38,38,38	0
56	MG	2A	3256	1/1	0.92	0.27	55,55,55,55	0
56	MG	1a	1658	1/1	0.92	0.14	65,65,65,65	0
56	MG	1A	3315	1/1	0.92	0.19	40,40,40,40	0
56	MG	2A	3034	1/1	0.92	0.12	34,34,34,34	0
56	MG	2A	3035	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3395	1/1	0.92	0.22	45,45,45,45	0
56	MG	2D	304	1/1	0.92	0.12	51,51,51,51	0
56	MG	2a	3242	1/1	0.92	0.28	64,64,64,64	0
56	MG	2A	3040	1/1	0.92	0.10	66,66,66,66	0
56	MG	2a	3244	1/1	0.92	0.14	90,90,90,90	0
56	MG	2a	3246	1/1	0.92	0.19	70,70,70,70	0
56	MG	1A	3891	1/1	0.92	0.08	55,55,55,55	0
56	MG	1a	1663	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	4080	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	3892	1/1	0.92	0.08	58,58,58,58	0
56	MG	1B	208	1/1	0.92	0.22	63,63,63,63	0
56	MG	2F	304	1/1	0.92	0.13	42,42,42,42	0
56	MG	2A	3274	1/1	0.92	0.22	58,58,58,58	0
56	MG	1a	1668	1/1	0.92	0.07	71,71,71,71	0
56	MG	2G	201	1/1	0.92	0.13	62,62,62,62	0
56	MG	2A	3054	1/1	0.92	0.18	43,43,43,43	0
56	MG	2A	3571	1/1	0.92	0.11	40,40,40,40	0
56	MG	2A	3278	1/1	0.92	0.08	39,39,39,39	0
56	MG	2A	3055	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3078	1/1	0.92	0.15	30,30,30,30	0
56	MG	1B	216	1/1	0.92	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3147	1/1	0.92	0.32	55,55,55,55	0
56	MG	1A	3721	1/1	0.92	0.15	33,33,33,33	0
56	MG	1B	225	1/1	0.92	0.10	45,45,45,45	0
56	MG	1A	3722	1/1	0.92	0.10	31,31,31,31	0
56	MG	1A	3233	1/1	0.92	0.07	42,42,42,42	0
56	MG	2x	104	1/1	0.92	0.27	72,72,72,72	0
56	MG	2a	3001	1/1	0.92	0.11	53,53,53,53	0
56	MG	2y	101	1/1	0.92	0.18	57,57,57,57	0
56	MG	1a	1685	1/1	0.92	0.12	56,56,56,56	0
56	MG	2A	3292	1/1	0.92	0.09	46,46,46,46	0
56	MG	2y	104	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3598	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3220	1/1	0.93	0.05	47,47,47,47	0
56	MG	1A	3997	1/1	0.93	0.10	45,45,45,45	0
56	MG	1A	3554	1/1	0.93	0.09	29,29,29,29	0
56	MG	1A	3341	1/1	0.93	0.10	43,43,43,43	0
56	MG	2A	3541	1/1	0.93	0.06	33,33,33,33	0
56	MG	1A	3207	1/1	0.93	0.08	44,44,44,44	0
56	MG	2T	202	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3225	1/1	0.93	0.07	50,50,50,50	0
56	MG	2Z	301	1/1	0.93	0.24	54,54,54,54	0
56	MG	1f	202	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3344	1/1	0.93	0.06	25,25,25,25	0
56	MG	1A	3064	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3348	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3434	1/1	0.93	0.17	50,50,50,50	0
56	MG	1w	103	1/1	0.93	0.15	61,61,61,61	0
56	MG	1A	4022	1/1	0.93	0.08	39,39,39,39	0
56	MG	1a	1623	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3572	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3241	1/1	0.93	0.19	59,59,59,59	0
56	MG	2A	3244	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3437	1/1	0.93	0.16	43,43,43,43	0
56	MG	1x	106	1/1	0.93	0.20	44,44,44,44	0
56	MG	2A	3248	1/1	0.93	0.27	62,62,62,62	0
56	MG	1A	3796	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3020	1/1	0.93	0.06	35,35,35,35	0
56	MG	1a	1630	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3288	1/1	0.93	0.09	43,43,43,43	0
56	MG	1a	1633	1/1	0.93	0.19	58,58,58,58	0
56	MG	1A	3151	1/1	0.93	0.10	41,41,41,41	0
56	MG	1A	3454	1/1	0.93	0.06	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	1638	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3461	1/1	0.93	0.07	40,40,40,40	0
56	MG	2A	3595	1/1	0.93	0.15	47,47,47,47	0
56	MG	2A	3596	1/1	0.93	0.07	55,55,55,55	0
56	MG	2a	3023	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3359	1/1	0.93	0.10	51,51,51,51	0
56	MG	2a	3027	1/1	0.93	0.35	69,69,69,69	0
56	MG	1a	1644	1/1	0.93	0.18	56,56,56,56	0
56	MG	2A	3599	1/1	0.93	0.21	73,73,73,73	0
56	MG	1A	3812	1/1	0.93	0.12	36,36,36,36	0
56	MG	1A	3361	1/1	0.93	0.08	41,41,41,41	0
56	MG	1A	4044	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3220	1/1	0.93	0.07	35,35,35,35	0
56	MG	1a	1651	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	4051	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3026	1/1	0.93	0.09	64,64,64,64	0
56	MG	2A	3611	1/1	0.93	0.10	66,66,66,66	0
56	MG	2a	3038	1/1	0.93	0.16	64,64,64,64	0
56	MG	2A	3272	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3816	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3032	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3033	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3818	1/1	0.93	0.10	31,31,31,31	0
56	MG	1A	3222	1/1	0.93	0.22	51,51,51,51	0
56	MG	2A	3037	1/1	0.93	0.32	68,68,68,68	0
56	MG	2A	3623	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3619	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3626	1/1	0.93	0.16	65,65,65,65	0
56	MG	2A	3629	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3368	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3152	1/1	0.93	0.15	43,43,43,43	0
56	MG	2a	3055	1/1	0.93	0.16	66,66,66,66	0
56	MG	2A	3042	1/1	0.93	0.22	58,58,58,58	0
56	MG	1A	3048	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3226	1/1	0.93	0.07	47,47,47,47	0
56	MG	2a	3061	1/1	0.93	0.07	66,66,66,66	0
56	MG	1A	3835	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3374	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3639	1/1	0.93	0.09	64,64,64,64	0
56	MG	1A	3304	1/1	0.93	0.30	36,36,36,36	0
56	MG	2A	3053	1/1	0.93	0.17	65,65,65,65	0
56	MG	1A	3033	1/1	0.93	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3645	1/1	0.93	0.15	30,30,30,30	0
56	MG	1A	3490	1/1	0.93	0.10	31,31,31,31	0
56	MG	1A	3024	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3650	1/1	0.93	0.06	64,64,64,64	0
56	MG	1a	1672	1/1	0.93	0.21	64,64,64,64	0
56	MG	2A	3059	1/1	0.93	0.07	46,46,46,46	0
56	MG	1B	201	1/1	0.93	0.10	58,58,58,58	0
56	MG	2A	3657	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3304	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3849	1/1	0.93	0.09	42,42,42,42	0
56	MG	2a	3083	1/1	0.93	0.13	66,66,66,66	0
56	MG	2A	3662	1/1	0.93	0.11	40,40,40,40	0
56	MG	2A	3065	1/1	0.93	0.08	56,56,56,56	0
56	MG	1B	212	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3666	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3069	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3672	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	3114	1/1	0.93	0.05	28,28,28,28	0
56	MG	2A	3073	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3675	1/1	0.93	0.09	53,53,53,53	0
56	MG	1a	1679	1/1	0.93	0.21	48,48,48,48	0
56	MG	1B	215	1/1	0.93	0.12	58,58,58,58	0
56	MG	2A	3679	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3667	1/1	0.93	0.07	33,33,33,33	0
56	MG	2A	3682	1/1	0.93	0.07	57,57,57,57	0
56	MG	2A	3686	1/1	0.93	0.10	61,61,61,61	0
56	MG	1A	3670	1/1	0.93	0.15	56,56,56,56	0
56	MG	2A	3080	1/1	0.93	0.06	45,45,45,45	0
56	MG	2A	3081	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3320	1/1	0.93	0.08	73,73,73,73	0
56	MG	1a	1686	1/1	0.93	0.25	55,55,55,55	0
56	MG	1A	3173	1/1	0.93	0.23	42,42,42,42	0
56	MG	2A	3084	1/1	0.93	0.11	47,47,47,47	0
56	MG	1B	223	1/1	0.93	0.18	48,48,48,48	0
56	MG	1A	3504	1/1	0.93	0.15	43,43,43,43	0
56	MG	2A	3088	1/1	0.93	0.18	36,36,36,36	0
56	MG	2A	3089	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	3389	1/1	0.93	0.28	33,33,33,33	0
56	MG	1A	3678	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3343	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3093	1/1	0.93	0.25	48,48,48,48	0
56	MG	2a	3119	1/1	0.93	0.31	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3345	1/1	0.93	0.07	71,71,71,71	0
56	MG	2A	3094	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	3118	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3889	1/1	0.93	0.12	20,20,20,20	0
56	MG	1A	3183	1/1	0.93	0.08	43,43,43,43	0
56	MG	1a	1698	1/1	0.93	0.42	69,69,69,69	0
56	MG	2A	3351	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3721	1/1	0.93	0.07	73,73,73,73	0
56	MG	2A	3722	1/1	0.93	0.07	67,67,67,67	0
56	MG	2A	3723	1/1	0.93	0.07	39,39,39,39	0
56	MG	1a	1700	1/1	0.93	0.15	32,32,32,32	0
56	MG	1A	3690	1/1	0.93	0.13	60,60,60,60	0
56	MG	2A	3730	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3103	1/1	0.93	0.10	45,45,45,45	0
56	MG	2a	3139	1/1	0.93	0.12	61,61,61,61	0
56	MG	2a	3140	1/1	0.93	0.14	64,64,64,64	0
56	MG	1A	3317	1/1	0.93	0.24	50,50,50,50	0
56	MG	1A	3897	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3359	1/1	0.93	0.19	49,49,49,49	0
56	MG	2a	3144	1/1	0.93	0.20	55,55,55,55	0
56	MG	2A	3739	1/1	0.93	0.09	67,67,67,67	0
56	MG	1D	305	1/1	0.93	0.13	26,26,26,26	0
56	MG	1A	3692	1/1	0.93	0.09	40,40,40,40	0
56	MG	1a	1709	1/1	0.93	0.18	55,55,55,55	0
56	MG	2a	3155	1/1	0.93	0.06	93,93,93,93	0
56	MG	1A	3517	1/1	0.93	0.22	43,43,43,43	0
56	MG	2A	3370	1/1	0.93	0.29	62,62,62,62	0
56	MG	2A	3751	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3758	1/1	0.93	0.08	33,33,33,33	0
56	MG	1A	3703	1/1	0.93	0.17	65,65,65,65	0
56	MG	1A	3028	1/1	0.93	0.08	28,28,28,28	0
56	MG	2a	3171	1/1	0.93	0.07	73,73,73,73	0
56	MG	2a	3172	1/1	0.93	0.11	82,82,82,82	0
56	MG	2A	3768	1/1	0.93	0.08	65,65,65,65	0
56	MG	2a	3175	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3715	1/1	0.93	0.09	15,15,15,15	0
56	MG	2A	3125	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3719	1/1	0.93	0.11	29,29,29,29	0
56	MG	1A	3720	1/1	0.93	0.10	29,29,29,29	0
56	MG	2a	3185	1/1	0.93	0.17	73,73,73,73	0
56	MG	2A	3783	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	3121	1/1	0.93	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1723	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3398	1/1	0.93	0.18	29,29,29,29	0
56	MG	1A	3923	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3138	1/1	0.93	0.14	61,61,61,61	0
56	MG	2A	3139	1/1	0.93	0.07	48,48,48,48	0
56	MG	1a	1728	1/1	0.93	0.10	61,61,61,61	0
56	MG	1a	1729	1/1	0.93	0.21	62,62,62,62	0
56	MG	2A	3394	1/1	0.93	0.07	61,61,61,61	0
56	MG	1a	1732	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3398	1/1	0.93	0.22	42,42,42,42	0
56	MG	1a	1735	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3524	1/1	0.93	0.14	39,39,39,39	0
56	MG	1A	3325	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	3725	1/1	0.93	0.10	35,35,35,35	0
56	MG	1a	1747	1/1	0.93	0.17	58,58,58,58	0
56	MG	2A	3152	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3253	1/1	0.93	0.25	31,31,31,31	0
