



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:40 AM UTC

PDB ID : 8G29 / pdb_00008g29
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.55Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

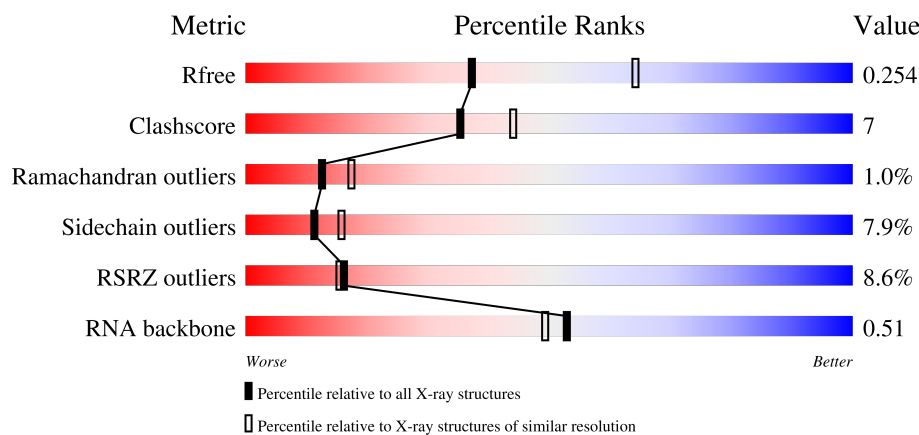
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

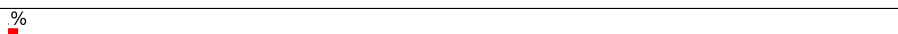
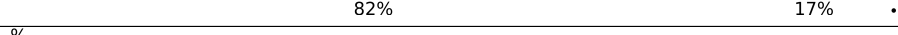
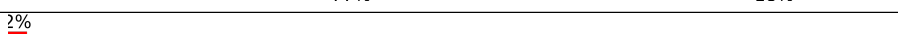
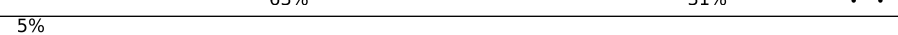
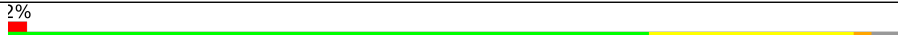
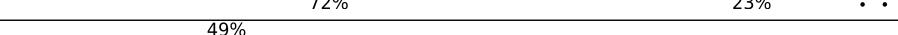
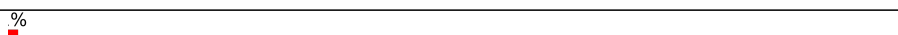
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	1A	2915	6% 69% 23% 6%
1	2A	2915	5% 60% 30% 6%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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

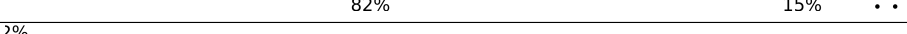
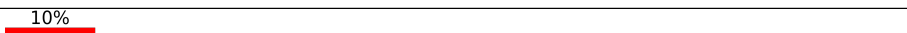
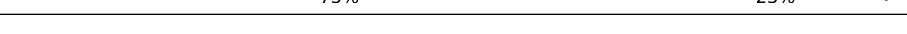
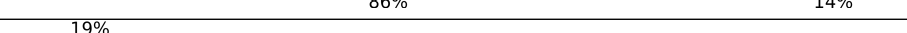
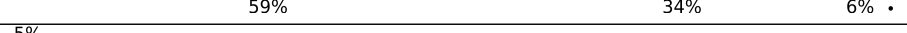
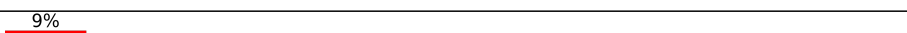
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Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24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

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

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

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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
57	MG	15	108	-	-	-	X
57	MG	1a	1659	-	-	-	X
57	MG	2A	3318	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299618 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
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	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 Aminoacylated Phe-tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1603	722	287	518	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1113	Total	Mg	0	0
			1113	1113		
57	1B	38	Total	Mg	0	0
			38	38		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	13	Total	Mg	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	4	Total 4	Mg 4	0	0
57	1P	5	Total 5	Mg 5	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	6	Total 6	Mg 6	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	6	Total 6	Mg 6	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	7	Total 7	Mg 7	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	3	Total 3	Mg 3	0	0
57	10	7	Total 7	Mg 7	0	0
57	11	6	Total 6	Mg 6	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	3	Total 3	Mg 3	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	2	Total 2	Mg 2	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	5	Total 5	Mg 5	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	220	Total 220	Mg 220	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1p	1	Total 1	Mg 1	0	0
57	1q	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	1	Total 1	Mg 1	0	0
57	1w	9	Total 9	Mg 9	0	0
57	1x	14	Total 14	Mg 14	0	0
57	2A	804	Total 804	Mg 804	0	0
57	2B	16	Total 16	Mg 16	0	0
57	2D	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	1	Total 1	Mg 1	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	3	Total 3	Mg 3	0	0
57	2V	1	Total 1	Mg 1	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	3	Total 3	Mg 3	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	3	Total 3	Mg 3	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	2	Total 2	Mg 2	0	0
57	2a	2	Total 2	Mg 2	0	0
57	2w	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2x	7	Total	Mg	0	0
			7	7		
57	2y	7	Total	Mg	0	0
			7	7		

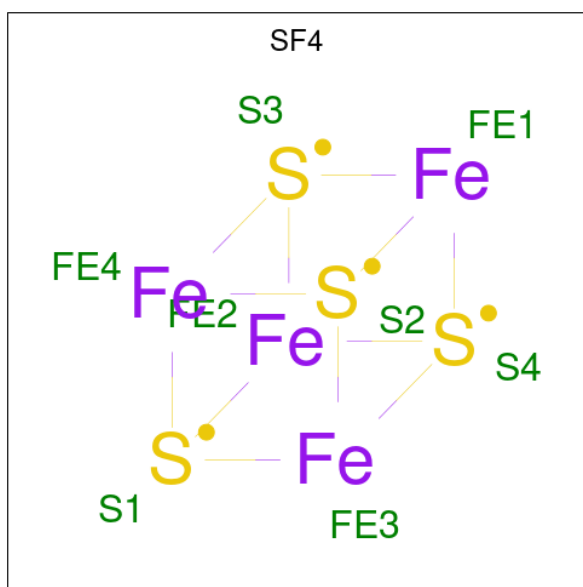
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total	K	0	0
			1	1		
58	2A	1	Total	K	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2067	Total	O	0	0
			2067	2067		
61	1B	61	Total	O	0	0
			61	61		
61	1D	32	Total	O	0	0
			32	32		
61	1E	26	Total	O	0	0
			26	26		
61	1F	20	Total	O	0	0
			20	20		
61	1G	1	Total	O	0	0
			1	1		
61	1H	2	Total	O	0	0
			2	2		
61	1N	6	Total	O	0	0
			6	6		
61	1O	6	Total	O	0	0
			6	6		
61	1P	21	Total	O	0	0
			21	21		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Q	7	Total 7	O 7	0	0
61	1R	7	Total 7	O 7	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	9	Total 9	O 9	0	0
61	1U	14	Total 14	O 14	0	0
61	1V	7	Total 7	O 7	0	0
61	1W	6	Total 6	O 6	0	0
61	1X	5	Total 5	O 5	0	0
61	1Y	3	Total 3	O 3	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	12	Total 12	O 12	0	0
61	11	7	Total 7	O 7	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	14	1	Total 1	O 1	0	0
61	15	10	Total 10	O 10	0	0
61	16	5	Total 5	O 5	0	0
61	17	10	Total 10	O 10	0	0
61	18	10	Total 10	O 10	0	0
61	1a	425	Total 425	O 425	0	0
61	1b	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1f	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	8	Total 8	O 8	0	0
61	1m	2	Total 2	O 2	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	3	Total 3	O 3	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1r	2	Total 2	O 2	0	0
61	1u	2	Total 2	O 2	0	0
61	1v	4	Total 4	O 4	0	0
61	1w	12	Total 12	O 12	0	0
61	1x	17	Total 17	O 17	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1094	Total 1094	O 1094	0	0
61	2B	18	Total 18	O 18	0	0
61	2D	22	Total 22	O 22	0	0
61	2E	9	Total 9	O 9	0	0
61	2F	11	Total 11	O 11	0	0
61	2I	3	Total 3	O 3	0	0
61	2N	1	Total 1	O 1	0	0

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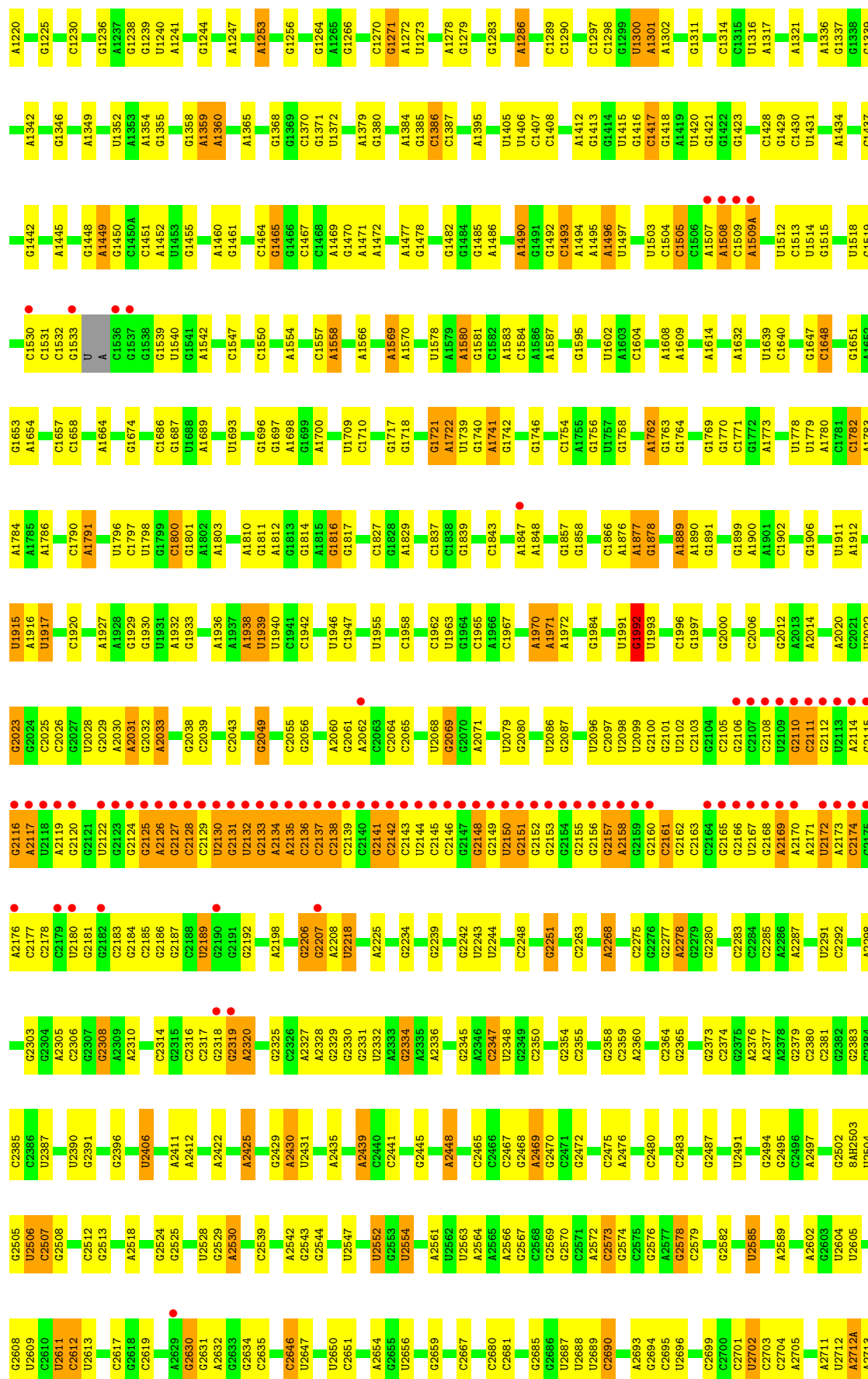
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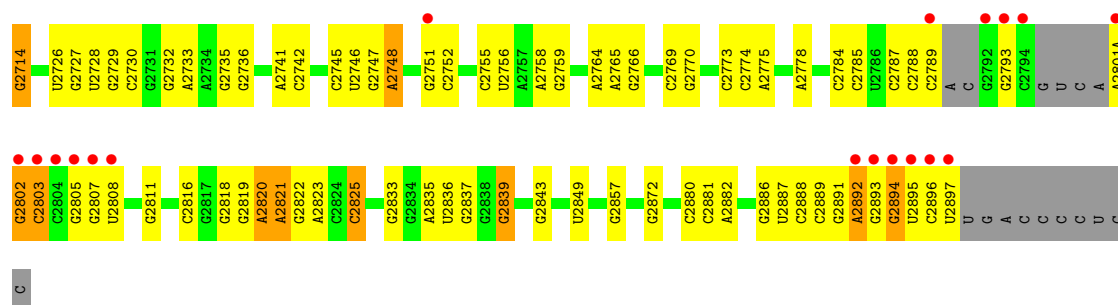
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2O	1	Total	O	0	0
			1	1		
61	2P	9	Total	O	0	0
			9	9		
61	2Q	1	Total	O	0	0
			1	1		
61	2R	1	Total	O	0	0
			1	1		
61	2T	5	Total	O	0	0
			5	5		
61	2U	3	Total	O	0	0
			3	3		
61	2W	3	Total	O	0	0
			3	3		
61	2X	2	Total	O	0	0
			2	2		
61	20	1	Total	O	0	0
			1	1		
61	21	6	Total	O	0	0
			6	6		
61	23	2	Total	O	0	0
			2	2		
61	27	5	Total	O	0	0
			5	5		
61	28	4	Total	O	0	0
			4	4		
61	29	1	Total	O	0	0
			1	1		
61	2w	1	Total	O	0	0
			1	1		
61	2x	6	Total	O	0	0
			6	6		
61	2y	2	Total	O	0	0
			2	2		