56	MG	1a	1752	1/1	0.93	0.22	47,47,47,47	0
56	MG	2A	3414	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3415	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3191	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3733	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3823	1/1	0.93	0.14	50,50,50,50	0
56	MG	1a	1756	1/1	0.93	0.21	71,71,71,71	0
56	MG	1A	3736	1/1	0.93	0.09	26,26,26,26	0
56	MG	1A	3951	1/1	0.93	0.09	44,44,44,44	0
56	MG	2A	3827	1/1	0.93	0.10	60,60,60,60	0
56	MG	2A	3828	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3952	1/1	0.93	0.06	24,24,24,24	0
56	MG	1A	3739	1/1	0.93	0.08	22,22,22,22	0
56	MG	1a	1769	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3433	1/1	0.93	0.14	48,48,48,48	0
56	MG	2a	3228	1/1	0.93	0.11	73,73,73,73	0
56	MG	2a	3230	1/1	0.93	0.07	66,66,66,66	0
56	MG	2A	3434	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3435	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3173	1/1	0.93	0.24	54,54,54,54	0
56	MG	2A	3441	1/1	0.93	0.11	63,63,63,63	0
56	MG	1A	3043	1/1	0.93	0.10	31,31,31,31	0
56	MG	1A	3331	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3194	1/1	0.93	0.30	57,57,57,57	0
56	MG	2A	3179	1/1	0.93	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3240	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	3063	1/1	0.93	0.05	27,27,27,27	0
56	MG	1a	1780	1/1	0.93	0.08	56,56,56,56	0
56	MG	2A	3184	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3202	1/1	0.93	0.17	50,50,50,50	0
56	MG	2B	201	1/1	0.93	0.26	60,60,60,60	0
56	MG	1A	3415	1/1	0.93	0.07	56,56,56,56	0
56	MG	1A	3758	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3465	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3190	1/1	0.93	0.12	37,37,37,37	0
56	MG	2f	202	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3544	1/1	0.93	0.17	43,43,43,43	0
56	MG	1A	3767	1/1	0.93	0.12	50,50,50,50	0
56	MG	14	101	1/1	0.93	0.12	57,57,57,57	0
56	MG	15	102	1/1	0.93	0.18	35,35,35,35	0
56	MG	1A	3337	1/1	0.93	0.36	50,50,50,50	0
56	MG	16	102	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3493	1/1	0.93	0.07	49,49,49,49	0
56	MG	2A	3200	1/1	0.93	0.10	45,45,45,45	0
56	MG	2A	3201	1/1	0.93	0.27	41,41,41,41	0
56	MG	2A	3202	1/1	0.93	0.13	45,45,45,45	0
56	MG	1A	3984	1/1	0.93	0.07	49,49,49,49	0
56	MG	1A	3546	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3275	1/1	0.93	0.08	41,41,41,41	0
56	MG	1a	1601	1/1	0.93	0.24	59,59,59,59	0
56	MG	2x	101	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3517	1/1	0.93	0.12	48,48,48,48	0
56	MG	1a	1602	1/1	0.93	0.15	45,45,45,45	0
56	MG	1a	1816	1/1	0.93	0.17	55,55,55,55	0
56	MG	1a	1817	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3339	1/1	0.93	0.07	40,40,40,40	0
56	MG	1a	1821	1/1	0.93	0.14	57,57,57,57	0
56	MG	2F	301	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3991	1/1	0.93	0.07	43,43,43,43	0
56	MG	1A	3994	1/1	0.93	0.09	40,40,40,40	0
56	MG	2T	203	1/1	0.94	0.09	39,39,39,39	0
56	MG	1A	4064	1/1	0.94	0.10	38,38,38,38	0
56	MG	2V	202	1/1	0.94	0.08	53,53,53,53	0
56	MG	2Y	201	1/1	0.94	0.12	43,43,43,43	0
56	MG	1A	4065	1/1	0.94	0.14	35,35,35,35	0
56	MG	1a	1657	1/1	0.94	0.10	60,60,60,60	0
56	MG	2I	103	1/1	0.94	0.15	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	3209	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3669	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3844	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3038	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	4075	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3299	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3300	1/1	0.94	0.10	50,50,50,50	0
56	MG	2a	3002	1/1	0.94	0.05	52,52,52,52	0
56	MG	2A	3586	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3590	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3117	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3850	1/1	0.94	0.09	27,27,27,27	0
56	MG	2A	3045	1/1	0.94	0.11	55,55,55,55	0
56	MG	1a	1667	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3515	1/1	0.94	0.16	41,41,41,41	0
56	MG	1a	1669	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3277	1/1	0.94	0.06	51,51,51,51	0
56	MG	2a	3014	1/1	0.94	0.14	62,62,62,62	0
56	MG	1A	3350	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	4084	1/1	0.94	0.19	45,45,45,45	0
56	MG	1A	3859	1/1	0.94	0.26	22,22,22,22	0
56	MG	2A	3604	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3605	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3519	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3056	1/1	0.94	0.33	66,66,66,66	0
56	MG	1A	3353	1/1	0.94	0.47	42,42,42,42	0
56	MG	1A	3416	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3244	1/1	0.94	0.14	37,37,37,37	0
56	MG	2A	3289	1/1	0.94	0.18	73,73,73,73	0
56	MG	2A	3061	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3303	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3875	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3696	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	3245	1/1	0.94	0.06	35,35,35,35	0
56	MG	1A	3526	1/1	0.94	0.10	37,37,37,37	0
56	MG	1a	1688	1/1	0.94	0.14	41,41,41,41	0
56	MG	1A	3705	1/1	0.94	0.06	38,38,38,38	0
56	MG	2A	3625	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3074	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3628	1/1	0.94	0.20	61,61,61,61	0
56	MG	1A	3421	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3303	1/1	0.94	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3248	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3529	1/1	0.94	0.14	46,46,46,46	0
56	MG	1B	233	1/1	0.94	0.07	52,52,52,52	0
56	MG	2A	3079	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3306	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3309	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3362	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3037	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3258	1/1	0.94	0.07	53,53,53,53	0
56	MG	2a	3052	1/1	0.94	0.14	48,48,48,48	0
56	MG	1a	1701	1/1	0.94	0.26	55,55,55,55	0
56	MG	2A	3644	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	3217	1/1	0.94	0.23	33,33,33,33	0
56	MG	1A	3435	1/1	0.94	0.23	46,46,46,46	0
56	MG	2A	3648	1/1	0.94	0.17	71,71,71,71	0
56	MG	2A	3087	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3919	1/1	0.94	0.07	66,66,66,66	0
56	MG	1A	3726	1/1	0.94	0.07	23,23,23,23	0
56	MG	2A	3321	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3322	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3323	1/1	0.94	0.18	63,63,63,63	0
56	MG	2a	3066	1/1	0.94	0.17	53,53,53,53	0
56	MG	1E	306	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3921	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3661	1/1	0.94	0.08	56,56,56,56	0
56	MG	2A	3328	1/1	0.94	0.17	60,60,60,60	0
56	MG	1E	309	1/1	0.94	0.07	22,22,22,22	0
56	MG	2a	3072	1/1	0.94	0.15	70,70,70,70	0
56	MG	1A	3541	1/1	0.94	0.12	43,43,43,43	0
56	MG	2a	3074	1/1	0.94	0.17	68,68,68,68	0
56	MG	1F	309	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3436	1/1	0.94	0.07	31,31,31,31	0
56	MG	1A	3927	1/1	0.94	0.12	60,60,60,60	0
56	MG	1A	3264	1/1	0.94	0.12	51,51,51,51	0
56	MG	1F	313	1/1	0.94	0.06	41,41,41,41	0
56	MG	2A	3342	1/1	0.94	0.20	42,42,42,42	0
56	MG	2A	3101	1/1	0.94	0.25	56,56,56,56	0
56	MG	1G	202	1/1	0.94	0.21	53,53,53,53	0
56	MG	2a	3085	1/1	0.94	0.20	59,59,59,59	0
56	MG	1A	3074	1/1	0.94	0.12	29,29,29,29	0
56	MG	1a	1726	1/1	0.94	0.26	55,55,55,55	0
56	MG	1A	3439	1/1	0.94	0.06	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	3108	1/1	0.94	0.08	67,67,67,67	0
56	MG	1N	202	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3445	1/1	0.94	0.14	52,52,52,52	0
56	MG	1O	201	1/1	0.94	0.06	46,46,46,46	0
56	MG	1a	1733	1/1	0.94	0.06	56,56,56,56	0
56	MG	1A	3936	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3937	1/1	0.94	0.10	60,60,60,60	0
56	MG	1P	205	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3941	1/1	0.94	0.07	25,25,25,25	0
56	MG	1a	1746	1/1	0.94	0.10	51,51,51,51	0
56	MG	1Q	201	1/1	0.94	0.12	33,33,33,33	0
56	MG	2a	3101	1/1	0.94	0.06	35,35,35,35	0
56	MG	2a	3102	1/1	0.94	0.10	59,59,59,59	0
56	MG	2A	3362	1/1	0.94	0.28	48,48,48,48	0
56	MG	2A	3363	1/1	0.94	0.32	59,59,59,59	0
56	MG	2A	3704	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3746	1/1	0.94	0.12	23,23,23,23	0
56	MG	1A	3094	1/1	0.94	0.10	38,38,38,38	0
56	MG	1R	202	1/1	0.94	0.11	45,45,45,45	0
56	MG	1a	1754	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3712	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3752	1/1	0.94	0.13	29,29,29,29	0
56	MG	1A	3753	1/1	0.94	0.08	21,21,21,21	0
56	MG	1T	202	1/1	0.94	0.08	35,35,35,35	0
56	MG	1V	201	1/1	0.94	0.11	32,32,32,32	0
56	MG	2A	3377	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3555	1/1	0.94	0.09	40,40,40,40	0
56	MG	1a	1765	1/1	0.94	0.17	68,68,68,68	0
56	MG	1V	206	1/1	0.94	0.10	33,33,33,33	0
56	MG	1A	3560	1/1	0.94	0.18	49,49,49,49	0
56	MG	1W	201	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3449	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	3450	1/1	0.94	0.11	32,32,32,32	0
56	MG	1Y	202	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3156	1/1	0.94	0.14	40,40,40,40	0
56	MG	1a	1778	1/1	0.94	0.14	67,67,67,67	0
56	MG	2A	3159	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3160	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3270	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3565	1/1	0.94	0.06	23,23,23,23	0
56	MG	1A	3375	1/1	0.94	0.20	60,60,60,60	0
56	MG	2A	3743	1/1	0.94	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3744	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3456	1/1	0.94	0.30	33,33,33,33	0
56	MG	2A	3748	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3569	1/1	0.94	0.08	17,17,17,17	0
56	MG	2A	3407	1/1	0.94	0.23	73,73,73,73	0
56	MG	2A	3757	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3377	1/1	0.94	0.07	42,42,42,42	0
56	MG	1a	1787	1/1	0.94	0.08	45,45,45,45	0
56	MG	1a	1788	1/1	0.94	0.09	73,73,73,73	0
56	MG	2a	3148	1/1	0.94	0.05	86,86,86,86	0
56	MG	1l	106	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3096	1/1	0.94	0.21	37,37,37,37	0
56	MG	2A	3770	1/1	0.94	0.10	46,46,46,46	0
56	MG	1a	1799	1/1	0.94	0.07	79,79,79,79	0
56	MG	1a	1800	1/1	0.94	0.12	81,81,81,81	0
56	MG	2A	3777	1/1	0.94	0.06	58,58,58,58	0
56	MG	2A	3178	1/1	0.94	0.17	62,62,62,62	0
56	MG	2a	3161	1/1	0.94	0.18	65,65,65,65	0
56	MG	2A	3419	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3420	1/1	0.94	0.06	50,50,50,50	0
56	MG	2A	3421	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3791	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3422	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3981	1/1	0.94	0.08	39,39,39,39	0
56	MG	1a	1803	1/1	0.94	0.10	77,77,77,77	0
56	MG	2A	3798	1/1	0.94	0.07	46,46,46,46	0
56	MG	2A	3181	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3427	1/1	0.94	0.32	64,64,64,64	0
56	MG	2A	3428	1/1	0.94	0.25	58,58,58,58	0
56	MG	2A	3182	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3324	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3778	1/1	0.94	0.14	33,33,33,33	0
56	MG	2A	3185	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3809	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3382	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3062	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3140	1/1	0.94	0.11	50,50,50,50	0
56	MG	2a	3195	1/1	0.94	0.18	62,62,62,62	0
56	MG	2A	3439	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3588	1/1	0.94	0.06	23,23,23,23	0
56	MG	1A	3595	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3995	1/1	0.94	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3470	1/1	0.94	0.14	33,33,33,33	0
56	MG	1a	1819	1/1	0.94	0.13	53,53,53,53	0
56	MG	1A	3104	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3788	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3199	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3789	1/1	0.94	0.08	29,29,29,29	0
56	MG	2A	3462	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	4004	1/1	0.94	0.13	55,55,55,55	0
56	MG	1a	1825	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3281	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3283	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	4016	1/1	0.94	0.05	26,26,26,26	0
56	MG	2A	3470	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3208	1/1	0.94	0.11	40,40,40,40	0
56	MG	2A	3833	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3482	1/1	0.94	0.25	50,50,50,50	0
56	MG	2A	3479	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3606	1/1	0.94	0.08	34,34,34,34	0
56	MG	1l	202	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3614	1/1	0.94	0.07	37,37,37,37	0
56	MG	1a	1621	1/1	0.94	0.28	47,47,47,47	0
56	MG	2a	3225	1/1	0.94	0.08	57,57,57,57	0
56	MG	2A	3494	1/1	0.94	0.13	65,65,65,65	0
56	MG	2A	3216	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3617	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3483	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3485	1/1	0.94	0.12	47,47,47,47	0
56	MG	2A	3507	1/1	0.94	0.19	43,43,43,43	0
56	MG	2A	3511	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3009	1/1	0.94	0.06	46,46,46,46	0
56	MG	1A	3079	1/1	0.94	0.23	34,34,34,34	0
56	MG	1a	1628	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3110	1/1	0.94	0.15	38,38,38,38	0
56	MG	1A	3489	1/1	0.94	0.33	29,29,29,29	0
56	MG	1A	4035	1/1	0.94	0.08	32,32,32,32	0
56	MG	1A	3637	1/1	0.94	0.06	25,25,25,25	0
56	MG	1A	4037	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3229	1/1	0.94	0.16	42,42,42,42	0
56	MG	2a	3245	1/1	0.94	0.20	63,63,63,63	0
56	MG	2A	3524	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3336	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3640	1/1	0.94	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1639	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3234	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4041	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	4042	1/1	0.94	0.14	52,52,52,52	0
56	MG	2B	218	1/1	0.94	0.09	63,63,63,63	0
56	MG	2B	219	1/1	0.94	0.15	67,67,67,67	0
56	MG	1A	3827	1/1	0.94	0.13	55,55,55,55	0
56	MG	2A	3542	1/1	0.94	0.06	61,61,61,61	0
56	MG	2A	3012	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3643	1/1	0.94	0.11	43,43,43,43	0
56	MG	1A	3291	1/1	0.94	0.20	54,54,54,54	0
56	MG	1A	3036	1/1	0.94	0.32	34,34,34,34	0
56	MG	2E	305	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3547	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3203	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3549	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3018	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3056	1/1	0.94	0.09	31,31,31,31	0
56	MG	2A	3021	1/1	0.94	0.13	43,43,43,43	0
56	MG	2F	306	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3836	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3507	1/1	0.94	0.38	43,43,43,43	0
56	MG	2A	3559	1/1	0.94	0.08	54,54,54,54	0
56	MG	2A	3024	1/1	0.94	0.07	40,40,40,40	0
56	MG	2P	201	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3839	1/1	0.94	0.06	20,20,20,20	0
56	MG	2A	3027	1/1	0.94	0.18	64,64,64,64	0
58	A1AIX	2A	3851	43/43	0.94	0.12	43,53,66,72	0
56	MG	2A	3583	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3845	1/1	0.95	0.08	38,38,38,38	0
56	MG	1A	3219	1/1	0.95	0.15	37,37,37,37	0
56	MG	1A	4070	1/1	0.95	0.08	42,42,42,42	0
56	MG	2I	102	1/1	0.95	0.13	44,44,44,44	0
56	MG	2A	3589	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3086	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3221	1/1	0.95	0.10	46,46,46,46	0
56	MG	27	101	1/1	0.95	0.12	41,41,41,41	0
56	MG	27	102	1/1	0.95	0.08	45,45,45,45	0
56	MG	27	103	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3025	1/1	0.95	0.08	57,57,57,57	0
56	MG	2A	3594	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3851	1/1	0.95	0.13	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	1661	1/1	0.95	0.19	52,52,52,52	0
56	MG	28	106	1/1	0.95	0.27	72,72,72,72	0
56	MG	1A	3852	1/1	0.95	0.16	31,31,31,31	0
56	MG	1A	3290	1/1	0.95	0.09	42,42,42,42	0
56	MG	2A	3288	1/1	0.95	0.16	54,54,54,54	0
56	MG	2A	3049	1/1	0.95	0.19	58,58,58,58	0
56	MG	1A	3172	1/1	0.95	0.06	23,23,23,23	0
56	MG	1A	3351	1/1	0.95	0.30	31,31,31,31	0
56	MG	1A	3068	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3864	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3174	1/1	0.95	0.06	42,42,42,42	0
56	MG	1B	202	1/1	0.95	0.12	45,45,45,45	0
56	MG	1B	203	1/1	0.95	0.15	48,48,48,48	0
56	MG	1B	205	1/1	0.95	0.23	51,51,51,51	0
56	MG	2A	3299	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3693	1/1	0.95	0.07	55,55,55,55	0
56	MG	1a	1674	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3616	1/1	0.95	0.08	48,48,48,48	0
56	MG	1B	209	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3869	1/1	0.95	0.06	39,39,39,39	0
56	MG	1B	213	1/1	0.95	0.08	44,44,44,44	0
56	MG	1a	1678	1/1	0.95	0.22	42,42,42,42	0
56	MG	1A	3428	1/1	0.95	0.25	37,37,37,37	0
56	MG	2a	3025	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3699	1/1	0.95	0.10	19,19,19,19	0
56	MG	1A	3355	1/1	0.95	0.22	30,30,30,30	0
56	MG	1A	3178	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3882	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3536	1/1	0.95	0.17	46,46,46,46	0
56	MG	2A	3313	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3297	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3229	1/1	0.95	0.06	32,32,32,32	0
56	MG	1B	228	1/1	0.95	0.06	31,31,31,31	0
56	MG	1A	3718	1/1	0.95	0.09	21,21,21,21	0
56	MG	1A	3896	1/1	0.95	0.08	68,68,68,68	0
56	MG	2A	3319	1/1	0.95	0.08	70,70,70,70	0
56	MG	1B	231	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3038	1/1	0.95	0.11	30,30,30,30	0
56	MG	1A	3231	1/1	0.95	0.08	50,50,50,50	0
56	MG	1a	1697	1/1	0.95	0.17	48,48,48,48	0
56	MG	1A	3542	1/1	0.95	0.15	50,50,50,50	0
56	MG	1a	1699	1/1	0.95	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3044	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3543	1/1	0.95	0.13	35,35,35,35	0
56	MG	2A	3646	1/1	0.95	0.06	52,52,52,52	0
56	MG	2A	3329	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3908	1/1	0.95	0.05	44,44,44,44	0
56	MG	1A	3363	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3365	1/1	0.95	0.07	49,49,49,49	0
56	MG	1D	307	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3914	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3441	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3444	1/1	0.95	0.22	24,24,24,24	0
56	MG	1E	304	1/1	0.95	0.25	28,28,28,28	0
56	MG	2a	3057	1/1	0.95	0.27	60,60,60,60	0
56	MG	1a	1712	1/1	0.95	0.24	54,54,54,54	0
56	MG	1A	3093	1/1	0.95	0.18	56,56,56,56	0
56	MG	1A	3729	1/1	0.95	0.08	27,27,27,27	0
56	MG	1a	1716	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3731	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3234	1/1	0.95	0.05	40,40,40,40	0
56	MG	1a	1719	1/1	0.95	0.19	47,47,47,47	0
56	MG	2A	3107	1/1	0.95	0.14	40,40,40,40	0
56	MG	1F	302	1/1	0.95	0.10	28,28,28,28	0
56	MG	1a	1721	1/1	0.95	0.09	60,60,60,60	0
56	MG	2A	3354	1/1	0.95	0.14	39,39,39,39	0
56	MG	1F	303	1/1	0.95	0.21	29,29,29,29	0
56	MG	1A	3184	1/1	0.95	0.12	21,21,21,21	0
56	MG	1A	3026	1/1	0.95	0.20	64,64,64,64	0
56	MG	1A	3737	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3049	1/1	0.95	0.12	42,42,42,42	0
56	MG	2a	3075	1/1	0.95	0.15	57,57,57,57	0
56	MG	2a	3076	1/1	0.95	0.14	65,65,65,65	0
56	MG	2A	3684	1/1	0.95	0.06	57,57,57,57	0
56	MG	1A	3453	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	3563	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3127	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3128	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3188	1/1	0.95	0.13	36,36,36,36	0
56	MG	2A	3368	1/1	0.95	0.16	42,42,42,42	0
56	MG	2A	3694	1/1	0.95	0.21	46,46,46,46	0
56	MG	1A	3307	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3938	1/1	0.95	0.07	31,31,31,31	0
56	MG	1a	1737	1/1	0.95	0.14	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	1N	203	1/1	0.95	0.09	40,40,40,40	0
56	MG	1a	1740	1/1	0.95	0.06	64,64,64,64	0
56	MG	1A	3458	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3567	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	3460	1/1	0.95	0.10	51,51,51,51	0