A2705	C2551	C2385	C2285	A2169	U2109	C1967	A1902	G1674	A1509A	C1386	G1256	A1098
U2712	U2552	U2406	A2286	A2170	G2110	C1970	A1803	C1686	U1518	U1394	G1264	G1099
A2712A	G2553	G2554	A2287	A2171	C2111	A1970	A1810	G1687	G1519	A1395	G1265	U1100
A2713	U2554	G2410	G2288	A2172	G2112	A1770	A1811	U1688	U1519	U1396	G1266	C1102
G2714	A2564	G2410	G2289	C2174	U2113	A1972	A1812	U1693	G1532	G1401	U1269	A1104
G2722	A2565	U2418	U2291	C2175	G2115	G1973	G1816	U1694	G	C1402	G1270	U1105
U2726	A2566	U2419	C2292	A2176	G2116	C1979	G1817	G1694	U	A1405	G1271	G1106
U2726	A2567	C2420	A2305	C2177	A2117	U1991	A1829	G1695	A	U1406	G1272	G1110
G2732	C2568	A2422	C2306	G2178	U2118	G1982	A1829	G1696	C	U1406	G1273	A1111
A2733	A2572	U2423	G2307	C2179	A2119	U1993	G1839	G1697	G1537	C1407	U1273	G1112
A2740	C2573	C2424	G2308	U2180	G2121	U1993	G1839	G1698	G1542	G1416	G1277	U1113
A2741	G2574	A2425	U2312	G2181	U2122	U1997	A1847	G1699	A1546	C1417	A1278	G1114
C2742	C2575	A2426	G2316	G2182	G2123	G1997	A1848	A1700	C1546	G1416	G1277	G1115
C2743	U2585	C2427	C2316	G2183	G2124	A2001	A1848	A1701	A1558	U1420	C1290	C1116
G2747	U2585	G2428	G2316	G2185	A2126	A2014	A1853	G1702	A1566	U1420	C1291	G1125
A2748	C2591	G2429	G2319	G2187	G2127	A2014	A1854	G1703	A1566	G1428	U1292	A1126
A2749	G2592	A2430	A2320	G2188	C2128	A2020	U1864	A1722	A1569	G1429	C1293	G1126
C2755	A2600	G2435	G2321	U2189	C2129	C2021	G1865	U1739	A1569	C1430	U1300	C1135
G2759	C2601	A2439	G2325	G2190	U2130	C2022	G1865	C1744	U1578	U1431	A1301	G1136
A2764	A2602	C2440	C2326	G2191	G2131	G2023	G1878	C1745	U1578	U1431	A1302	G1139
A2765	U2605	C2441	A2327	G2192	U2132	A2043	G1878	G1745	G1581	G1442	G1303	G1139
C2774	G2609	G2445	A2328	A2198	A2134	A2030	A1889	G1756	C1582	U1453	G1332	A1155
A2775	C2610	G2446	G2329	G2206	A2135	A2031	A1890	U1757	A1583	G1455	G1338	A1156
A2778	U2611	G2447	G2330	G2207	C2136	A2032	A1900	G1758	C1584	U1459	U1341	U1175
A2781	C2612	A2448	G2331	A2208	C2137	A2033	A1899	G1759	A1586	G1448	U1341	G1176
C2787	G2616	G2458	G2334	U2218	G2138	C2043	A1900	A1762	A1587	U1449	C1345	U1177
C2788	C2617	U2461	A2335	G2222	G2140	C2055	G1906	G1763	C1588	G1450	U1352	C1178
U2790	A2629	U2462	A2336	G2223	G2141	G2056	U1911	G1769	G1594	U1453	U1352	C1180
C2791	G2630	U2462	G2341	A2225	C2142	A2060	U1911	A1773	U1602	G1455	U1357	G1183
G2792	C2646	A2476	G2342	G2235	U2144	G2061	U1915	G1774	G1607	G1466	U1358	C1184
G2793	U2647	A2477	C2347	G2238	C2145	G2061	A1916	U1775	A1608	C1467	A1369	C1185
C2794	C2648	A2478	C2350	G2239	C2146	A2062	U1917	U1778	A1609	U1474	A1360	G1187
G	U2649	U2491	G2354	U2243	G2147	U2074	U1929	U1779	A1610	C1475	G1364	U1188
U	U2650	U2491	G2355	U2244	U2148	U2075	G1930	G1782	A1615	G1475	A1486	C1201
C	A2654	G2502	C2359	G2248	G2153	G2088	A1932	A1783	G1622	G1478	G1364	G1188
A	G2659	8AH2503	A2360	G2251	G2154	U2089	G1933	A1784	C1636	G1482	A1365	C1188
G2802	G2663	U2504	A2361	G2251	G2155	G2094	A1936	A1786	A1637	A1486	G1365	G1188
C2803	A2664	G2505	C2364	A2268	G2156	C2094	A1937	C1790	G1647	G1487	G1371	C1201
G2804	A2665	U2506	G2365	A2269	A2158	C2097	A1938	A1791	C1643	G1487	U1372	G1223
G2805	C2666	A2518	A2366	G2270	G2159	U2098	U1939	U1794	G1651	C1493	U1372	G1224
G2807	C2667	U2522	G2372	U2272	G2160	G2100	C1942	U1795	A1494	A1494	G1377	G1225
U2808	U2689	G2529	A2376	A2273	G2161	G2101	U1955	U1796	A1496	A1496	A1378	A1226
A2809	C2691	A2533	A2377	A2274	C2163	U2102	U1955	C1797	A1664	A1665	A1379	G1243
A2810	U2702	G2549	A2378	G2277	G2165	C2105	C1958	U1798	A1669	C1506	G1380	G1244
G2811		G2550	G2383	C2283	G2166	C2106	C1962	G1799	A1507	A1507	A1384	G1244
			G2384	C2284	G2168	C2108	U1963	G1801	C1509	C1509	G1385	A1253

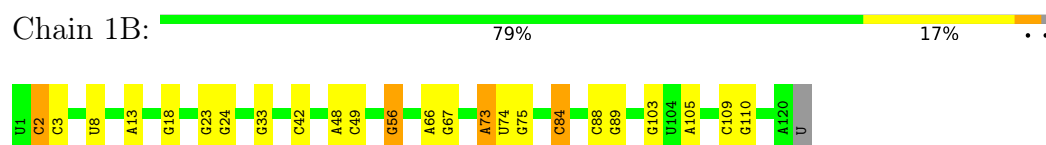
Chain 2A:



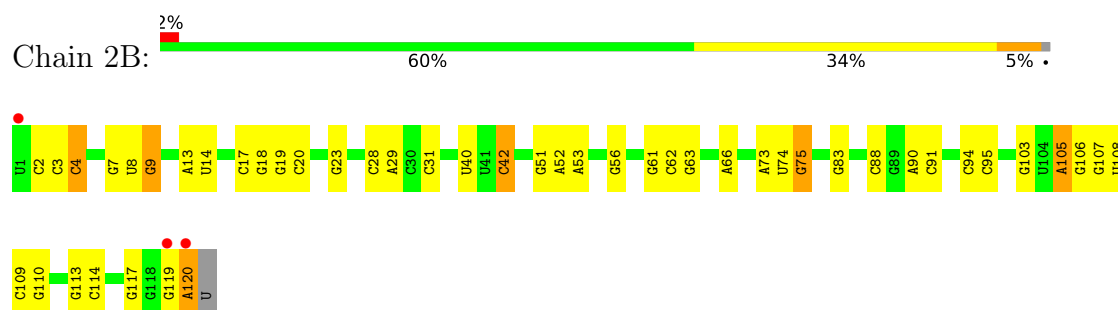




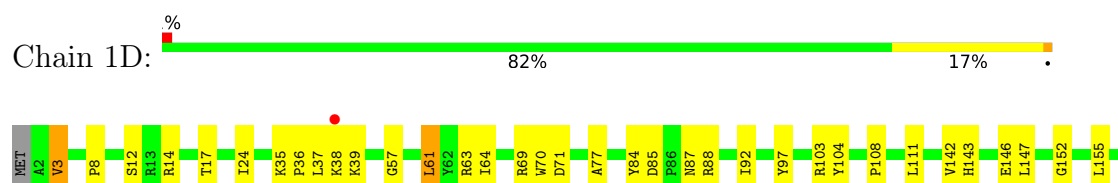
• Molecule 2: 5S Ribosomal RNA



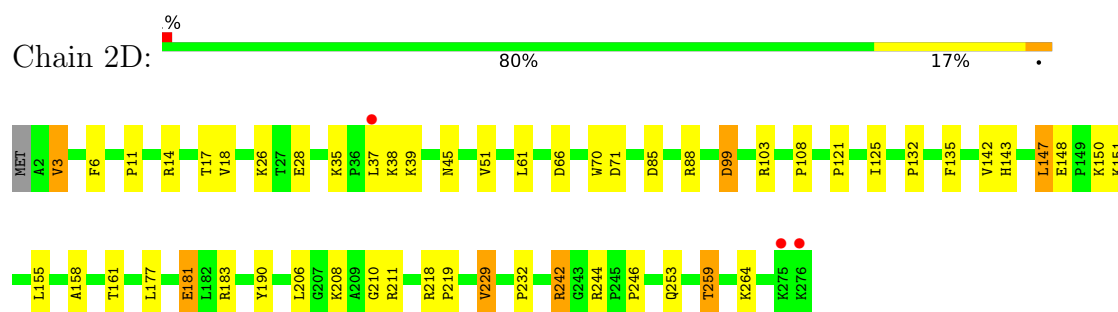
• Molecule 2: 5S Ribosomal RNA



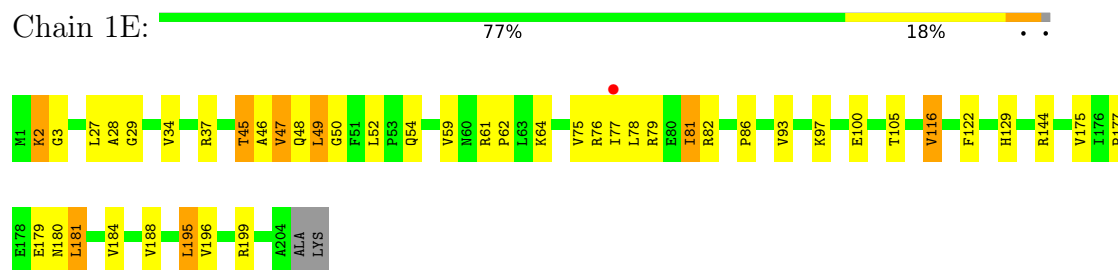
• Molecule 3: 50S ribosomal protein L2



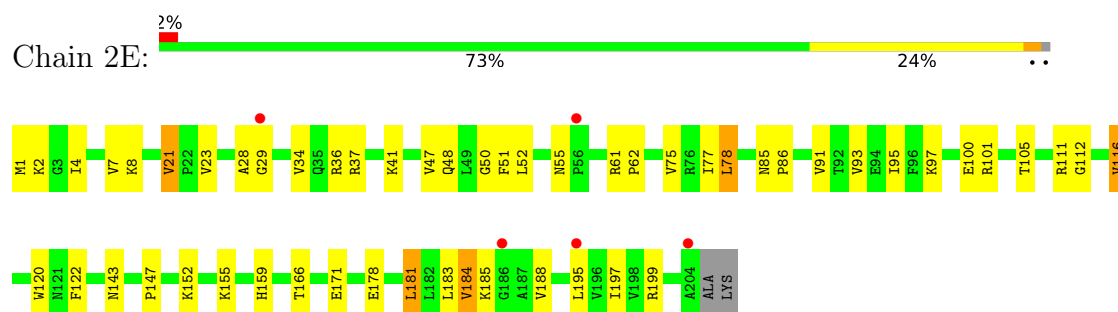
• Molecule 3: 50S ribosomal protein L2



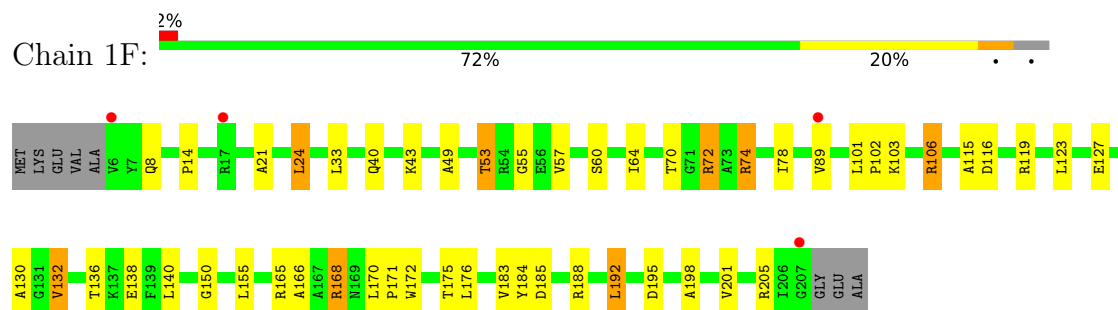
• Molecule 4: 50S ribosomal protein L3



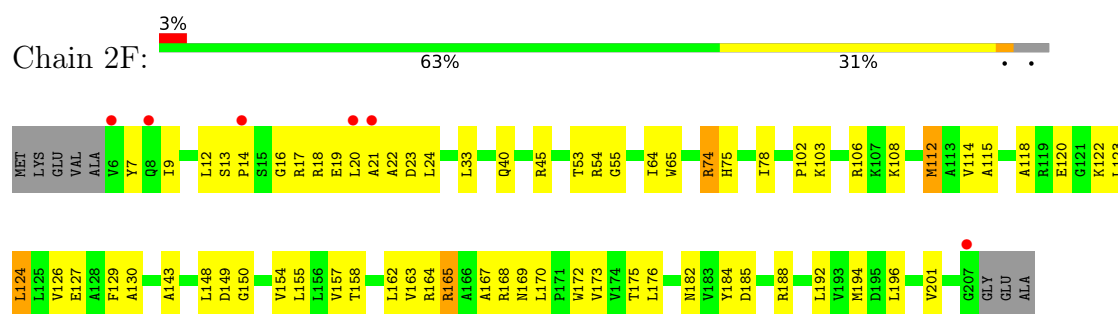
• Molecule 4: 50S ribosomal protein L3



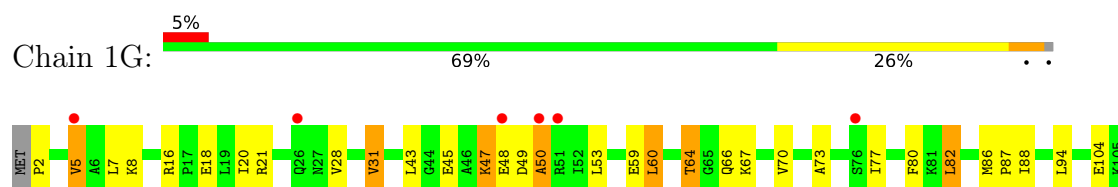
• Molecule 5: 50S ribosomal protein L4

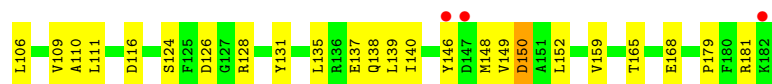


• Molecule 5: 50S ribosomal protein L4

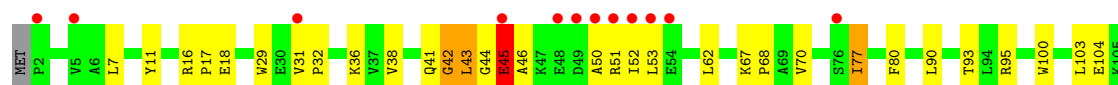


• Molecule 6: 50S ribosomal protein L5

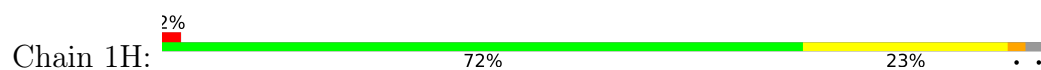




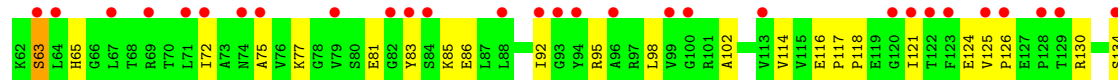
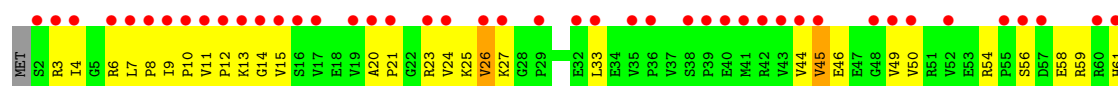
- Molecule 6: 50S ribosomal protein L5