56	MG	2A	3379	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3189	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3709	1/1	0.95	0.10	60,60,60,60	0
56	MG	1P	204	1/1	0.95	0.23	31,31,31,31	0
56	MG	2A	3382	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3462	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3190	1/1	0.95	0.12	26,26,26,26	0
56	MG	1A	3953	1/1	0.95	0.09	24,24,24,24	0
56	MG	1A	3761	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3580	1/1	0.95	0.09	28,28,28,28	0
56	MG	2A	3390	1/1	0.95	0.28	48,48,48,48	0
56	MG	1R	201	1/1	0.95	0.20	38,38,38,38	0
56	MG	2A	3392	1/1	0.95	0.22	48,48,48,48	0
56	MG	1a	1761	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3134	1/1	0.95	0.08	30,30,30,30	0
56	MG	2A	3724	1/1	0.95	0.09	72,72,72,72	0
56	MG	2A	3396	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3727	1/1	0.95	0.06	60,60,60,60	0
56	MG	1R	203	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3158	1/1	0.95	0.09	30,30,30,30	0
56	MG	1S	201	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3314	1/1	0.95	0.18	51,51,51,51	0
56	MG	2A	3162	1/1	0.95	0.10	42,42,42,42	0
56	MG	2a	3117	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3771	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3164	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	3772	1/1	0.95	0.05	18,18,18,18	0
56	MG	1U	203	1/1	0.95	0.21	39,39,39,39	0
56	MG	1a	1772	1/1	0.95	0.07	71,71,71,71	0
56	MG	1A	3380	1/1	0.95	0.21	51,51,51,51	0
56	MG	2A	3413	1/1	0.95	0.08	35,35,35,35	0
56	MG	1a	1774	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3746	1/1	0.95	0.07	54,54,54,54	0
56	MG	1a	1775	1/1	0.95	0.06	86,86,86,86	0
56	MG	2a	3129	1/1	0.95	0.29	51,51,51,51	0
56	MG	1a	1776	1/1	0.95	0.10	74,74,74,74	0
56	MG	1A	3381	1/1	0.95	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3756	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3973	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3098	1/1	0.95	0.08	34,34,34,34	0
56	MG	2a	3137	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3251	1/1	0.95	0.09	28,28,28,28	0
56	MG	1W	202	1/1	0.95	0.26	49,49,49,49	0
56	MG	2A	3761	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3767	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3597	1/1	0.95	0.06	18,18,18,18	0
56	MG	1X	102	1/1	0.95	0.29	33,33,33,33	0
56	MG	1A	3099	1/1	0.95	0.22	39,39,39,39	0
56	MG	1A	3983	1/1	0.95	0.11	58,58,58,58	0
56	MG	1A	3386	1/1	0.95	0.06	39,39,39,39	0
56	MG	2A	3775	1/1	0.95	0.11	63,63,63,63	0
56	MG	2a	3149	1/1	0.95	0.07	70,70,70,70	0
56	MG	2a	3150	1/1	0.95	0.06	78,78,78,78	0
56	MG	1Z	301	1/1	0.95	0.06	50,50,50,50	0
56	MG	1a	1794	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3985	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3187	1/1	0.95	0.05	43,43,43,43	0
56	MG	1A	3387	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3318	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3792	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3256	1/1	0.95	0.07	32,32,32,32	0
56	MG	1a	1802	1/1	0.95	0.06	64,64,64,64	0
56	MG	2a	3167	1/1	0.95	0.05	75,75,75,75	0
56	MG	10	105	1/1	0.95	0.07	48,48,48,48	0
56	MG	2a	3170	1/1	0.95	0.09	79,79,79,79	0
56	MG	2A	3797	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3443	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3195	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3445	1/1	0.95	0.29	59,59,59,59	0
56	MG	2A	3449	1/1	0.95	0.08	54,54,54,54	0
56	MG	2A	3451	1/1	0.95	0.13	47,47,47,47	0
56	MG	2A	3195	1/1	0.95	0.23	42,42,42,42	0
56	MG	2a	3182	1/1	0.95	0.14	54,54,54,54	0
56	MG	1a	1805	1/1	0.95	0.06	51,51,51,51	0
56	MG	2a	3184	1/1	0.95	0.10	59,59,59,59	0
56	MG	11	102	1/1	0.95	0.11	45,45,45,45	0
56	MG	2A	3808	1/1	0.95	0.12	71,71,71,71	0
56	MG	11	105	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3607	1/1	0.95	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3609	1/1	0.95	0.13	39,39,39,39	0
56	MG	2A	3812	1/1	0.95	0.05	38,38,38,38	0
56	MG	1A	3996	1/1	0.95	0.08	18,18,18,18	0
56	MG	1A	3259	1/1	0.95	0.17	32,32,32,32	0
56	MG	1A	3790	1/1	0.95	0.07	34,34,34,34	0
56	MG	16	101	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3262	1/1	0.95	0.06	46,46,46,46	0
56	MG	2A	3207	1/1	0.95	0.10	52,52,52,52	0
56	MG	17	104	1/1	0.95	0.07	32,32,32,32	0
56	MG	2A	3210	1/1	0.95	0.21	54,54,54,54	0
56	MG	1A	3199	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3141	1/1	0.95	0.21	21,21,21,21	0
56	MG	1A	4007	1/1	0.95	0.09	12,12,12,12	0
56	MG	19	102	1/1	0.95	0.19	50,50,50,50	0
56	MG	2A	3481	1/1	0.95	0.08	35,35,35,35	0
56	MG	2A	3482	1/1	0.95	0.10	64,64,64,64	0
56	MG	1A	4008	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3487	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3396	1/1	0.95	0.08	35,35,35,35	0
56	MG	2a	3210	1/1	0.95	0.06	64,64,64,64	0
56	MG	1d	301	1/1	0.95	0.06	30,30,30,30	0
56	MG	1a	1605	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3492	1/1	0.95	0.11	32,32,32,32	0
56	MG	1A	4013	1/1	0.95	0.07	46,46,46,46	0
56	MG	2a	3216	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	4014	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3629	1/1	0.95	0.10	20,20,20,20	0
56	MG	1A	4017	1/1	0.95	0.08	41,41,41,41	0
56	MG	2A	3509	1/1	0.95	0.09	58,58,58,58	0
56	MG	1a	1614	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3397	1/1	0.95	0.35	44,44,44,44	0
56	MG	2A	3226	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3145	1/1	0.95	0.38	35,35,35,35	0
56	MG	1A	3076	1/1	0.95	0.16	30,30,30,30	0
56	MG	1w	106	1/1	0.95	0.07	64,64,64,64	0
56	MG	2A	3849	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3638	1/1	0.95	0.06	31,31,31,31	0
56	MG	1x	103	1/1	0.95	0.12	41,41,41,41	0
56	MG	2a	3232	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	4026	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3506	1/1	0.95	0.11	32,32,32,32	0
56	MG	1A	3058	1/1	0.95	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3817	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3402	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3820	1/1	0.95	0.12	18,18,18,18	0
56	MG	2A	3534	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3645	1/1	0.95	0.06	38,38,38,38	0
56	MG	2A	3243	1/1	0.95	0.06	41,41,41,41	0
56	MG	1A	3824	1/1	0.95	0.24	29,29,29,29	0
56	MG	1A	3649	1/1	0.95	0.06	20,20,20,20	0
56	MG	1A	3826	1/1	0.95	0.15	33,33,33,33	0
56	MG	1A	3651	1/1	0.95	0.05	21,21,21,21	0
56	MG	2A	3005	1/1	0.95	0.19	41,41,41,41	0
56	MG	1A	3653	1/1	0.95	0.06	20,20,20,20	0
56	MG	1A	3829	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3656	1/1	0.95	0.07	14,14,14,14	0
56	MG	1A	3061	1/1	0.95	0.23	51,51,51,51	0
56	MG	1a	1636	1/1	0.95	0.17	44,44,44,44	0
56	MG	1A	3510	1/1	0.95	0.36	27,27,27,27	0
56	MG	2D	303	1/1	0.95	0.09	30,30,30,30	0
56	MG	1A	4046	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3659	1/1	0.95	0.05	42,42,42,42	0
56	MG	2A	3260	1/1	0.95	0.10	43,43,43,43	0
56	MG	1a	1642	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3558	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3016	1/1	0.95	0.13	31,31,31,31	0
56	MG	2A	3560	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3052	1/1	0.95	0.16	33,33,33,33	0
56	MG	1A	3514	1/1	0.95	0.19	49,49,49,49	0
56	MG	1a	1647	1/1	0.95	0.06	54,54,54,54	0
56	MG	2A	3566	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3568	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3569	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3276	1/1	0.95	0.05	52,52,52,52	0
56	MG	1A	4059	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3031	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3841	1/1	0.95	0.06	21,21,21,21	0
56	MG	1A	4062	1/1	0.95	0.10	50,50,50,50	0
56	MG	2T	201	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3111	1/1	0.95	0.11	31,31,31,31	0
56	MG	1A	3162	1/1	0.95	0.08	32,32,32,32	0
56	MG	2T	204	1/1	0.95	0.27	67,67,67,67	0
58	A1AIX	1A	4085	43/43	0.95	0.11	22,41,58,59	0
56	MG	2A	3036	1/1	0.95	0.06	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	14	102	1/1	0.95	0.11	98,98,98,98	0
56	MG	1A	3957	1/1	0.96	0.06	37,37,37,37	0
56	MG	20	101	1/1	0.96	0.07	60,60,60,60	0
56	MG	1a	1706	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3961	1/1	0.96	0.05	54,54,54,54	0
56	MG	1A	3289	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3610	1/1	0.96	0.09	51,51,51,51	0
56	MG	25	101	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3601	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3964	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3611	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3613	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3495	1/1	0.96	0.21	48,48,48,48	0
56	MG	1A	3232	1/1	0.96	0.19	46,46,46,46	0
56	MG	1A	3500	1/1	0.96	0.09	27,27,27,27	0
56	MG	28	104	1/1	0.96	0.08	51,51,51,51	0
56	MG	1P	202	1/1	0.96	0.19	29,29,29,29	0
56	MG	1A	3408	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	3410	1/1	0.96	0.33	37,37,37,37	0
56	MG	2A	3612	1/1	0.96	0.06	52,52,52,52	0
56	MG	2a	3004	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3787	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3621	1/1	0.96	0.05	21,21,21,21	0
56	MG	2A	3092	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3617	1/1	0.96	0.06	55,55,55,55	0
56	MG	1Q	203	1/1	0.96	0.04	39,39,39,39	0
56	MG	1A	3345	1/1	0.96	0.43	37,37,37,37	0
56	MG	1A	3626	1/1	0.96	0.06	34,34,34,34	0
56	MG	1Q	206	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3087	1/1	0.96	0.10	36,36,36,36	0
56	MG	2A	3327	1/1	0.96	0.18	46,46,46,46	0
56	MG	2A	3098	1/1	0.96	0.18	59,59,59,59	0
56	MG	1A	3795	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1730	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3331	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3413	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3333	1/1	0.96	0.05	57,57,57,57	0
56	MG	1R	204	1/1	0.96	0.09	19,19,19,19	0
56	MG	1R	205	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3634	1/1	0.96	0.07	23,23,23,23	0
56	MG	1A	3347	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3635	1/1	0.96	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1739	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	3292	1/1	0.96	0.18	44,44,44,44	0
56	MG	2A	3110	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3801	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3802	1/1	0.96	0.11	57,57,57,57	0
56	MG	1U	204	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3803	1/1	0.96	0.04	48,48,48,48	0
56	MG	2A	3115	1/1	0.96	0.04	50,50,50,50	0
56	MG	2A	3116	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3804	1/1	0.96	0.08	22,22,22,22	0
56	MG	2A	3119	1/1	0.96	0.09	41,41,41,41	0
56	MG	1a	1749	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3353	1/1	0.96	0.06	48,48,48,48	0
56	MG	1a	1750	1/1	0.96	0.06	61,61,61,61	0
56	MG	2A	3123	1/1	0.96	0.17	38,38,38,38	0
56	MG	1a	1751	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3656	1/1	0.96	0.11	49,49,49,49	0
56	MG	2A	3126	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3658	1/1	0.96	0.04	46,46,46,46	0
56	MG	1A	3998	1/1	0.96	0.05	44,44,44,44	0
56	MG	1A	3511	1/1	0.96	0.07	31,31,31,31	0
56	MG	1A	3293	1/1	0.96	0.17	44,44,44,44	0
56	MG	2A	3361	1/1	0.96	0.09	48,48,48,48	0
56	MG	2a	3050	1/1	0.96	0.05	69,69,69,69	0
56	MG	1A	3417	1/1	0.96	0.16	36,36,36,36	0
56	MG	1A	3641	1/1	0.96	0.05	30,30,30,30	0
56	MG	1W	205	1/1	0.96	0.05	35,35,35,35	0
56	MG	2A	3668	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3101	1/1	0.96	0.24	24,24,24,24	0
56	MG	2A	3670	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3671	1/1	0.96	0.25	75,75,75,75	0
56	MG	2a	3058	1/1	0.96	0.19	73,73,73,73	0
56	MG	1a	1762	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3137	1/1	0.96	0.16	57,57,57,57	0
56	MG	1X	106	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3192	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3648	1/1	0.96	0.11	32,32,32,32	0
56	MG	2A	3141	1/1	0.96	0.05	46,46,46,46	0
56	MG	2A	3374	1/1	0.96	0.37	53,53,53,53	0
56	MG	2A	3375	1/1	0.96	0.14	65,65,65,65	0
56	MG	2A	3681	1/1	0.96	0.05	69,69,69,69	0
56	MG	1A	3516	1/1	0.96	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3155	1/1	0.96	0.13	36,36,36,36	0
56	MG	2A	3685	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	3042	1/1	0.96	0.08	35,35,35,35	0
56	MG	1Z	303	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3146	1/1	0.96	0.22	45,45,45,45	0
56	MG	1A	4015	1/1	0.96	0.06	22,22,22,22	0
56	MG	2A	3691	1/1	0.96	0.08	55,55,55,55	0
56	MG	2A	3148	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3821	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3158	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	3159	1/1	0.96	0.05	36,36,36,36	0
56	MG	10	106	1/1	0.96	0.12	60,60,60,60	0
56	MG	2A	3155	1/1	0.96	0.11	42,42,42,42	0
56	MG	10	107	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3699	1/1	0.96	0.10	57,57,57,57	0
56	MG	2A	3700	1/1	0.96	0.11	57,57,57,57	0
56	MG	1A	3425	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	4021	1/1	0.96	0.11	37,37,37,37	0
56	MG	11	103	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3200	1/1	0.96	0.11	34,34,34,34	0
56	MG	2A	3395	1/1	0.96	0.12	46,46,46,46	0
56	MG	2A	3161	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	4023	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3662	1/1	0.96	0.07	17,17,17,17	0
56	MG	2A	3400	1/1	0.96	0.12	27,27,27,27	0
56	MG	2A	3401	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3360	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3429	1/1	0.96	0.11	43,43,43,43	0
56	MG	2a	3097	1/1	0.96	0.19	62,62,62,62	0
56	MG	15	104	1/1	0.96	0.24	49,49,49,49	0
56	MG	2A	3405	1/1	0.96	0.05	33,33,33,33	0
56	MG	1a	1789	1/1	0.96	0.06	63,63,63,63	0
56	MG	1a	1791	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3169	1/1	0.96	0.06	71,71,71,71	0
56	MG	1A	3090	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3431	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3124	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3725	1/1	0.96	0.08	59,59,59,59	0
56	MG	2A	3412	1/1	0.96	0.13	53,53,53,53	0
56	MG	17	103	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3166	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3671	1/1	0.96	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3204	1/1	0.96	0.11	51,51,51,51	0
56	MG	2A	3732	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	3254	1/1	0.96	0.14	50,50,50,50	0
56	MG	2A	3418	1/1	0.96	0.25	46,46,46,46	0
56	MG	1A	3535	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3738	1/1	0.96	0.14	72,72,72,72	0
56	MG	1A	3255	1/1	0.96	0.12	30,30,30,30	0
56	MG	1a	1806	1/1	0.96	0.09	59,59,59,59	0
56	MG	1a	1807	1/1	0.96	0.06	65,65,65,65	0
56	MG	1a	1808	1/1	0.96	0.06	58,58,58,58	0
56	MG	1A	3169	1/1	0.96	0.06	32,32,32,32	0
56	MG	1a	1604	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3309	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3687	1/1	0.96	0.05	38,38,38,38	0
56	MG	2A	3747	1/1	0.96	0.04	43,43,43,43	0
56	MG	2a	3126	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3846	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3105	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3131	1/1	0.96	0.04	46,46,46,46	0
56	MG	2A	3752	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3754	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3260	1/1	0.96	0.08	19,19,19,19	0
56	MG	2a	3134	1/1	0.96	0.14	50,50,50,50	0
56	MG	1a	1612	1/1	0.96	0.06	52,52,52,52	0
56	MG	1a	1820	1/1	0.96	0.05	50,50,50,50	0
56	MG	2A	3436	1/1	0.96	0.33	56,56,56,56	0
56	MG	1A	4050	1/1	0.96	0.05	45,45,45,45	0
56	MG	1A	3446	1/1	0.96	0.05	40,40,40,40	0
56	MG	2A	3764	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3694	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3313	1/1	0.96	0.15	28,28,28,28	0
56	MG	1A	4057	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	3853	1/1	0.96	0.10	65,65,65,65	0
56	MG	2A	3447	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3697	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3450	1/1	0.96	0.05	51,51,51,51	0
56	MG	1A	4060	1/1	0.96	0.12	29,29,29,29	0
56	MG	2A	3203	1/1	0.96	0.20	47,47,47,47	0
56	MG	2a	3151	1/1	0.96	0.08	67,67,67,67	0
56	MG	1A	3261	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3213	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3785	1/1	0.96	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3787	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3547	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3789	1/1	0.96	0.07	53,53,53,53	0
56	MG	2A	3790	1/1	0.96	0.18	53,53,53,53	0
56	MG	1A	3008	1/1	0.96	0.04	23,23,23,23	0
56	MG	1m	3001	1/1	0.96	0.07	60,60,60,60	0
56	MG	2A	3209	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3794	1/1	0.96	0.06	56,56,56,56	0
56	MG	2a	3169	1/1	0.96	0.05	74,74,74,74	0
56	MG	1A	3452	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	4067	1/1	0.96	0.06	40,40,40,40	0
56	MG	1t	201	1/1	0.96	0.24	49,49,49,49	0
56	MG	1A	4068	1/1	0.96	0.06	27,27,27,27	0
56	MG	1A	3714	1/1	0.96	0.05	44,44,44,44	0
56	MG	1A	3867	1/1	0.96	0.05	60,60,60,60	0
56	MG	2a	3178	1/1	0.96	0.13	53,53,53,53	0
56	MG	2a	3179	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	3868	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	3044	1/1	0.96	0.07	25,25,25,25	0
56	MG	1x	101	1/1	0.96	0.06	51,51,51,51	0
56	MG	2A	3478	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3265	1/1	0.96	0.05	37,37,37,37	0
56	MG	1A	3873	1/1	0.96	0.06	33,33,33,33	0
56	MG	1a	1637	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3557	1/1	0.96	0.07	30,30,30,30	0
56	MG	1A	3319	1/1	0.96	0.08	37,37,37,37	0
56	MG	2A	3485	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3876	1/1	0.96	0.07	41,41,41,41	0
56	MG	2A	3488	1/1	0.96	0.12	55,55,55,55	0
56	MG	2a	3192	1/1	0.96	0.13	57,57,57,57	0
56	MG	1a	1641	1/1	0.96	0.04	41,41,41,41	0
56	MG	1A	3457	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3879	1/1	0.96	0.06	68,68,68,68	0
56	MG	1A	3175	1/1	0.96	0.28	28,28,28,28	0
56	MG	1A	3883	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3502	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3002	1/1	0.96	0.19	44,44,44,44	0
56	MG	1a	1646	1/1	0.96	0.09	69,69,69,69	0
56	MG	1A	3888	1/1	0.96	0.05	12,12,12,12	0
56	MG	1A	3177	1/1	0.96	0.21	54,54,54,54	0
56	MG	2A	3510	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3006	1/1	0.96	0.14	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	3512	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3385	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3008	1/1	0.96	0.07	58,58,58,58	0
56	MG	1B	207	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3323	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3242	1/1	0.96	0.05	45,45,45,45	0
56	MG	2A	3834	1/1	0.96	0.09	49,49,49,49	0
56	MG	1A	3109	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	3081	1/1	0.96	0.23	38,38,38,38	0
56	MG	1A	3273	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3730	1/1	0.96	0.09	14,14,14,14	0
56	MG	1A	3901	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3182	1/1	0.96	0.09	34,34,34,34	0
56	MG	2A	3526	1/1	0.96	0.08	24,24,24,24	0
56	MG	1A	3082	1/1	0.96	0.16	50,50,50,50	0
56	MG	2A	3530	1/1	0.96	0.08	51,51,51,51	0
56	MG	1B	220	1/1	0.96	0.04	27,27,27,27	0
56	MG	1A	3075	1/1	0.96	0.14	25,25,25,25	0
56	MG	2A	3848	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3911	1/1	0.96	0.08	26,26,26,26	0
56	MG	1A	3734	1/1	0.96	0.07	20,20,20,20	0
56	MG	2a	3229	1/1	0.96	0.06	87,87,87,87	0
56	MG	1A	3575	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3540	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3578	1/1	0.96	0.13	12,12,12,12	0
56	MG	2A	3257	1/1	0.96	0.29	61,61,61,61	0
56	MG	1A	3393	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3278	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3745	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3582	1/1	0.96	0.10	28,28,28,28	0
56	MG	1A	3050	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3477	1/1	0.96	0.25	52,52,52,52	0
56	MG	1A	3479	1/1	0.96	0.08	18,18,18,18	0
56	MG	1A	3481	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3551	1/1	0.96	0.05	61,61,61,61	0
56	MG	1A	3592	1/1	0.96	0.05	17,17,17,17	0
56	MG	1D	302	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3594	1/1	0.96	0.10	21,21,21,21	0
56	MG	2A	3043	1/1	0.96	0.18	34,34,34,34	0