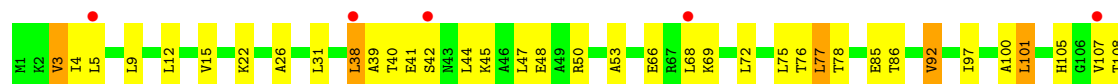
- Molecule 7: 50S ribosomal protein L6



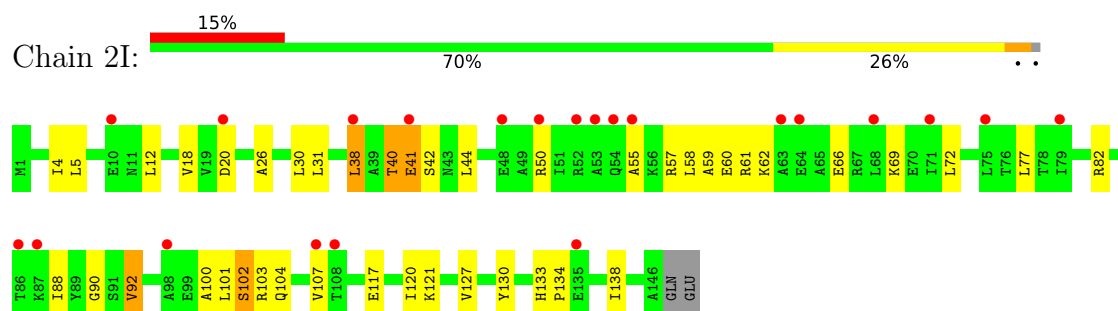
- Molecule 7: 50S ribosomal protein L6



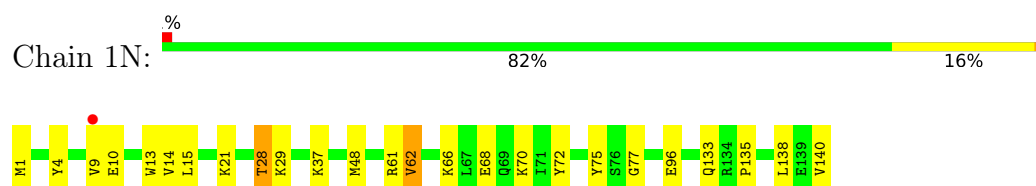
- Molecule 8: 50S ribosomal protein L9



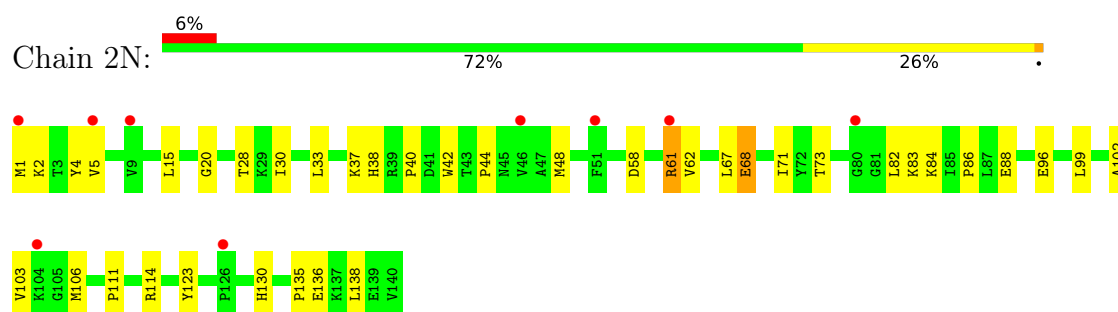
- Molecule 8: 50S ribosomal protein L9



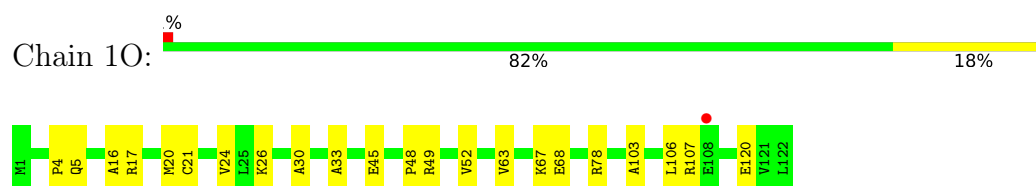
- Molecule 9: 50S ribosomal protein L13



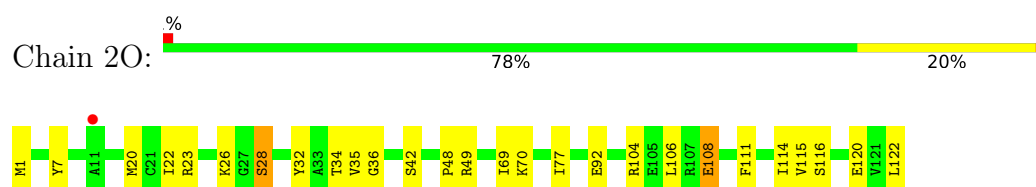
- Molecule 9: 50S ribosomal protein L13



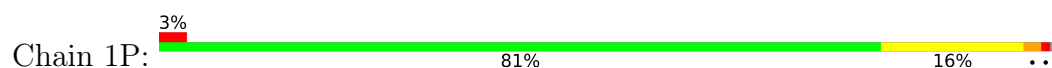
- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

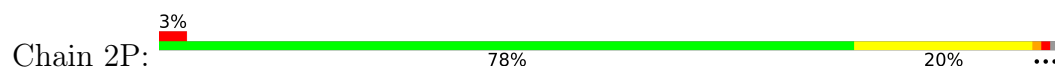


- Molecule 11: 50S ribosomal protein L15

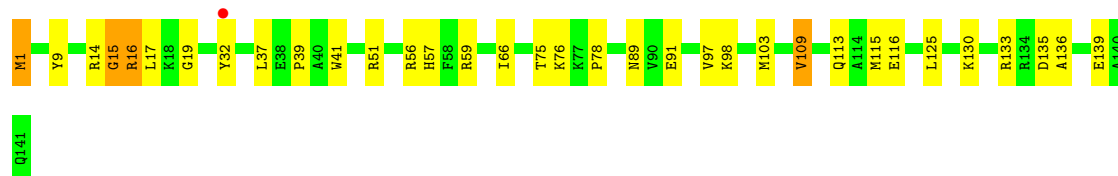
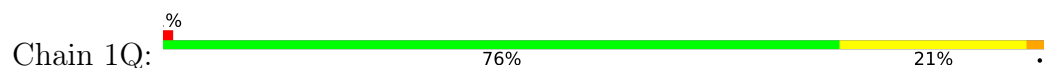




- Molecule 11: 50S ribosomal protein L15



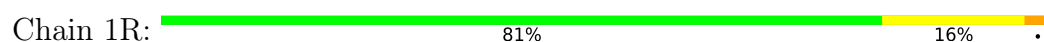
- Molecule 12: 50S ribosomal protein L16



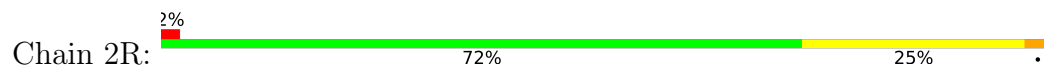
- Molecule 12: 50S ribosomal protein L16



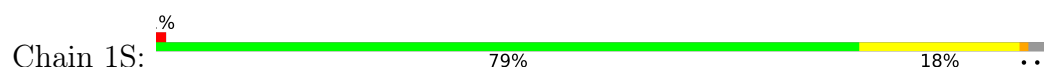
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

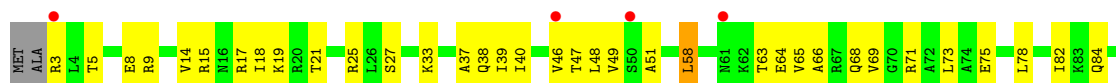


- Molecule 14: 50S ribosomal protein L18

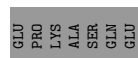
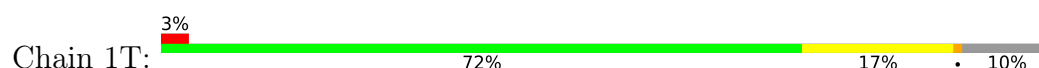




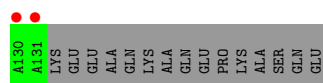
- Molecule 14: 50S ribosomal protein L18



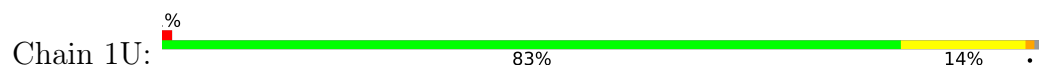
- Molecule 15: 50S ribosomal protein L19



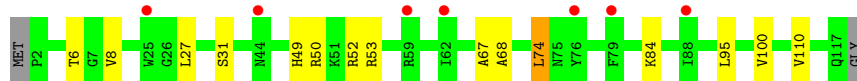
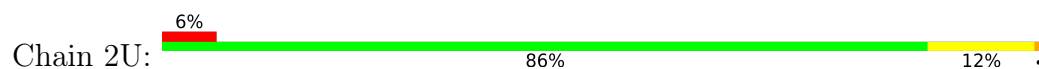
- Molecule 15: 50S ribosomal protein L19



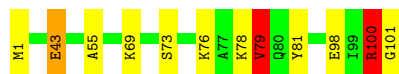
- Molecule 16: 50S ribosomal protein L20



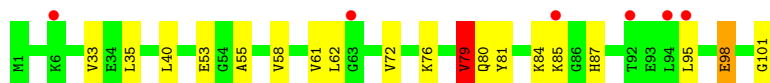
- Molecule 16: 50S ribosomal protein L20



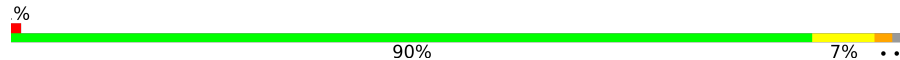
• Molecule 17: 50S ribosomal protein L21

Chain 1V:  88% 9% ..

• Molecule 17: 50S ribosomal protein L21

Chain 2V:  6% 81% 17% ..

• Molecule 18: 50S ribosomal protein L22

Chain 1W:  % 90% 7% ..

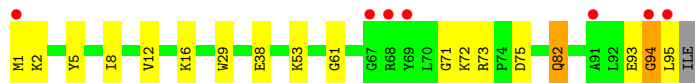
• Molecule 18: 50S ribosomal protein L22

Chain 2W:  3% 78% 20% ..

• Molecule 19: 50S ribosomal protein L23

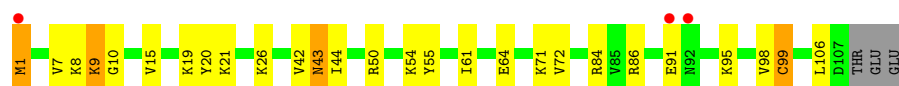
Chain 1X:  3% 82% 16% ..

• Molecule 19: 50S ribosomal protein L23

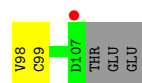
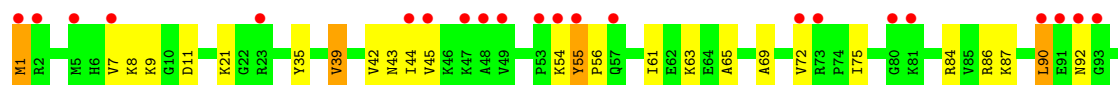
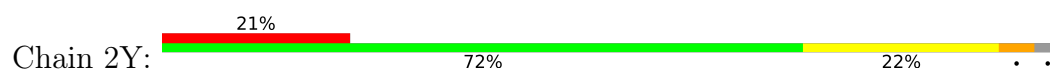
Chain 2X:  7% 80% 17% ..

• Molecule 20: 50S ribosomal protein L24

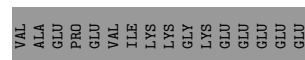
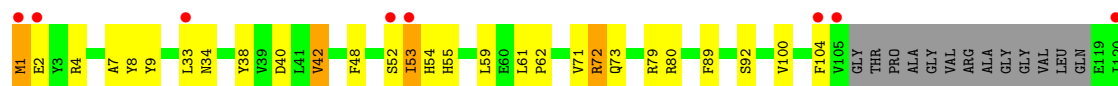
Chain 1Y:  3% 73% 21% ..