56	MG	1D	306	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3932	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3334	1/1	0.96	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3596	1/1	0.96	0.07	24,24,24,24	0
56	MG	1A	3186	1/1	0.96	0.15	35,35,35,35	0
56	MG	1E	302	1/1	0.96	0.27	34,34,34,34	0
56	MG	1E	303	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3282	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3766	1/1	0.96	0.06	47,47,47,47	0
56	MG	2E	304	1/1	0.96	0.07	51,51,51,51	0
56	MG	1E	307	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	3228	1/1	0.96	0.18	52,52,52,52	0
56	MG	1A	3768	1/1	0.96	0.11	59,59,59,59	0
56	MG	1A	3400	1/1	0.96	0.10	26,26,26,26	0
56	MG	1a	1693	1/1	0.96	0.21	47,47,47,47	0
56	MG	2A	3579	1/1	0.96	0.11	36,36,36,36	0
56	MG	1E	312	1/1	0.96	0.21	45,45,45,45	0
56	MG	2A	3062	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3148	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3950	1/1	0.96	0.11	53,53,53,53	0
56	MG	1F	304	1/1	0.96	0.07	26,26,26,26	0
56	MG	2A	3066	1/1	0.96	0.11	32,32,32,32	0
56	MG	1F	306	1/1	0.96	0.10	24,24,24,24	0
56	MG	2x	105	1/1	0.96	0.10	66,66,66,66	0
56	MG	2Q	201	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3587	1/1	0.96	0.12	41,41,41,41	0
56	MG	2A	3588	1/1	0.96	0.08	52,52,52,52	0
56	MG	1F	308	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3070	1/1	0.96	0.09	56,56,56,56	0
57	K	1A	3497	1/1	0.96	0.08	67,67,67,67	0
56	MG	1A	3150	1/1	0.96	0.05	23,23,23,23	0
56	MG	1A	3115	1/1	0.96	0.12	23,23,23,23	0
56	MG	1A	3404	1/1	0.96	0.21	54,54,54,54	0
56	MG	1A	3608	1/1	0.96	0.07	27,27,27,27	0
56	MG	2A	3121	1/1	0.97	0.12	39,39,39,39	0
56	MG	1A	3877	1/1	0.97	0.06	28,28,28,28	0
56	MG	1a	1766	1/1	0.97	0.05	63,63,63,63	0
56	MG	2A	3124	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3235	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3030	1/1	0.97	0.23	30,30,30,30	0
56	MG	1A	4048	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	4049	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3750	1/1	0.97	0.07	17,17,17,17	0
56	MG	1A	3116	1/1	0.97	0.23	42,42,42,42	0
56	MG	2a	3003	1/1	0.97	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4053	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	4054	1/1	0.97	0.13	48,48,48,48	0
56	MG	2A	3636	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3886	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3134	1/1	0.97	0.07	56,56,56,56	0
56	MG	13	102	1/1	0.97	0.09	38,38,38,38	0
56	MG	13	104	1/1	0.97	0.05	30,30,30,30	0
56	MG	1A	3053	1/1	0.97	0.06	33,33,33,33	0
56	MG	15	101	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3455	1/1	0.97	0.17	31,31,31,31	0
56	MG	15	103	1/1	0.97	0.17	40,40,40,40	0
56	MG	1a	1784	1/1	0.97	0.06	62,62,62,62	0
56	MG	1A	3343	1/1	0.97	0.04	30,30,30,30	0
56	MG	1A	3011	1/1	0.97	0.08	30,30,30,30	0
56	MG	1A	3622	1/1	0.97	0.07	16,16,16,16	0
56	MG	1A	3895	1/1	0.97	0.05	77,77,77,77	0
56	MG	17	101	1/1	0.97	0.09	33,33,33,33	0
56	MG	1a	1790	1/1	0.97	0.04	65,65,65,65	0
56	MG	2A	3654	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3623	1/1	0.97	0.08	51,51,51,51	0
56	MG	2a	3024	1/1	0.97	0.19	61,61,61,61	0
56	MG	1A	3759	1/1	0.97	0.04	19,19,19,19	0
56	MG	1A	3898	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3531	1/1	0.97	0.30	52,52,52,52	0
56	MG	18	103	1/1	0.97	0.06	30,30,30,30	0
56	MG	1A	4066	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3196	1/1	0.97	0.18	27,27,27,27	0
56	MG	1A	3903	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3904	1/1	0.97	0.04	30,30,30,30	0
56	MG	1A	3243	1/1	0.97	0.18	33,33,33,33	0
56	MG	2A	3665	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3386	1/1	0.97	0.30	47,47,47,47	0
56	MG	1A	3906	1/1	0.97	0.05	49,49,49,49	0
56	MG	2A	3388	1/1	0.97	0.24	53,53,53,53	0
56	MG	1A	3630	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	4073	1/1	0.97	0.13	45,45,45,45	0
56	MG	1A	3631	1/1	0.97	0.08	43,43,43,43	0
56	MG	1a	1809	1/1	0.97	0.17	48,48,48,48	0
56	MG	1A	3909	1/1	0.97	0.10	55,55,55,55	0
56	MG	1a	1610	1/1	0.97	0.05	59,59,59,59	0
56	MG	2A	3676	1/1	0.97	0.04	42,42,42,42	0
56	MG	1A	3910	1/1	0.97	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3769	1/1	0.97	0.04	25,25,25,25	0
56	MG	1a	1613	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	3534	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3198	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3160	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3161	1/1	0.97	0.06	19,19,19,19	0
56	MG	1A	3012	1/1	0.97	0.27	22,22,22,22	0
56	MG	2A	3176	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3918	1/1	0.97	0.07	65,65,65,65	0
56	MG	2A	3688	1/1	0.97	0.12	66,66,66,66	0
56	MG	1A	3775	1/1	0.97	0.13	34,34,34,34	0
56	MG	1A	3539	1/1	0.97	0.15	41,41,41,41	0
56	MG	1B	206	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3352	1/1	0.97	0.29	32,32,32,32	0
56	MG	1A	3467	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3779	1/1	0.97	0.05	35,35,35,35	0
56	MG	1B	210	1/1	0.97	0.09	42,42,42,42	0
56	MG	1a	1627	1/1	0.97	0.08	32,32,32,32	0
56	MG	1f	201	1/1	0.97	0.15	50,50,50,50	0
56	MG	1B	211	1/1	0.97	0.08	34,34,34,34	0
56	MG	1A	3925	1/1	0.97	0.05	60,60,60,60	0
56	MG	1A	3926	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3034	1/1	0.97	0.11	19,19,19,19	0
56	MG	1A	3165	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3122	1/1	0.97	0.09	46,46,46,46	0
56	MG	2A	3193	1/1	0.97	0.07	47,47,47,47	0
56	MG	2A	3705	1/1	0.97	0.05	38,38,38,38	0
56	MG	1B	217	1/1	0.97	0.06	41,41,41,41	0
56	MG	2A	3423	1/1	0.97	0.07	61,61,61,61	0
56	MG	2A	3708	1/1	0.97	0.05	61,61,61,61	0
56	MG	1A	3931	1/1	0.97	0.05	19,19,19,19	0
56	MG	1w	102	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3205	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3472	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3934	1/1	0.97	0.08	23,23,23,23	0
56	MG	1B	224	1/1	0.97	0.09	44,44,44,44	0
56	MG	1w	107	1/1	0.97	0.07	66,66,66,66	0
56	MG	1A	3167	1/1	0.97	0.16	53,53,53,53	0
56	MG	2A	3718	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3548	1/1	0.97	0.14	46,46,46,46	0
56	MG	1B	227	1/1	0.97	0.05	26,26,26,26	0
56	MG	1A	3549	1/1	0.97	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	1x	105	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3123	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3940	1/1	0.97	0.04	40,40,40,40	0
56	MG	2A	3440	1/1	0.97	0.12	56,56,56,56	0
56	MG	1A	3476	1/1	0.97	0.24	45,45,45,45	0
56	MG	2A	3442	1/1	0.97	0.22	46,46,46,46	0
56	MG	2A	3728	1/1	0.97	0.07	71,71,71,71	0
56	MG	1A	3553	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3791	1/1	0.97	0.19	52,52,52,52	0
56	MG	1x	111	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3446	1/1	0.97	0.17	53,53,53,53	0
56	MG	1A	3947	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3448	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3210	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3211	1/1	0.97	0.11	24,24,24,24	0
56	MG	1A	3556	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3480	1/1	0.97	0.14	30,30,30,30	0
56	MG	1D	303	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3668	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3559	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3046	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3459	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3958	1/1	0.97	0.05	27,27,27,27	0
56	MG	2A	3009	1/1	0.97	0.04	44,44,44,44	0
56	MG	2A	3010	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3011	1/1	0.97	0.11	46,46,46,46	0
56	MG	1A	3125	1/1	0.97	0.15	35,35,35,35	0
56	MG	1A	3018	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3467	1/1	0.97	0.08	66,66,66,66	0
56	MG	2A	3755	1/1	0.97	0.06	34,34,34,34	0
56	MG	1E	301	1/1	0.97	0.15	29,29,29,29	0
56	MG	1A	3215	1/1	0.97	0.23	23,23,23,23	0
56	MG	2A	3230	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3127	1/1	0.97	0.18	31,31,31,31	0
56	MG	2A	3473	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3100	1/1	0.97	0.26	32,32,32,32	0
56	MG	2A	3763	1/1	0.97	0.08	62,62,62,62	0
56	MG	2A	3476	1/1	0.97	0.05	33,33,33,33	0
56	MG	2A	3765	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3766	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3477	1/1	0.97	0.04	45,45,45,45	0
56	MG	1E	305	1/1	0.97	0.12	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	3020	1/1	0.97	0.07	41,41,41,41	0
56	MG	2a	3131	1/1	0.97	0.23	49,49,49,49	0
56	MG	1A	3269	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3682	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3176	1/1	0.97	0.13	29,29,29,29	0
56	MG	2A	3238	1/1	0.97	0.17	56,56,56,56	0
56	MG	2A	3239	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3486	1/1	0.97	0.06	41,41,41,41	0
56	MG	2A	3782	1/1	0.97	0.04	45,45,45,45	0
56	MG	1a	1670	1/1	0.97	0.13	52,52,52,52	0
56	MG	1A	3685	1/1	0.97	0.04	41,41,41,41	0
56	MG	1E	310	1/1	0.97	0.10	18,18,18,18	0
56	MG	2A	3786	1/1	0.97	0.09	36,36,36,36	0
56	MG	2A	3492	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3686	1/1	0.97	0.06	47,47,47,47	0
56	MG	2A	3029	1/1	0.97	0.04	44,44,44,44	0
56	MG	2A	3030	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3496	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3246	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3499	1/1	0.97	0.09	25,25,25,25	0
56	MG	1A	3976	1/1	0.97	0.04	46,46,46,46	0
56	MG	2A	3503	1/1	0.97	0.10	41,41,41,41	0
56	MG	2a	3153	1/1	0.97	0.05	76,76,76,76	0
56	MG	1F	301	1/1	0.97	0.17	28,28,28,28	0
56	MG	2A	3505	1/1	0.97	0.08	43,43,43,43	0
56	MG	2a	3156	1/1	0.97	0.04	78,78,78,78	0
56	MG	1A	3133	1/1	0.97	0.21	30,30,30,30	0
56	MG	1A	3979	1/1	0.97	0.06	54,54,54,54	0
56	MG	2A	3508	1/1	0.97	0.10	65,65,65,65	0
56	MG	1A	3426	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3819	1/1	0.97	0.16	50,50,50,50	0
56	MG	2a	3163	1/1	0.97	0.05	79,79,79,79	0
56	MG	2a	3164	1/1	0.97	0.06	44,44,44,44	0
56	MG	1a	1681	1/1	0.97	0.08	39,39,39,39	0
56	MG	1F	307	1/1	0.97	0.19	30,30,30,30	0
56	MG	1A	3570	1/1	0.97	0.05	48,48,48,48	0
56	MG	2A	3807	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3059	1/1	0.97	0.16	35,35,35,35	0