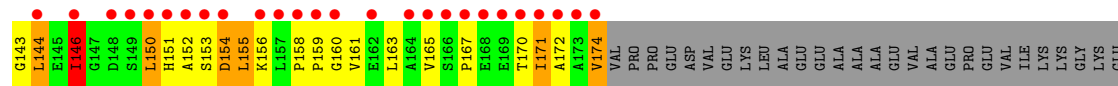
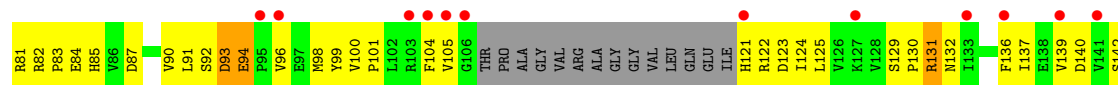
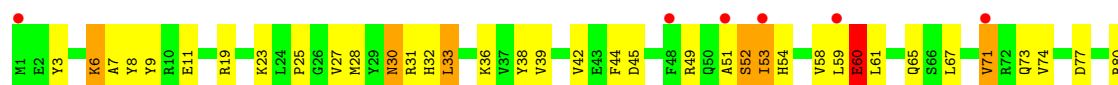
- Molecule 20: 50S ribosomal protein L24



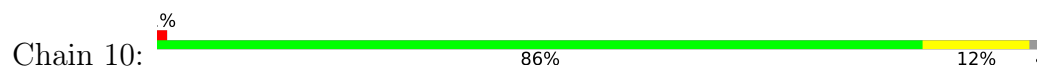
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

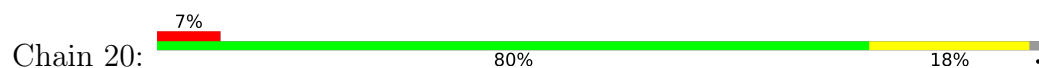


- Molecule 22: 50S ribosomal protein L27

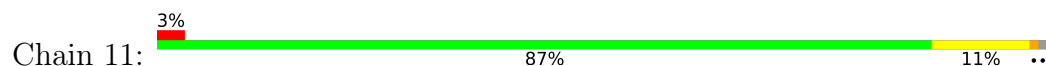




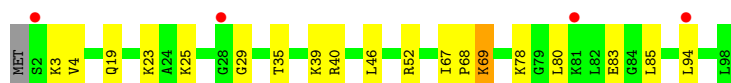
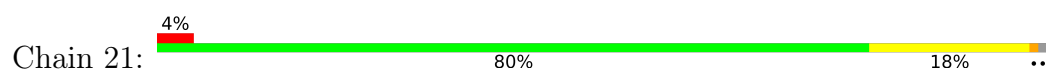
- Molecule 22: 50S ribosomal protein L27



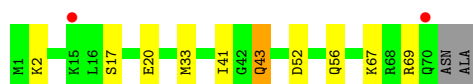
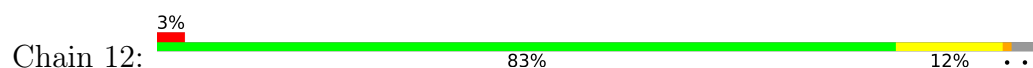
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



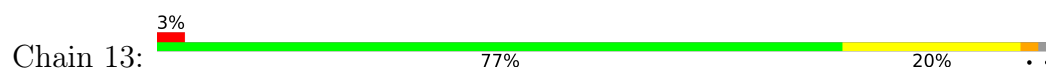
- Molecule 24: 50S ribosomal protein L29



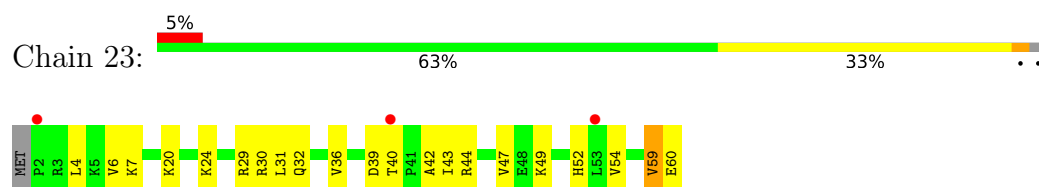
- Molecule 24: 50S ribosomal protein L29



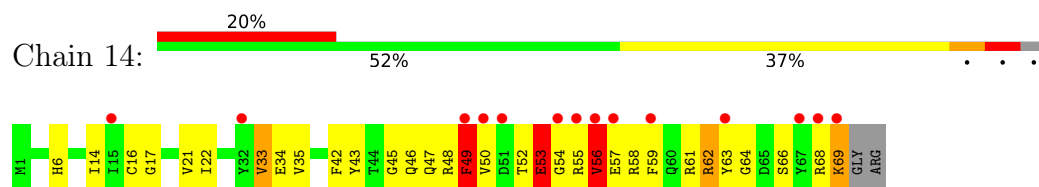
- Molecule 25: 50S ribosomal protein L30



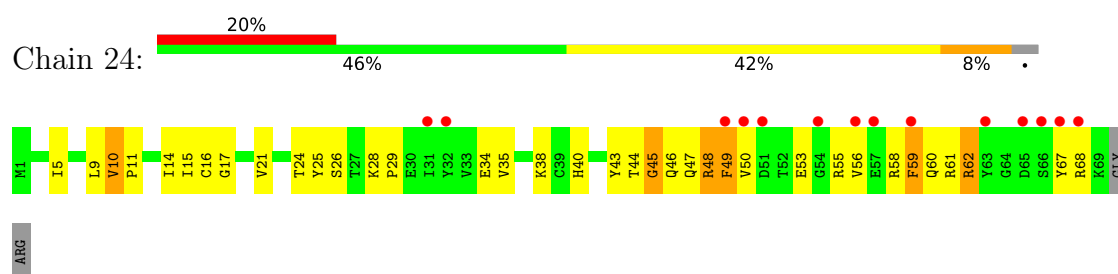
- Molecule 25: 50S ribosomal protein L30



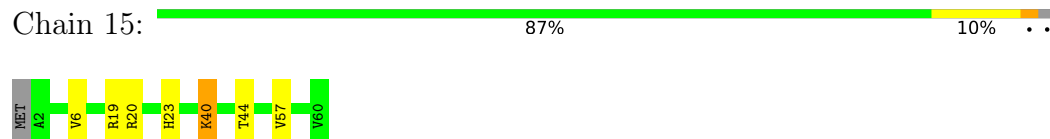
- Molecule 26: 50S ribosomal protein L31



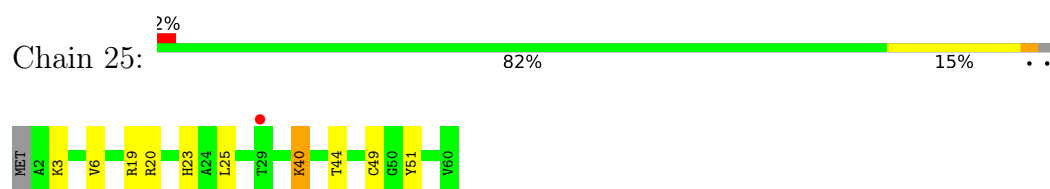
- Molecule 26: 50S ribosomal protein L31



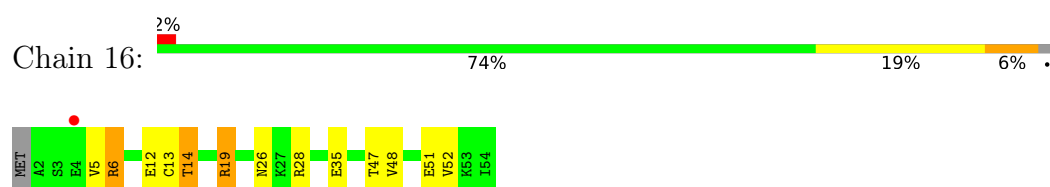
- Molecule 27: 50S ribosomal protein L32



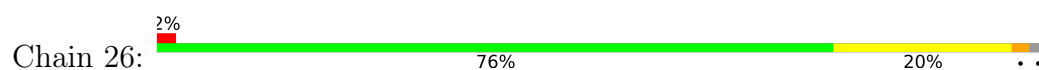
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

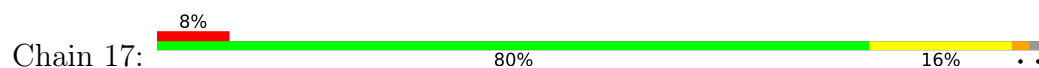


- Molecule 28: 50S ribosomal protein L33

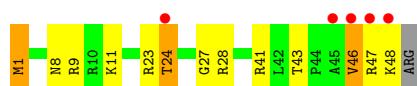
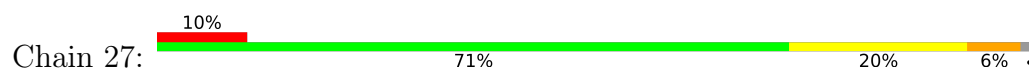




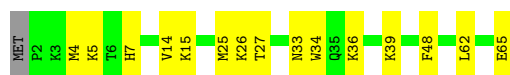
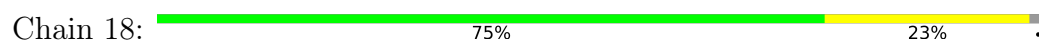
- Molecule 29: 50S ribosomal protein L34



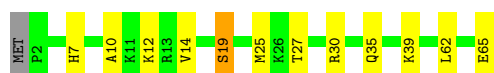
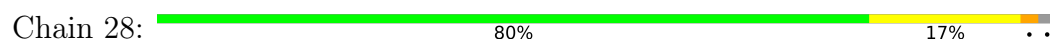
- Molecule 29: 50S ribosomal protein L34



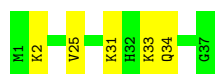
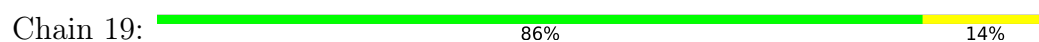
- Molecule 30: 50S ribosomal protein L35



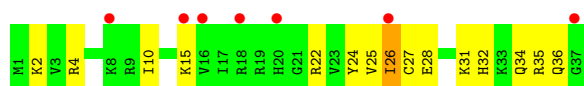
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

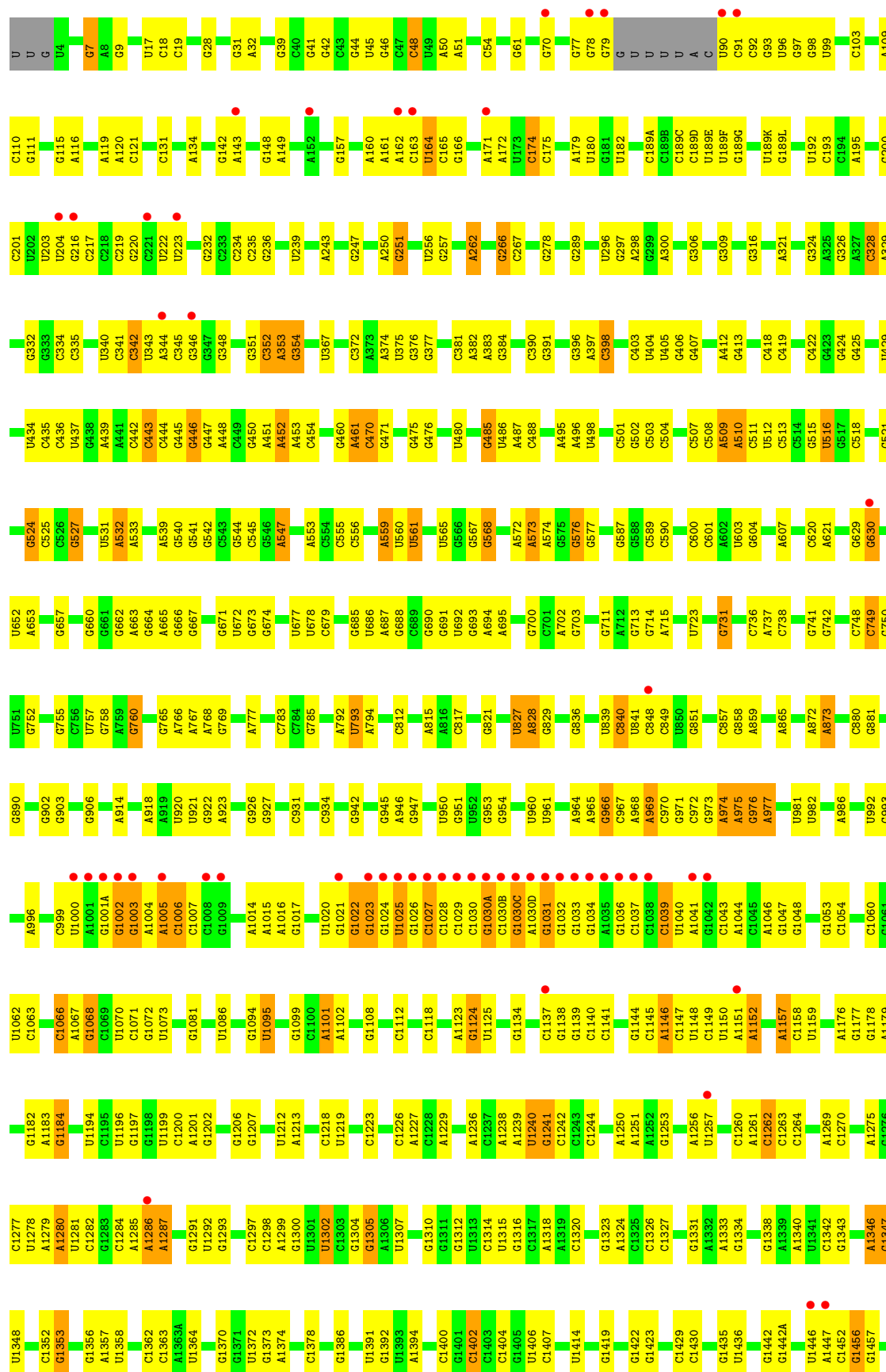


- Molecule 31: 50S ribosomal protein L36



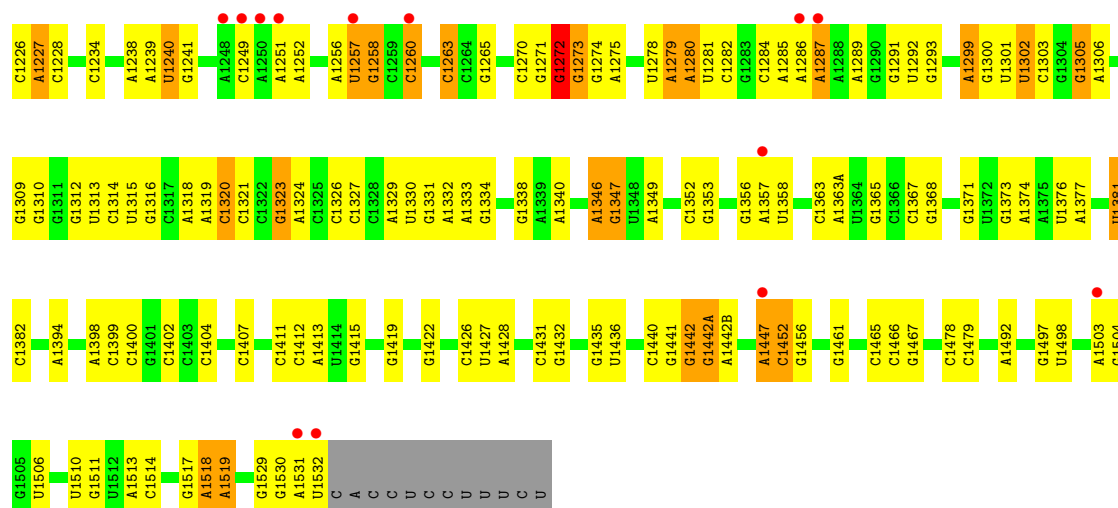
- Molecule 32: 16S Ribosomal RNA



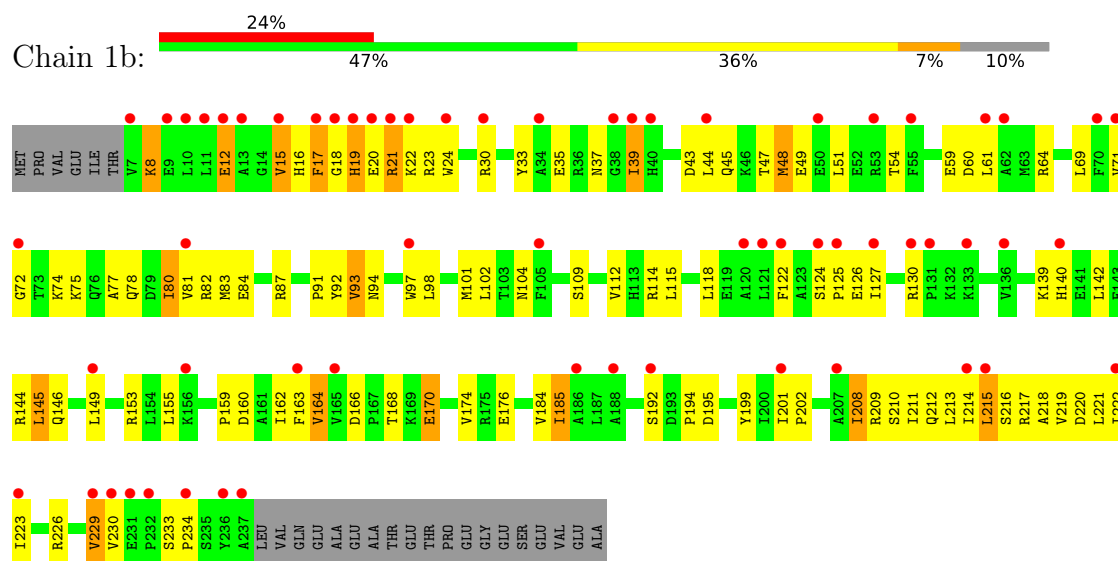


Chain 2a:

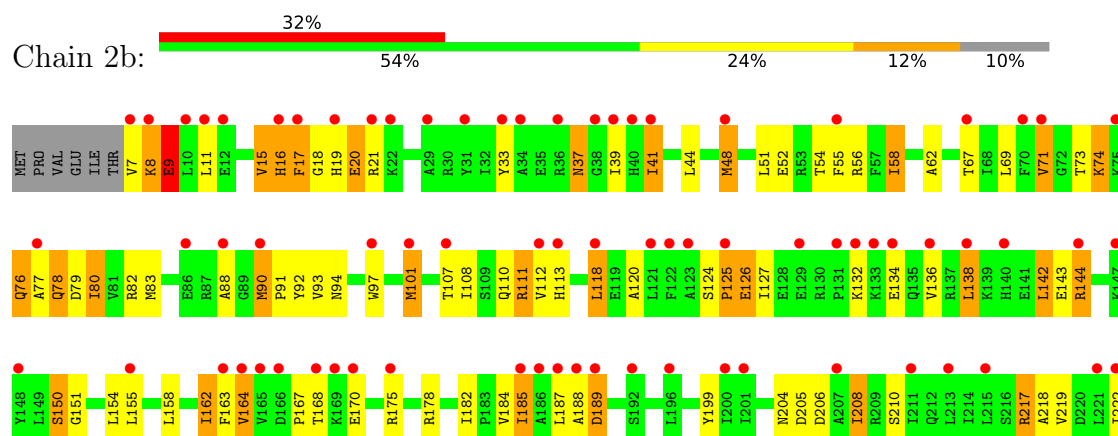


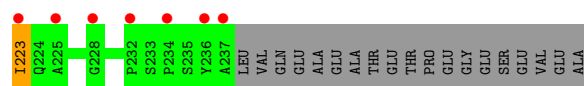


• Molecule 33: 30S ribosomal protein S2

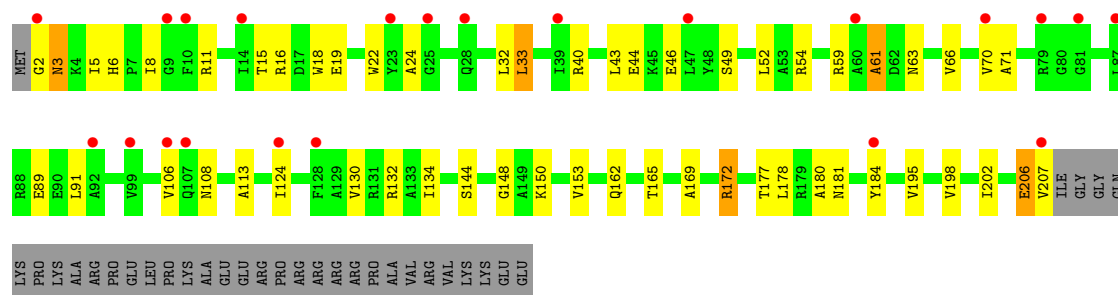


• Molecule 33: 30S ribosomal protein S2

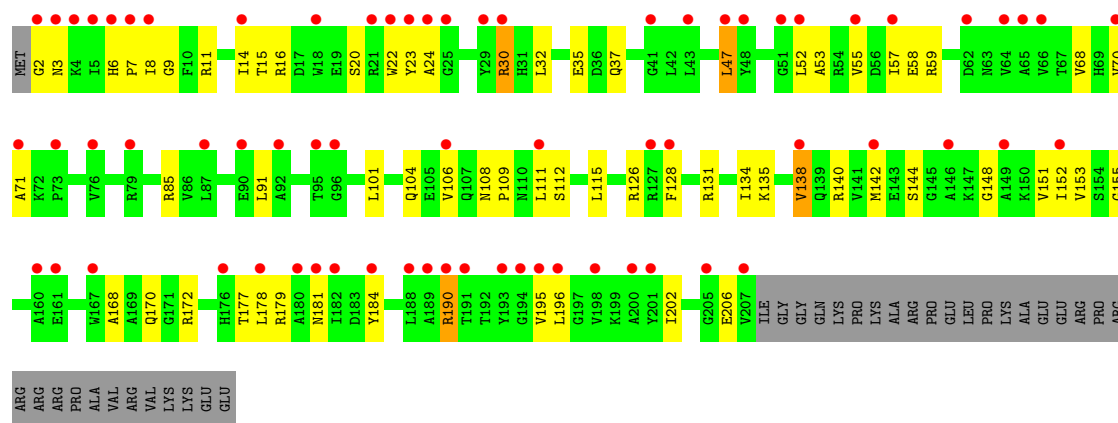




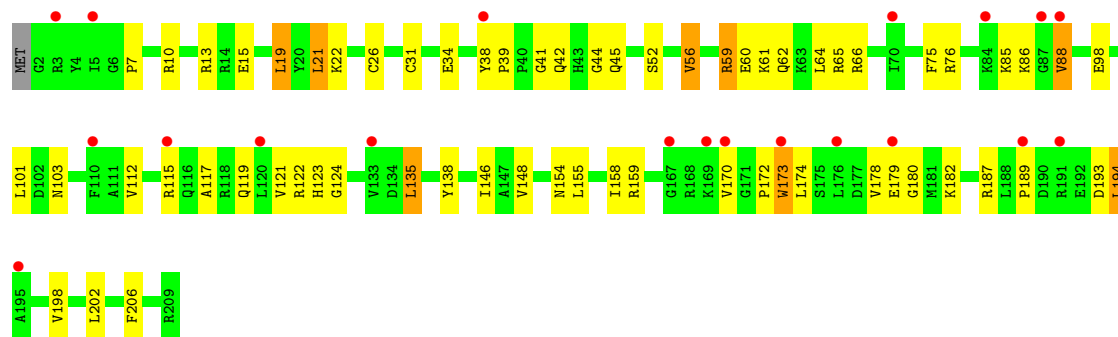
• Molecule 34: 30S ribosomal protein S3



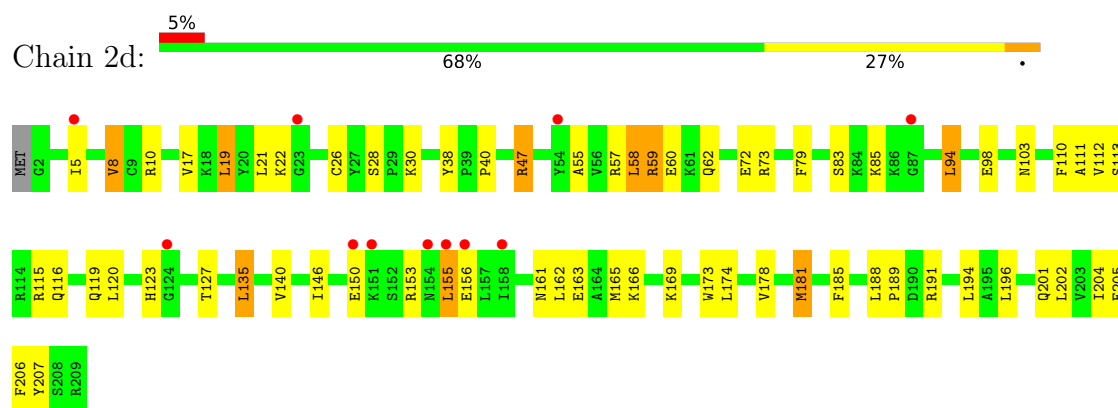
• Molecule 34: 30S ribosomal protein S3



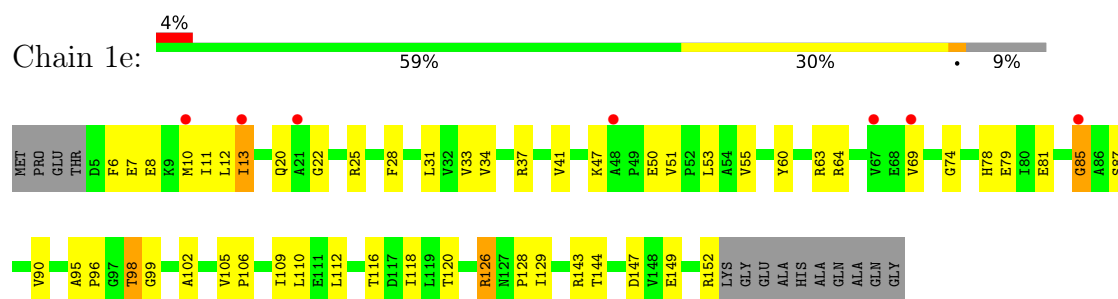
• Molecule 35: 30S ribosomal protein S4



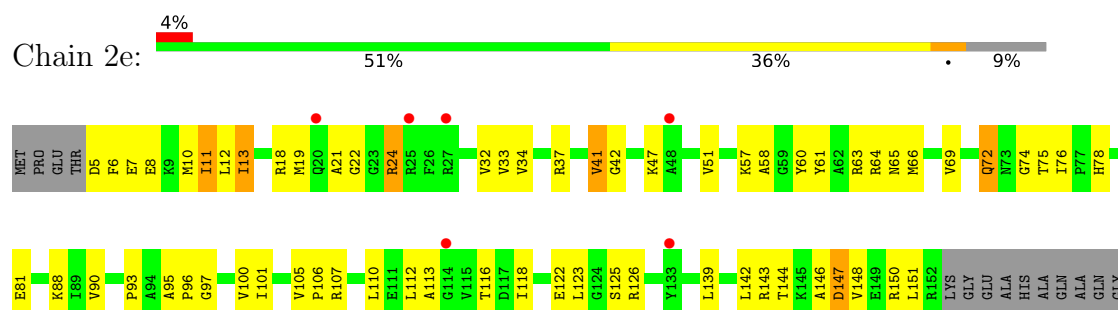
• Molecule 35: 30S ribosomal protein S4



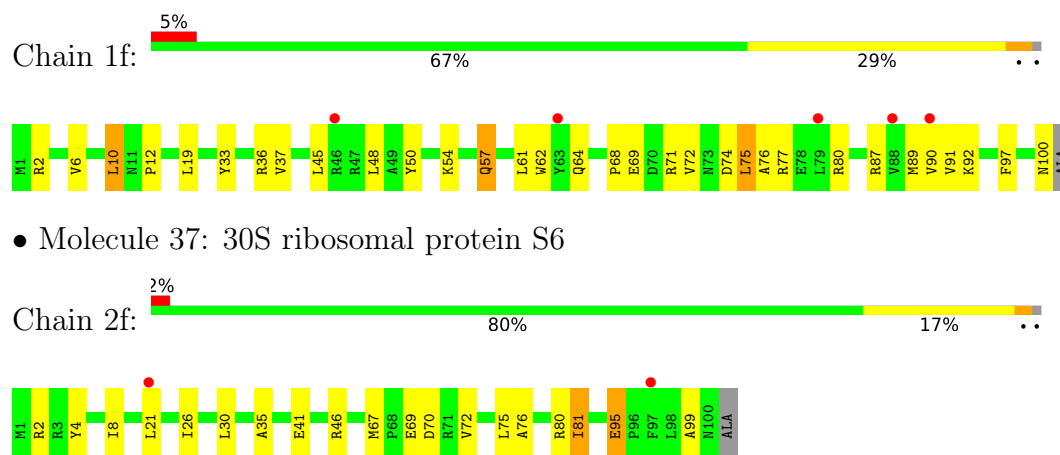
- Molecule 36: 30S ribosomal protein S5



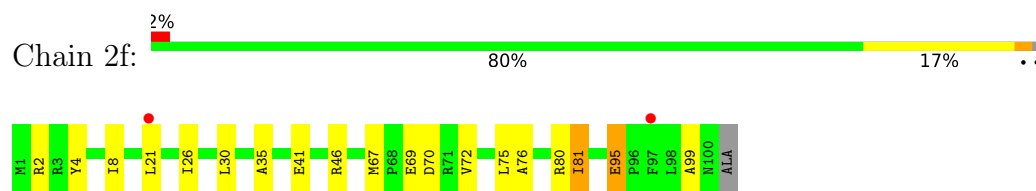
- Molecule 36: 30S ribosomal protein S5



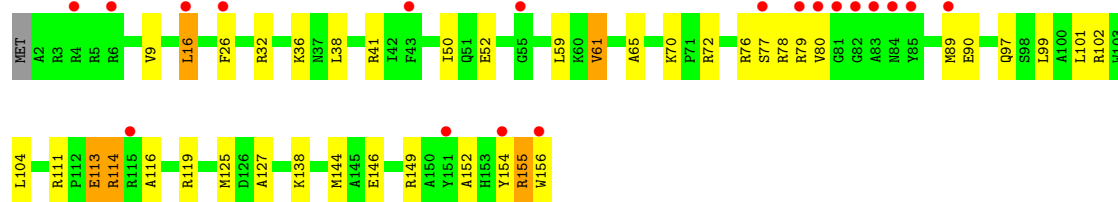
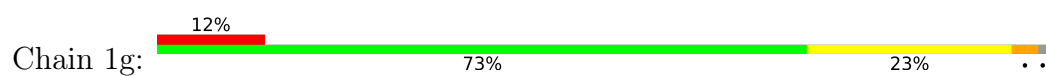
- Molecule 37: 30S ribosomal protein S6