56	MG	1A	3493	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3494	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3259	1/1	0.97	0.07	61,61,61,61	0
56	MG	2a	3174	1/1	0.97	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	1A	3695	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3987	1/1	0.97	0.13	28,28,28,28	0
56	MG	1A	3576	1/1	0.97	0.05	27,27,27,27	0
56	MG	2A	3263	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3264	1/1	0.97	0.09	57,57,57,57	0
56	MG	1G	203	1/1	0.97	0.12	31,31,31,31	0
56	MG	2A	3818	1/1	0.97	0.17	46,46,46,46	0
56	MG	1A	3577	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3527	1/1	0.97	0.04	59,59,59,59	0
56	MG	2A	3048	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3529	1/1	0.97	0.06	48,48,48,48	0
56	MG	1H	201	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3698	1/1	0.97	0.04	41,41,41,41	0
56	MG	2A	3051	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3993	1/1	0.97	0.05	21,21,21,21	0
56	MG	1A	3320	1/1	0.97	0.13	41,41,41,41	0
56	MG	2A	3537	1/1	0.97	0.04	39,39,39,39	0
56	MG	1A	3700	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3376	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3499	1/1	0.97	0.15	27,27,27,27	0
56	MG	2a	3196	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3704	1/1	0.97	0.06	39,39,39,39	0
56	MG	1P	201	1/1	0.97	0.06	28,28,28,28	0
56	MG	1a	1702	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3060	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3060	1/1	0.97	0.11	37,37,37,37	0
56	MG	2A	3281	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3837	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3180	1/1	0.97	0.14	26,26,26,26	0
56	MG	1A	4002	1/1	0.97	0.05	22,22,22,22	0
56	MG	2A	3841	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3711	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3713	1/1	0.97	0.17	44,44,44,44	0
56	MG	2A	3844	1/1	0.97	0.07	53,53,53,53	0
56	MG	1A	3103	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3842	1/1	0.97	0.07	24,24,24,24	0
56	MG	2A	3556	1/1	0.97	0.08	27,27,27,27	0
56	MG	2a	3213	1/1	0.97	0.06	64,64,64,64	0
56	MG	1A	3505	1/1	0.97	0.18	42,42,42,42	0
56	MG	2A	3071	1/1	0.97	0.06	53,53,53,53	0
56	MG	1a	1713	1/1	0.97	0.21	48,48,48,48	0
56	MG	1A	3716	1/1	0.97	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3561	1/1	0.97	0.05	39,39,39,39	0
56	MG	2A	3294	1/1	0.97	0.19	54,54,54,54	0
56	MG	1A	3277	1/1	0.97	0.20	45,45,45,45	0
56	MG	2A	3564	1/1	0.97	0.15	37,37,37,37	0
56	MG	1A	3590	1/1	0.97	0.03	26,26,26,26	0
56	MG	1A	3591	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3080	1/1	0.97	0.12	19,19,19,19	0
56	MG	1A	3326	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3013	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3301	1/1	0.97	0.07	39,39,39,39	0
56	MG	2A	3572	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3280	1/1	0.97	0.13	31,31,31,31	0
56	MG	1T	201	1/1	0.97	0.05	56,56,56,56	0
56	MG	2A	3576	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3577	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	3015	1/1	0.97	0.17	47,47,47,47	0
56	MG	1T	203	1/1	0.97	0.07	24,24,24,24	0
56	MG	1a	1725	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3440	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3039	1/1	0.97	0.06	31,31,31,31	0
56	MG	1U	205	1/1	0.97	0.13	39,39,39,39	0
56	MG	1U	208	1/1	0.97	0.34	30,30,30,30	0
56	MG	2D	305	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3857	1/1	0.97	0.10	40,40,40,40	0
56	MG	1V	202	1/1	0.97	0.37	38,38,38,38	0
56	MG	1V	203	1/1	0.97	0.11	31,31,31,31	0
56	MG	1a	1734	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3728	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	4028	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3443	1/1	0.97	0.09	53,53,53,53	0
56	MG	1V	208	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3029	1/1	0.97	0.14	24,24,24,24	0
56	MG	2F	303	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3284	1/1	0.97	0.19	42,42,42,42	0
56	MG	1a	1742	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3605	1/1	0.97	0.16	31,31,31,31	0
56	MG	1W	204	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3065	1/1	0.97	0.09	26,26,26,26	0
56	MG	1W	207	1/1	0.97	0.11	26,26,26,26	0
56	MG	2A	3104	1/1	0.97	0.16	67,67,67,67	0
56	MG	1X	101	1/1	0.97	0.04	29,29,29,29	0
56	MG	1A	4034	1/1	0.97	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1X	103	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3518	1/1	0.97	0.08	29,29,29,29	0
56	MG	2A	3109	1/1	0.97	0.04	59,59,59,59	0
56	MG	1A	3066	1/1	0.97	0.12	18,18,18,18	0
56	MG	2A	3334	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	3448	1/1	0.97	0.10	51,51,51,51	0
56	MG	2A	3336	1/1	0.97	0.06	49,49,49,49	0
56	MG	2X	101	1/1	0.97	0.07	62,62,62,62	0
56	MG	2X	102	1/1	0.97	0.12	53,53,53,53	0
56	MG	1A	3089	1/1	0.97	0.15	23,23,23,23	0
56	MG	2A	3338	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3741	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	4040	1/1	0.97	0.12	47,47,47,47	0
56	MG	1a	1759	1/1	0.97	0.05	53,53,53,53	0
56	MG	1A	3067	1/1	0.97	0.19	29,29,29,29	0
56	MG	1A	3744	1/1	0.97	0.04	40,40,40,40	0
56	MG	23	102	1/1	0.97	0.04	59,59,59,59	0
56	MG	2A	3118	1/1	0.97	0.28	41,41,41,41	0
56	MG	10	102	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3612	1/1	0.97	0.10	31,31,31,31	0
59	ZN	24	501	1/1	0.97	0.11	127,127,127,127	0
56	MG	2A	3438	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3208	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3929	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	3625	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3502	1/1	0.98	0.15	31,31,31,31	0
56	MG	2A	3627	1/1	0.98	0.08	60,60,60,60	0
56	MG	1A	3628	1/1	0.98	0.04	14,14,14,14	0
56	MG	1A	3136	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3240	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3357	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3822	1/1	0.98	0.09	36,36,36,36	0
56	MG	1U	201	1/1	0.98	0.12	30,30,30,30	0
56	MG	1U	202	1/1	0.98	0.22	30,30,30,30	0
56	MG	1A	3137	1/1	0.98	0.14	25,25,25,25	0
56	MG	2A	3287	1/1	0.98	0.07	58,58,58,58	0
56	MG	1l	201	1/1	0.98	0.06	61,61,61,61	0
56	MG	1A	3633	1/1	0.98	0.13	18,18,18,18	0
56	MG	1A	3939	1/1	0.98	0.08	35,35,35,35	0
56	MG	2A	3456	1/1	0.98	0.05	50,50,50,50	0
56	MG	1U	206	1/1	0.98	0.15	30,30,30,30	0
56	MG	1U	207	1/1	0.98	0.34	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3643	1/1	0.98	0.05	55,55,55,55	0
56	MG	1A	3138	1/1	0.98	0.05	27,27,27,27	0
56	MG	2A	3136	1/1	0.98	0.04	40,40,40,40	0
56	MG	1a	1680	1/1	0.98	0.23	40,40,40,40	0
56	MG	1A	3139	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3004	1/1	0.98	0.03	24,24,24,24	0
56	MG	1A	3943	1/1	0.98	0.10	18,18,18,18	0
56	MG	1a	1684	1/1	0.98	0.22	51,51,51,51	0
56	MG	1V	204	1/1	0.98	0.21	28,28,28,28	0
56	MG	1A	3084	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	3407	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	4074	1/1	0.98	0.10	49,49,49,49	0
56	MG	2A	3471	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3246	1/1	0.98	0.14	22,22,22,22	0
56	MG	1A	3409	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3247	1/1	0.98	0.06	49,49,49,49	0
56	MG	2A	3475	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3459	1/1	0.98	0.10	15,15,15,15	0
56	MG	2A	3150	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3646	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3647	1/1	0.98	0.04	18,18,18,18	0
56	MG	1W	206	1/1	0.98	0.06	31,31,31,31	0
56	MG	2A	3154	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	4081	1/1	0.98	0.05	26,26,26,26	0
56	MG	1A	3955	1/1	0.98	0.06	16,16,16,16	0
56	MG	2A	3484	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3573	1/1	0.98	0.04	20,20,20,20	0
56	MG	1A	3163	1/1	0.98	0.03	35,35,35,35	0
56	MG	1X	104	1/1	0.98	0.04	33,33,33,33	0
56	MG	1X	105	1/1	0.98	0.03	31,31,31,31	0
56	MG	2A	3489	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3740	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3650	1/1	0.98	0.04	12,12,12,12	0
56	MG	1B	204	1/1	0.98	0.03	32,32,32,32	0
56	MG	2D	301	1/1	0.98	0.07	54,54,54,54	0
56	MG	1A	3287	1/1	0.98	0.13	33,33,33,33	0
56	MG	1A	3743	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3965	1/1	0.98	0.11	49,49,49,49	0
56	MG	2A	3497	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3683	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3652	1/1	0.98	0.06	52,52,52,52	0
56	MG	2a	3146	1/1	0.98	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3326	1/1	0.98	0.07	50,50,50,50	0
56	MG	2A	3500	1/1	0.98	0.08	32,32,32,32	0
56	MG	2A	3501	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	3967	1/1	0.98	0.03	49,49,49,49	0
56	MG	1a	1710	1/1	0.98	0.25	47,47,47,47	0
56	MG	1A	3250	1/1	0.98	0.20	25,25,25,25	0
56	MG	1A	3654	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3655	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3748	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3749	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3369	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	3751	1/1	0.98	0.06	18,18,18,18	0
56	MG	1A	3978	1/1	0.98	0.07	45,45,45,45	0
56	MG	1B	218	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3513	1/1	0.98	0.06	39,39,39,39	0
56	MG	11	104	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	3370	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3216	1/1	0.98	0.20	31,31,31,31	0
56	MG	2A	3025	1/1	0.98	0.06	56,56,56,56	0
56	MG	1A	3466	1/1	0.98	0.11	48,48,48,48	0
56	MG	13	101	1/1	0.98	0.08	32,32,32,32	0
56	MG	1A	3856	1/1	0.98	0.06	31,31,31,31	0
56	MG	2U	201	1/1	0.98	0.04	63,63,63,63	0
56	MG	13	103	1/1	0.98	0.12	44,44,44,44	0
56	MG	1A	3660	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	3661	1/1	0.98	0.05	12,12,12,12	0
56	MG	1A	3252	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3862	1/1	0.98	0.07	17,17,17,17	0
56	MG	1a	1731	1/1	0.98	0.04	50,50,50,50	0
56	MG	1A	3584	1/1	0.98	0.04	27,27,27,27	0
56	MG	1A	3664	1/1	0.98	0.10	22,22,22,22	0
56	MG	21	101	1/1	0.98	0.22	54,54,54,54	0
56	MG	2A	3715	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3989	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3760	1/1	0.98	0.07	26,26,26,26	0