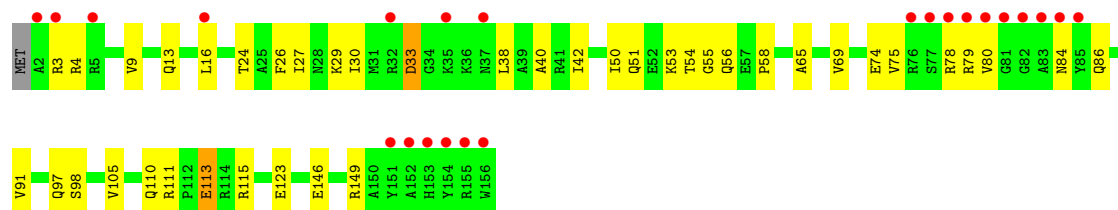
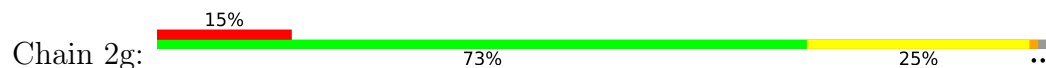
- Molecule 37: 30S ribosomal protein S6



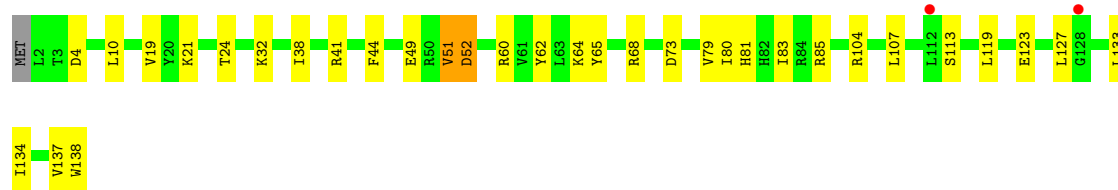
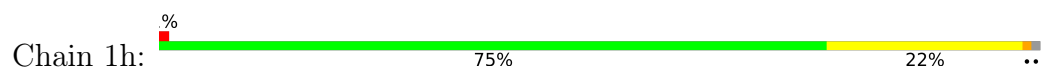
- Molecule 38: 30S ribosomal protein S7



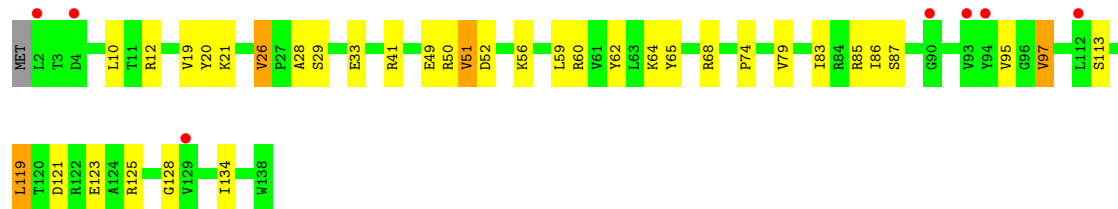
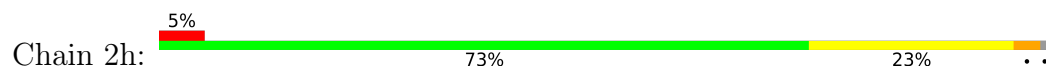
• Molecule 38: 30S ribosomal protein S7



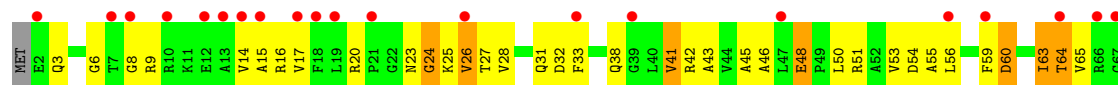
• Molecule 39: 30S ribosomal protein S8

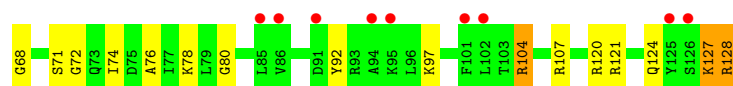


• Molecule 39: 30S ribosomal protein S8

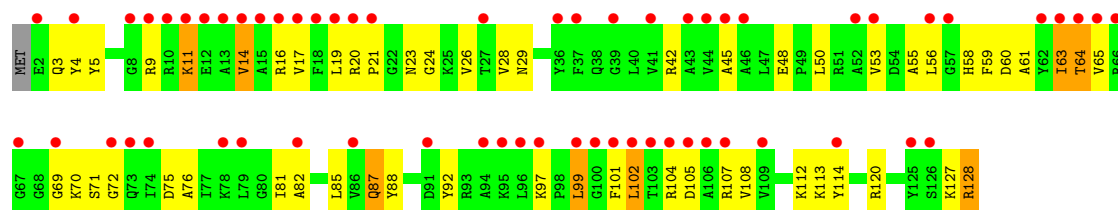


• Molecule 40: 30S ribosomal protein S9

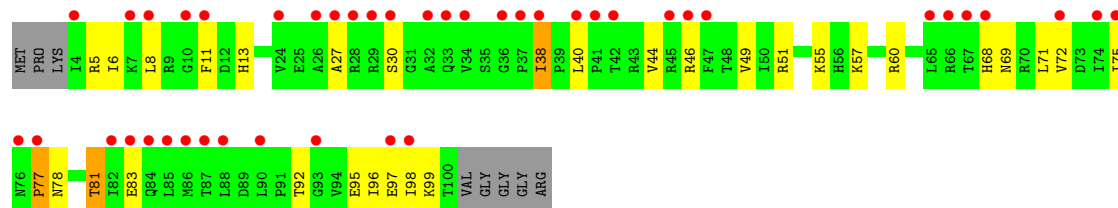
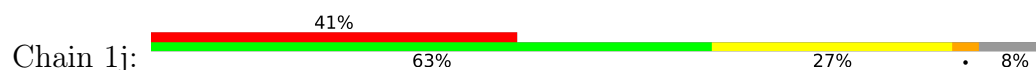




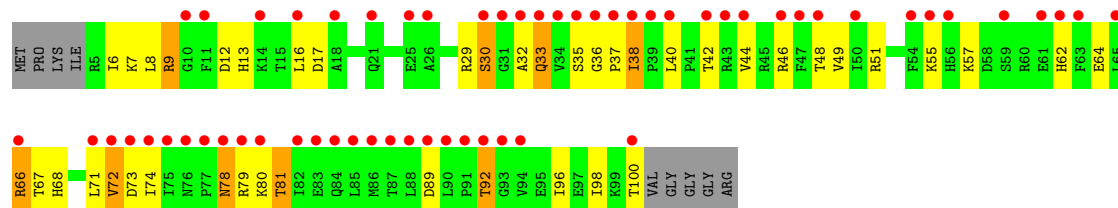
- Molecule 40: 30S ribosomal protein S9



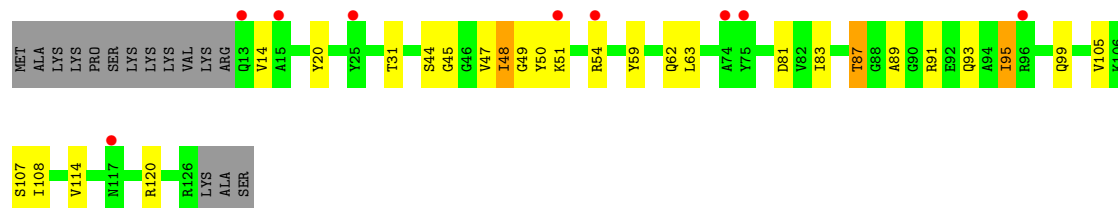
- Molecule 41: 30S ribosomal protein S10



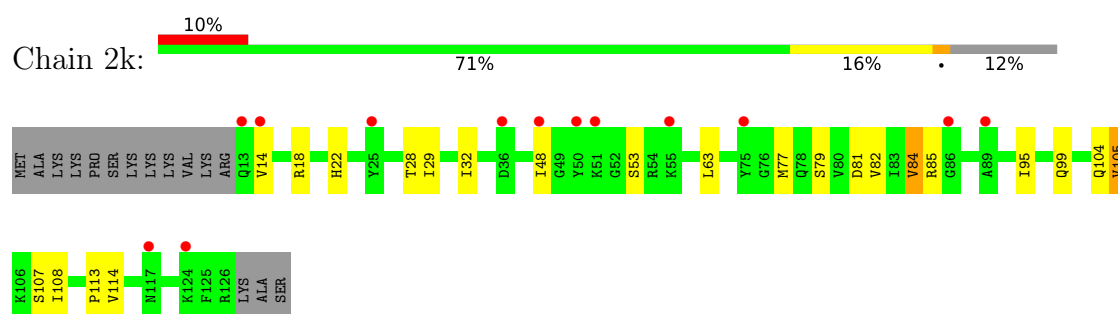
- Molecule 41: 30S ribosomal protein S10



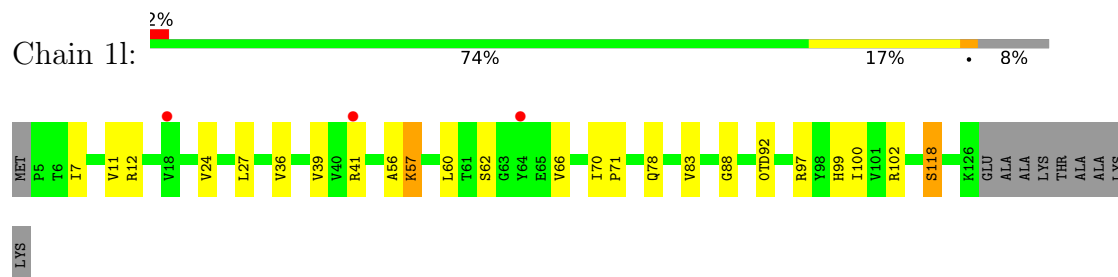
- Molecule 42: 30S ribosomal protein S11



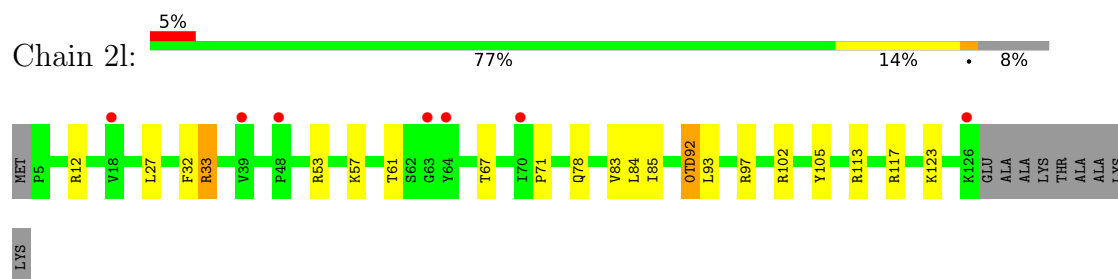
- Molecule 42: 30S ribosomal protein S11



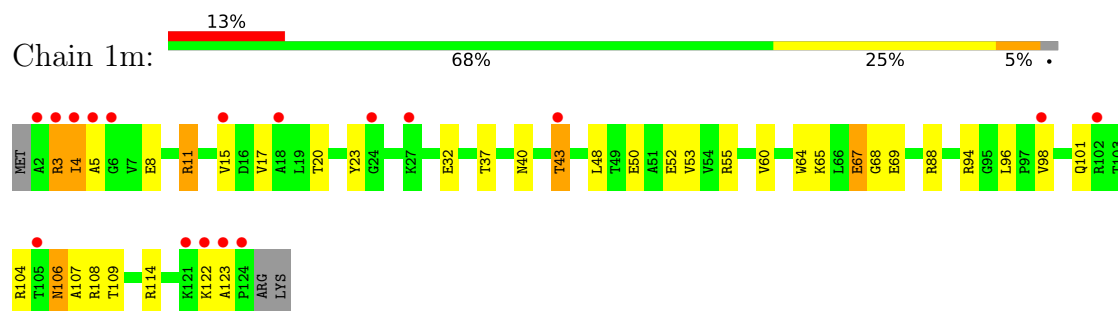
- Molecule 43: 30S ribosomal protein S12



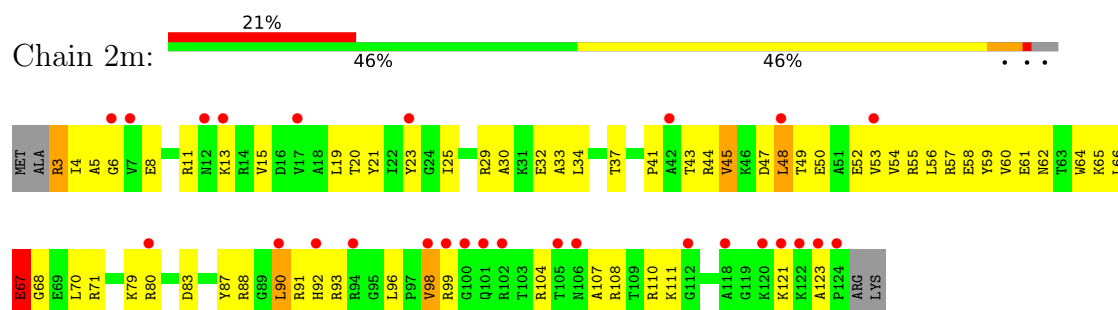
- Molecule 43: 30S ribosomal protein S12



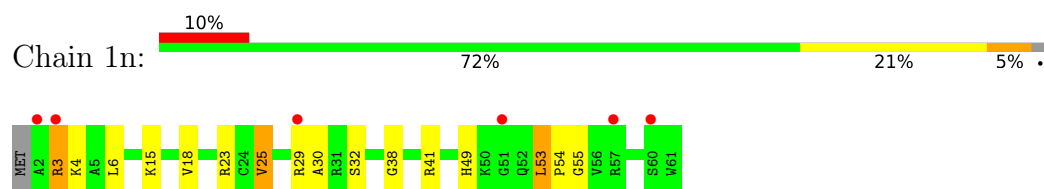
- Molecule 44: 30S ribosomal protein S13



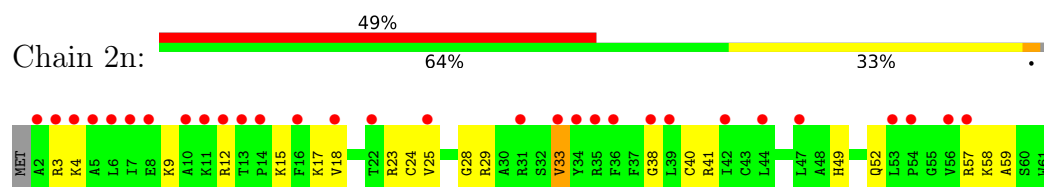
- Molecule 44: 30S ribosomal protein S13



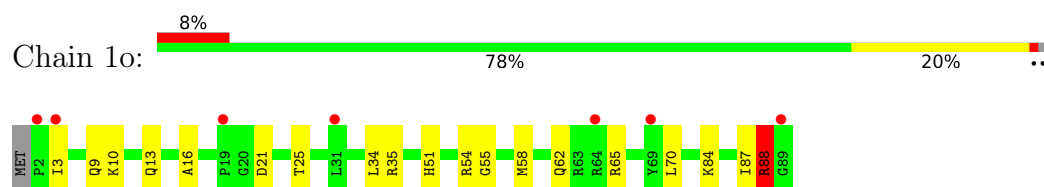
- Molecule 45: 30S ribosomal protein S14 type Z



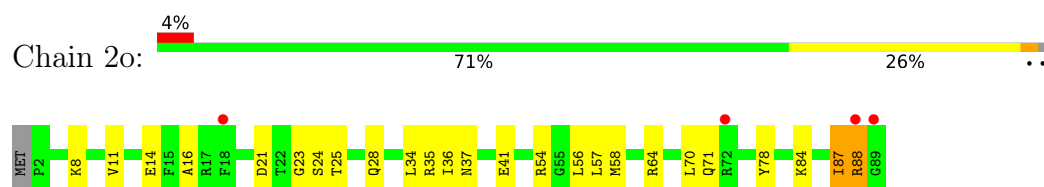
- Molecule 45: 30S ribosomal protein S14 type Z



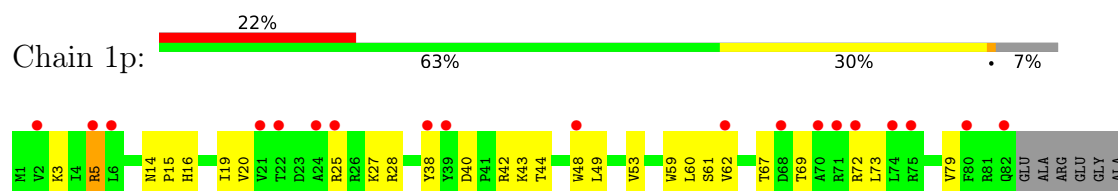
- Molecule 46: 30S ribosomal protein S15



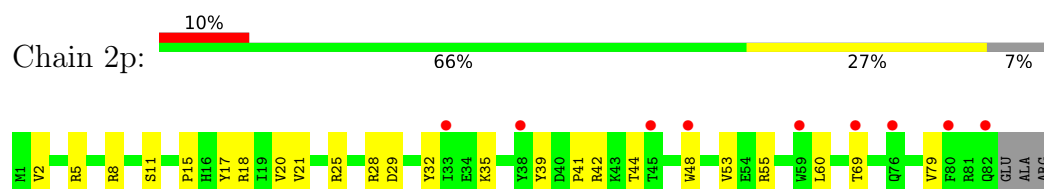
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

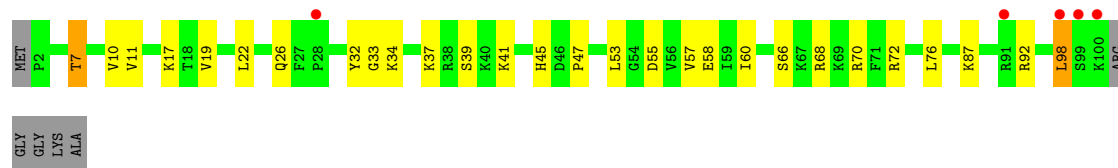


- Molecule 47: 30S ribosomal protein S16

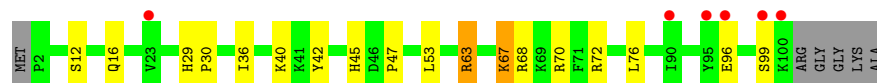
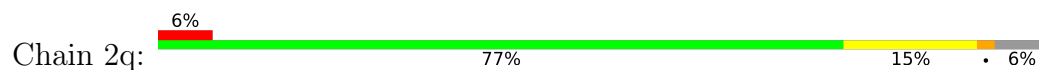


- Molecule 48: 30S ribosomal protein S17

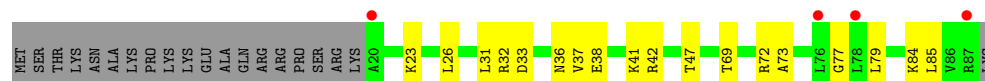




- Molecule 48: 30S ribosomal protein S17



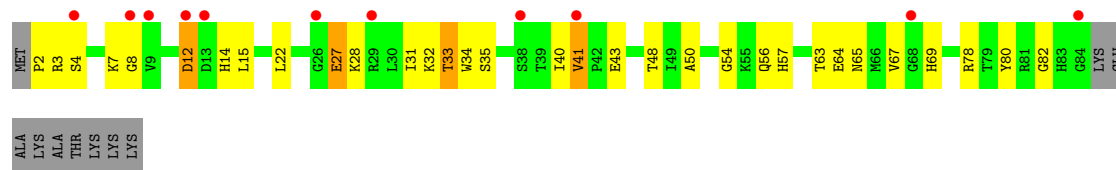
- Molecule 49: 30S ribosomal protein S18



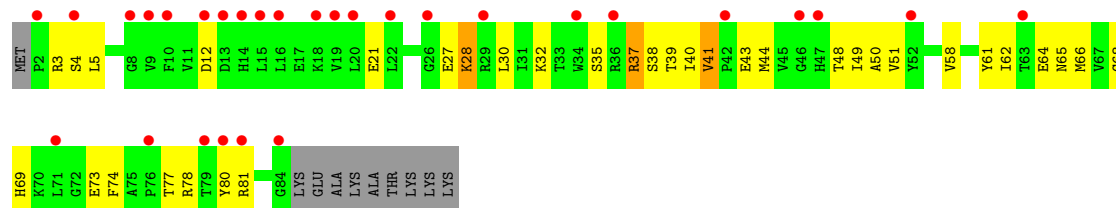
- Molecule 49: 30S ribosomal protein S18



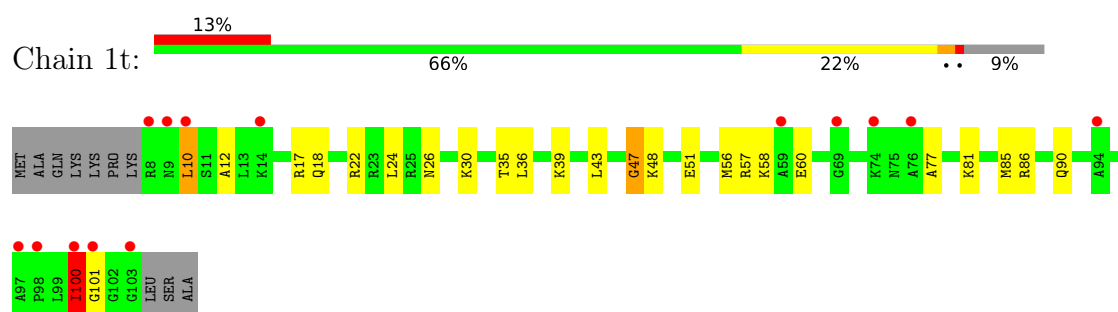
- Molecule 50: 30S ribosomal protein S19



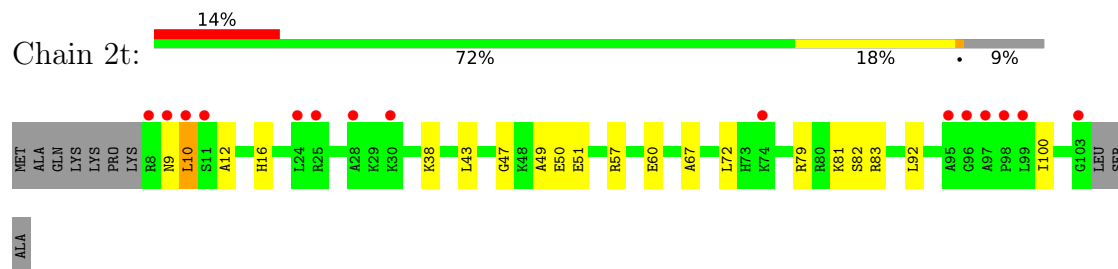
- Molecule 50: 30S ribosomal protein S19



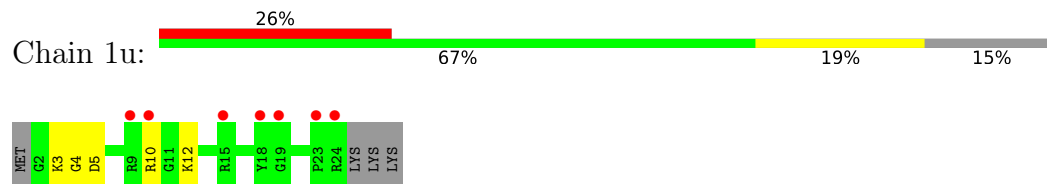
- Molecule 51: 30S ribosomal protein S20



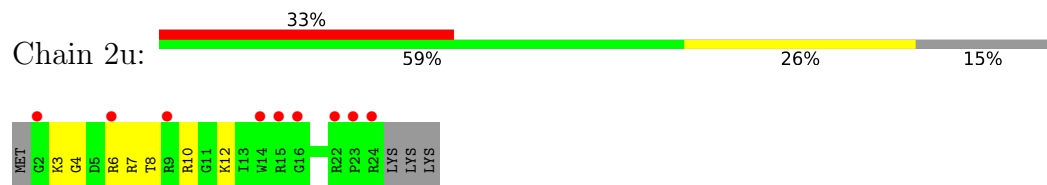
- Molecule 51: 30S ribosomal protein S20



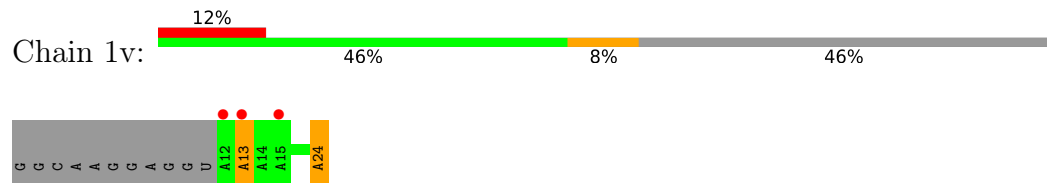
- Molecule 52: 30S ribosomal protein Thx



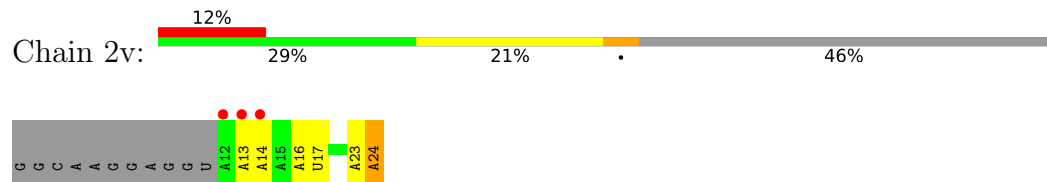
- Molecule 52: 30S ribosomal protein Thx



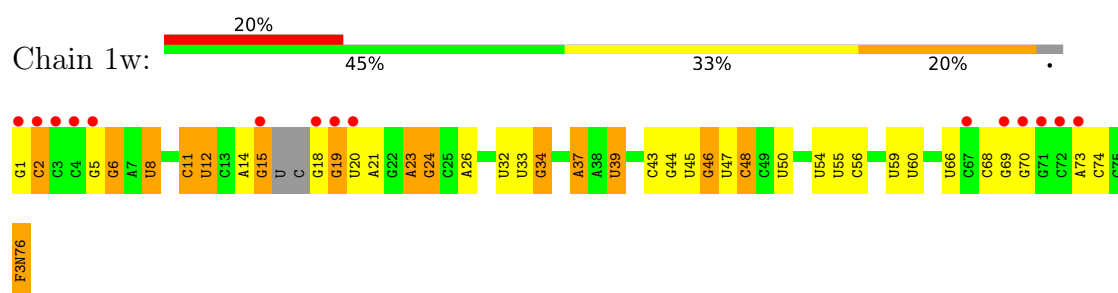
- Molecule 53: MF-mRNA



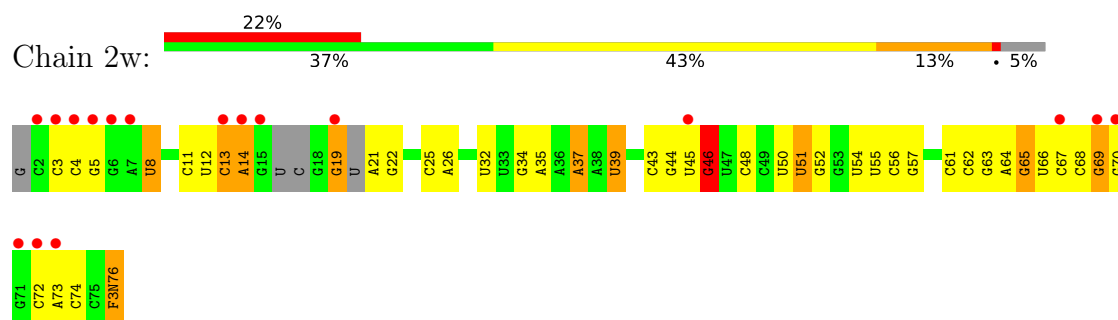
- Molecule 53: MF-mRNA



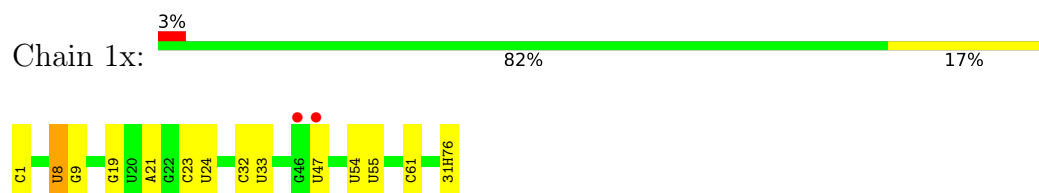
- Molecule 54: A-site Aminoacylated Phe-tRNAphe