56	MG	1a	1736	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3142	1/1	0.98	0.12	26,26,26,26	0
56	MG	1A	3992	1/1	0.98	0.10	22,22,22,22	0
56	MG	17	102	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3763	1/1	0.98	0.18	22,22,22,22	0
56	MG	1A	3586	1/1	0.98	0.11	34,34,34,34	0
56	MG	1B	236	1/1	0.98	0.04	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	17	106	1/1	0.98	0.03	44,44,44,44	0
56	MG	18	101	1/1	0.98	0.04	32,32,32,32	0
56	MG	28	103	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3765	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3366	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3330	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3143	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	3144	1/1	0.98	0.07	32,32,32,32	0
56	MG	1D	304	1/1	0.98	0.09	28,28,28,28	0
56	MG	2A	3733	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3003	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3168	1/1	0.98	0.05	31,31,31,31	0
56	MG	2A	3552	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3474	1/1	0.98	0.15	31,31,31,31	0
56	MG	1A	3006	1/1	0.98	0.06	38,38,38,38	0
56	MG	1D	309	1/1	0.98	0.12	14,14,14,14	0
56	MG	1A	3674	1/1	0.98	0.04	17,17,17,17	0
56	MG	1A	3676	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3031	1/1	0.98	0.21	34,34,34,34	0
56	MG	1A	4010	1/1	0.98	0.03	28,28,28,28	0
56	MG	1A	3884	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3885	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3129	1/1	0.98	0.09	16,16,16,16	0
56	MG	1A	3478	1/1	0.98	0.28	34,34,34,34	0
56	MG	2A	3749	1/1	0.98	0.07	45,45,45,45	0
56	MG	1a	1767	1/1	0.98	0.06	50,50,50,50	0
56	MG	2A	3067	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3197	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3753	1/1	0.98	0.07	63,63,63,63	0
56	MG	2A	3567	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3890	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3600	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3684	1/1	0.98	0.06	45,45,45,45	0
56	MG	1A	3149	1/1	0.98	0.12	31,31,31,31	0
56	MG	2a	3226	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	4020	1/1	0.98	0.03	39,39,39,39	0
56	MG	1A	3602	1/1	0.98	0.06	17,17,17,17	0
56	MG	1A	3340	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3575	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3095	1/1	0.98	0.20	27,27,27,27	0
56	MG	1A	4024	1/1	0.98	0.13	39,39,39,39	0
56	MG	1F	305	1/1	0.98	0.05	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	1779	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3432	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3484	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3132	1/1	0.98	0.12	28,28,28,28	0
56	MG	2A	3771	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3902	1/1	0.98	0.04	37,37,37,37	0
56	MG	1a	1631	1/1	0.98	0.26	42,42,42,42	0
56	MG	1A	3266	1/1	0.98	0.11	26,26,26,26	0
56	MG	2A	3776	1/1	0.98	0.08	65,65,65,65	0
56	MG	1A	3120	1/1	0.98	0.18	33,33,33,33	0
56	MG	2A	3778	1/1	0.98	0.06	58,58,58,58	0
56	MG	2A	3779	1/1	0.98	0.04	56,56,56,56	0
56	MG	2A	3780	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3112	1/1	0.98	0.05	23,23,23,23	0
56	MG	1A	3154	1/1	0.98	0.07	45,45,45,45	0
56	MG	1G	201	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	3007	1/1	0.98	0.04	21,21,21,21	0
56	MG	1A	3793	1/1	0.98	0.05	39,39,39,39	0
56	MG	2A	3592	1/1	0.98	0.12	39,39,39,39	0
56	MG	1A	3794	1/1	0.98	0.06	35,35,35,35	0
56	MG	1a	1793	1/1	0.98	0.04	60,60,60,60	0
56	MG	1A	3271	1/1	0.98	0.16	43,43,43,43	0
56	MG	1A	3349	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3701	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3616	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3156	1/1	0.98	0.08	30,30,30,30	0
56	MG	1N	205	1/1	0.98	0.03	33,33,33,33	0
56	MG	1A	3915	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3551	1/1	0.98	0.13	35,35,35,35	0
56	MG	1A	3442	1/1	0.98	0.15	32,32,32,32	0
56	MG	1A	3706	1/1	0.98	0.04	26,26,26,26	0
56	MG	1A	4045	1/1	0.98	0.04	34,34,34,34	0
56	MG	2A	3800	1/1	0.98	0.11	53,53,53,53	0
56	MG	1P	203	1/1	0.98	0.19	23,23,23,23	0
56	MG	1A	3206	1/1	0.98	0.12	33,33,33,33	0
56	MG	1A	3709	1/1	0.98	0.06	29,29,29,29	0
56	MG	1P	206	1/1	0.98	0.05	31,31,31,31	0
56	MG	2A	3610	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3236	1/1	0.98	0.13	59,59,59,59	0
56	MG	1A	3810	1/1	0.98	0.09	44,44,44,44	0
56	MG	1a	1814	1/1	0.98	0.05	49,49,49,49	0
56	MG	1A	3712	1/1	0.98	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3432	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3924	1/1	0.98	0.08	58,58,58,58	0
56	MG	1A	4052	1/1	0.98	0.04	36,36,36,36	0
56	MG	1A	3498	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	3813	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3181	1/1	0.98	0.09	29,29,29,29	0
59	ZN	29	501	1/1	0.98	0.04	81,81,81,81	0
60	SF4	2d	302	8/8	0.98	0.04	67,80,92,98	0
56	MG	1A	3809	1/1	0.99	0.06	34,34,34,34	0
56	MG	1A	3520	1/1	0.99	0.19	35,35,35,35	0
56	MG	1A	3045	1/1	0.99	0.07	22,22,22,22	0
56	MG	1A	3972	1/1	0.99	0.04	51,51,51,51	0
56	MG	1A	3593	1/1	0.99	0.06	19,19,19,19	0
56	MG	1A	3974	1/1	0.99	0.06	38,38,38,38	0
56	MG	1A	3308	1/1	0.99	0.06	28,28,28,28	0
56	MG	1A	3501	1/1	0.99	0.12	23,23,23,23	0
56	MG	1A	3257	1/1	0.99	0.11	26,26,26,26	0
56	MG	2A	3365	1/1	0.99	0.05	36,36,36,36	0
56	MG	2A	3522	1/1	0.99	0.03	32,32,32,32	0
56	MG	1B	221	1/1	0.99	0.03	28,28,28,28	0
56	MG	1A	3364	1/1	0.99	0.09	38,38,38,38	0
56	MG	1A	3130	1/1	0.99	0.09	40,40,40,40	0
56	MG	1A	3627	1/1	0.99	0.05	22,22,22,22	0
56	MG	1A	3735	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3170	1/1	0.99	0.09	37,37,37,37	0
56	MG	1A	3870	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3871	1/1	0.99	0.04	44,44,44,44	0
56	MG	2A	3614	1/1	0.99	0.04	46,46,46,46	0
56	MG	2A	3531	1/1	0.99	0.03	44,44,44,44	0
56	MG	1A	3424	1/1	0.99	0.06	37,37,37,37	0
56	MG	2A	3533	1/1	0.99	0.03	57,57,57,57	0
56	MG	1A	3738	1/1	0.99	0.06	34,34,34,34	0
56	MG	2A	3453	1/1	0.99	0.04	56,56,56,56	0
56	MG	1Q	202	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	3574	1/1	0.99	0.09	30,30,30,30	0
56	MG	2A	3538	1/1	0.99	0.03	52,52,52,52	0
56	MG	1A	3097	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3108	1/1	0.99	0.08	28,28,28,28	0
56	MG	1A	3071	1/1	0.99	0.08	19,19,19,19	0
56	MG	1A	3035	1/1	0.99	0.14	34,34,34,34	0
56	MG	1A	3579	1/1	0.99	0.05	26,26,26,26	0
56	MG	1B	237	1/1	0.99	0.04	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3880	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	3881	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3636	1/1	0.99	0.06	20,20,20,20	0
56	MG	1A	3073	1/1	0.99	0.12	28,28,28,28	0
56	MG	2A	3466	1/1	0.99	0.07	41,41,41,41	0
56	MG	1a	1796	1/1	0.99	0.07	37,37,37,37	0
56	MG	1a	1797	1/1	0.99	0.04	64,64,64,64	0
56	MG	1a	1798	1/1	0.99	0.04	50,50,50,50	0
56	MG	2A	3015	1/1	0.99	0.07	68,68,68,68	0
56	MG	1A	3027	1/1	0.99	0.15	22,22,22,22	0
56	MG	1A	3832	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3833	1/1	0.99	0.03	24,24,24,24	0
56	MG	1A	3887	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3249	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	4003	1/1	0.99	0.06	42,42,42,42	0
56	MG	1A	3710	1/1	0.99	0.04	20,20,20,20	0
56	MG	1A	4005	1/1	0.99	0.05	40,40,40,40	0
56	MG	1A	3558	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3021	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	4009	1/1	0.99	0.06	19,19,19,19	0
56	MG	1A	3945	1/1	0.99	0.09	12,12,12,12	0
56	MG	2A	3736	1/1	0.99	0.03	60,60,60,60	0
56	MG	1a	1603	1/1	0.99	0.03	49,49,49,49	0
56	MG	1A	3946	1/1	0.99	0.03	33,33,33,33	0
56	MG	1A	3642	1/1	0.99	0.06	18,18,18,18	0
56	MG	2a	3165	1/1	0.99	0.04	66,66,66,66	0
56	MG	1A	3675	1/1	0.99	0.03	27,27,27,27	0
56	MG	1A	3949	1/1	0.99	0.02	51,51,51,51	0
56	MG	1A	3019	1/1	0.99	0.04	17,17,17,17	0
56	MG	1a	1743	1/1	0.99	0.04	33,33,33,33	0
56	MG	1a	1744	1/1	0.99	0.08	36,36,36,36	0
56	MG	2A	3491	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	3644	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3717	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3085	1/1	0.99	0.07	16,16,16,16	0
56	MG	1A	3899	1/1	0.99	0.04	51,51,51,51	0
56	MG	2a	3176	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3014	1/1	0.99	0.07	30,30,30,30	0
56	MG	1A	4083	1/1	0.99	0.05	42,42,42,42	0
56	MG	1A	3956	1/1	0.99	0.03	17,17,17,17	0
56	MG	2A	3667	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3680	1/1	0.99	0.06	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	3800	1/1	0.99	0.06	12,12,12,12	0
56	MG	1A	3960	1/1	0.99	0.06	42,42,42,42	0
56	MG	1A	3681	1/1	0.99	0.04	43,43,43,43	0
56	MG	1A	3615	1/1	0.99	0.04	26,26,26,26	0
56	MG	1A	3762	1/1	0.99	0.03	27,27,27,27	0
56	MG	1a	1758	1/1	0.99	0.09	65,65,65,65	0
56	MG	1A	3128	1/1	0.99	0.03	24,24,24,24	0
56	MG	2A	3762	1/1	0.99	0.08	40,40,40,40	0
56	MG	1a	1760	1/1	0.99	0.04	36,36,36,36	0
59	ZN	1Y	204	1/1	0.99	0.03	84,84,84,84	0
56	MG	1A	3805	1/1	0.99	0.07	31,31,31,31	0
59	ZN	15	106	1/1	0.99	0.07	52,52,52,52	0
59	ZN	1n	103	1/1	0.99	0.03	60,60,60,60	0
59	ZN	2Y	202	1/1	0.99	0.06	109,109,109,109	0
56	MG	1A	3589	1/1	0.99	0.04	39,39,39,39	0
59	ZN	25	103	1/1	0.99	0.03	69,69,69,69	0
59	ZN	26	501	1/1	0.99	0.05	67,67,67,67	0
56	MG	1A	3807	1/1	0.99	0.04	35,35,35,35	0
59	ZN	2n	501	1/1	0.99	0.03	98,98,98,98	0
60	SF4	1d	302	8/8	0.99	0.03	59,68,73,74	0
56	MG	1A	3224	1/1	0.99	0.13	31,31,31,31	0
56	MG	1A	3689	1/1	1.00	0.04	13,13,13,13	0
56	MG	1A	3708	1/1	1.00	0.01	31,31,31,31	0
56	MG	1A	3975	1/1	1.00	0.03	17,17,17,17	0
56	MG	1A	4006	1/1	1.00	0.03	35,35,35,35	0
56	MG	1A	3893	1/1	1.00	0.03	42,42,42,42	0
59	ZN	16	103	1/1	1.00	0.01	40,40,40,40	0
59	ZN	19	103	1/1	1.00	0.04	43,43,43,43	0
56	MG	1A	3069	1/1	1.00	0.05	23,23,23,23	0
56	MG	2A	3651	1/1	1.00	0.09	31,31,31,31	0
56	MG	1A	3959	1/1	1.00	0.03	24,24,24,24	0
56	MG	1A	3688	1/1	1.00	0.01	20,20,20,20	0
56	MG	2A	3774	1/1	1.00	0.03	33,33,33,33	0
56	MG	2a	3162	1/1	1.00	0.05	44,44,44,44	0
56	MG	1A	3860	1/1	1.00	0.03	26,26,26,26	0
56	MG	1A	3861	1/1	1.00	0.02	24,24,24,24	0
56	MG	1A	3855	1/1	1.00	0.04	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.