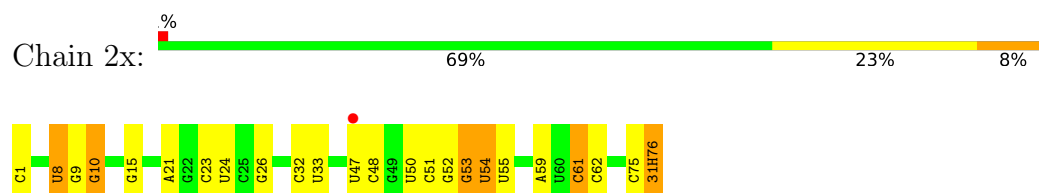
- Molecule 54: A-site Aminoacylated Phe-tRNAphe



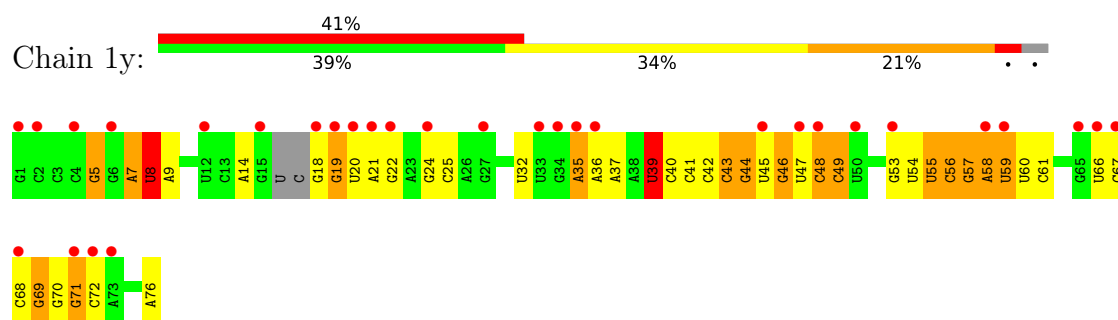
- Molecule 55: P-site Aminoacylated fMet-tRNAmet



- Molecule 55: P-site Aminoacylated fMet-tRNAmet

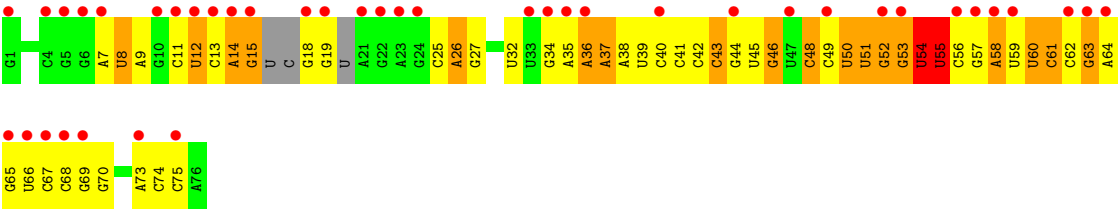


- Molecule 56: E-site Deacylated tRNAphe



- Molecule 56: E-site Deacylated tRNAphe





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.09Å 449.74Å 625.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.52 – 2.55 153.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (153.52-2.55) 99.1 (153.52-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.252 0.216 , 0.254	Depositor DCC
R_{free} test set	94286 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299618	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 1.55% 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: ZN, MG, MIA, 4SU, 5MU, SF4, 31H, UR3, F3N, 2MU, OMC, 2MG, 5MC, K, 4OC, 0TD, G7M, PSU, 8AH, OMG, MA6, M2G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.27	0/69010	0.46	2/107716 (0.0%)
1	2A	0.21	0/67294	0.40	3/105038 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.26	0/2186	0.51	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.49	0/2149
4	2E	0.19	0/1592	0.42	0/2149
5	1F	0.25	0/1618	0.50	0/2191
5	2F	0.20	0/1614	0.45	0/2186
6	1G	0.22	0/1448	0.45	0/1957
6	2G	0.19	0/1453	0.39	0/1963
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.19	0/1356	0.39	0/1834
8	1I	0.19	0/1112	0.44	0/1514
8	2I	0.19	0/1079	0.40	0/1475
9	1N	0.25	0/1144	0.48	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.19	0/943	0.42	0/1269
11	1P	0.24	0/1152	0.54	0/1533
11	2P	0.20	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.27	0/982	0.51	0/1312
13	2R	0.19	0/982	0.45	0/1312
14	1S	0.23	0/883	0.46	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.44	0/1477
15	2T	0.20	0/1097	0.42	0/1468
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.38	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.17	0/782	0.38	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.24	0/764	0.50	2/1025 (0.2%)
19	2X	0.22	0/764	0.48	2/1025 (0.2%)
20	1Y	0.23	0/819	0.50	0/1095
20	2Y	0.20	0/819	0.46	0/1095
21	1Z	0.22	0/1267	0.45	0/1717
21	2Z	0.23	0/1299	0.44	0/1763
22	10	0.25	0/662	0.50	0/881
22	20	0.18	0/662	0.41	0/881
23	11	0.25	0/762	0.46	0/1014
23	21	0.22	0/762	0.40	0/1014
24	12	0.30	0/590	0.50	0/781
24	22	0.19	0/590	0.36	0/781
25	13	0.27	0/474	0.47	0/635
25	23	0.18	0/469	0.41	0/630
26	14	0.24	0/565	0.56	0/761
26	24	0.25	0/545	0.54	0/737
27	15	0.27	0/469	0.46	0/635
27	25	0.20	0/469	0.40	0/635
28	16	0.26	0/460	0.47	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.31	0/426	0.51	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.24	0/525	0.45	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.29	0/310	0.52	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.19	1/35886 (0.0%)	0.38	3/56005 (0.0%)
33	1b	0.21	0/1881	0.47	0/2542
33	2b	0.21	0/1860	0.45	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.20	0/1566	0.40	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.44	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.19	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.17	0/1108	0.39	0/1494
40	1i	0.19	0/1002	0.48	0/1346
40	2i	0.20	0/997	0.49	0/1343
41	1j	0.20	0/722	0.40	0/982
41	2j	0.20	0/727	0.46	0/988
42	1k	0.18	0/844	0.41	0/1145
42	2k	0.18	0/848	0.41	0/1149
43	1l	0.21	0/937	0.40	0/1260
43	2l	0.18	0/937	0.39	0/1260
44	1m	0.19	0/969	0.51	0/1302
44	2m	0.20	0/961	0.45	0/1291
45	1n	0.19	0/501	0.43	0/664
45	2n	0.20	0/501	0.41	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.33	0/985
47	1p	0.21	0/697	0.52	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.20	0/836	0.47	0/1117
48	2q	0.18	0/836	0.42	0/1117
49	1r	0.20	0/560	0.38	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.20	0/667	0.50	0/900
50	2s	0.22	0/661	0.50	0/893
51	1t	0.20	0/730	0.47	0/965
51	2t	0.20	0/729	0.47	0/965
52	1u	0.18	0/203	0.43	0/266
52	2u	0.19	0/203	0.42	0/266
53	1v	0.23	0/310	0.40	0/480
53	2v	0.22	0/310	0.46	0/480
54	1w	0.29	1/1581 (0.1%)	0.41	0/2458
54	2w	0.30	1/1531 (0.1%)	0.39	0/2379
55	1x	0.27	1/1723 (0.1%)	0.42	0/2684
55	2x	0.25	0/1723	0.38	0/2684
56	1y	0.31	2/1606 (0.1%)	0.38	0/2497
56	2y	0.31	1/1583 (0.1%)	0.40	0/2459
All	All	0.23	7/316632 (0.0%)	0.42	12/474029 (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
21	1Z	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	5.64	1.61	1.56
54	2w	46	G7M	O3'-P	5.55	1.61	1.56
56	1y	46	G7M	O3'-P	5.46	1.61	1.56
56	2y	46	G7M	O3'-P	5.31	1.61	1.56
55	1x	8	4SU	O3'-P	5.22	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.63	119.45	109.50
32	2a	1272	G	N1-C2-N2	-6.41	96.97	116.20
32	2a	1263	C	N1-C2-O2	5.80	136.31	118.90
32	2a	1272	G	N3-C2-N2	5.75	137.14	119.90
1	2A	271(M)	G	P-O3'-C3'	5.32	126.08	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	136	PHE	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	61853	0	31183	477	0
1	2A	60323	0	30412	625	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	28	0
3	1D	2136	0	2218	35	0
3	2D	2136	0	2218	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	37	0
5	1F	1583	0	1625	31	0
5	2F	1579	0	1619	44	0
6	1G	1423	0	1436	34	0
6	2G	1428	0	1438	40	0
7	1H	1330	0	1407	27	0
7	2H	1330	0	1407	39	0
8	1I	1097	0	1140	31	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	17	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	22	0
11	2P	1135	0	1212	22	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	34	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	14	0
14	2S	870	0	923	33	0
15	1T	1091	0	1151	15	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	10	0
17	1V	771	0	830	10	0
17	2V	771	0	830	13	0
18	1W	886	0	940	5	0
18	2W	886	0	940	16	0
19	1X	750	0	814	11	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	14	0
21	1Z	1240	0	1240	35	0
21	2Z	1271	0	1273	63	0
22	10	653	0	674	9	0
22	20	653	0	674	9	0
23	11	755	0	826	6	0
23	21	755	0	826	12	0
24	12	588	0	643	7	0
24	22	588	0	643	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	5	0
25	23	464	0	514	10	0
26	14	552	0	533	25	0
26	24	532	0	503	27	0
27	15	455	0	465	4	0
27	25	455	0	465	6	0
28	16	453	0	473	7	0
28	26	449	0	469	8	0
29	17	418	0	467	5	0
29	27	418	0	467	8	0
30	18	517	0	582	11	0
30	28	517	0	582	9	0
31	19	307	0	335	4	0
31	29	307	0	335	9	0
32	1a	32246	0	16295	373	0
32	2a	32327	0	16338	376	0
33	1b	1846	0	1867	65	0
33	2b	1825	0	1828	64	0
34	1c	1548	0	1535	32	0
34	2c	1542	0	1517	37	0
35	1d	1655	0	1672	43	0
35	2d	1674	0	1714	40	0
36	1e	1129	0	1185	33	0
36	2e	1133	0	1191	42	0
37	1f	810	0	804	16	0
37	2f	816	0	808	13	0
38	1g	1231	0	1238	27	0
38	2g	1235	0	1249	20	0
39	1h	1088	0	1126	18	0
39	2h	1088	0	1126	21	0
40	1i	983	0	986	36	0
40	2i	978	0	966	40	0
41	1j	709	0	650	19	0
41	2j	714	0	672	30	0
42	1k	829	0	825	17	0
42	2k	833	0	836	9	0
43	1l	932	0	981	13	0
43	2l	932	0	981	14	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	48	0
45	1n	492	0	529	12	0
45	2n	492	0	529	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	13	0
46	2o	728	0	760	14	0
47	1p	681	0	697	18	0
47	2p	677	0	686	16	0
48	1q	823	0	891	17	0
48	2q	823	0	891	10	0
49	1r	555	0	618	11	0
49	2r	555	0	618	10	0
50	1s	652	0	662	24	0
50	2s	646	0	644	25	0
51	1t	728	0	798	21	0
51	2t	727	0	796	13	0
52	1u	199	0	208	5	0
52	2u	199	0	208	7	0
53	1v	277	0	140	2	0
53	2v	277	0	140	3	0
54	1w	1603	0	828	21	0
54	2w	1555	0	797	20	0
55	1x	1656	0	849	7	0
55	2x	1656	0	849	16	0
56	1y	1585	0	803	26	0
56	2y	1565	0	794	34	0
57	10	7	0	0	0	0
57	11	6	0	0	0	0
57	12	2	0	0	0	0
57	13	3	0	0	0	0
57	14	1	0	0	0	0
57	15	8	0	0	0	0
57	16	2	0	0	0	0
57	17	6	0	0	0	0
57	18	5	0	0	0	0
57	19	1	0	0	0	0
57	1A	1113	0	0	0	0
57	1B	38	0	0	0	0
57	1D	12	0	0	0	0
57	1E	14	0	0	0	0
57	1F	13	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	4	0	0	0	0
57	1P	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1Q	7	0	0	0	0
57	1R	6	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	6	0	0	0	0
57	1V	7	0	0	0	0
57	1W	6	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	220	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1p	1	0	0	0	0
57	1q	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	9	0	0	0	0
57	1x	14	0	0	0	0
57	20	2	0	0	0	0
57	21	3	0	0	0	0
57	23	2	0	0	0	0
57	25	3	0	0	0	0
57	27	2	0	0	0	0
57	28	2	0	0	0	0
57	2A	804	0	0	0	0
57	2B	16	0	0	0	0
57	2D	6	0	0	0	0
57	2E	7	0	0	0	0
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	2	0	0	0	0
57	2T	3	0	0	0	0
57	2U	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2V	1	0	0	0	0
57	2W	3	0	0	0	0
57	2X	2	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	2	0	0	0	0
57	2w	6	0	0	0	0
57	2x	7	0	0	0	0
57	2y	7	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	12	0	0	1	0
61	11	7	0	0	0	0
61	12	4	0	0	0	0
61	13	4	0	0	0	0
61	14	1	0	0	0	0
61	15	10	0	0	0	0
61	16	5	0	0	0	0
61	17	10	0	0	1	0
61	18	10	0	0	0	0
61	1A	2067	0	0	62	0
61	1B	61	0	0	2	0
61	1D	32	0	0	1	0
61	1E	26	0	0	1	0
61	1F	20	0	0	1	0
61	1G	1	0	0	0	0
61	1H	2	0	0	0	0
61	1N	6	0	0	0	0
61	1O	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1P	21	0	0	2	0
61	1Q	7	0	0	0	0
61	1R	7	0	0	1	0
61	1S	5	0	0	1	0
61	1T	9	0	0	0	0
61	1U	14	0	0	1	0
61	1V	7	0	0	0	0
61	1W	6	0	0	1	0
61	1X	5	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	1	0
61	1a	425	0	0	25	0
61	1b	1	0	0	0	0
61	1f	1	0	0	0	0
61	1i	1	0	0	0	0
61	1l	8	0	0	0	0
61	1m	2	0	0	1	0
61	1n	1	0	0	0	0
61	1o	3	0	0	0	0
61	1p	1	0	0	0	0
61	1q	2	0	0	0	0
61	1r	2	0	0	0	0
61	1u	2	0	0	1	0
61	1v	4	0	0	0	0
61	1w	12	0	0	1	0
61	1x	17	0	0	0	0
61	1y	1	0	0	0	0
61	20	1	0	0	0	0
61	21	6	0	0	0	0
61	23	2	0	0	0	0
61	27	5	0	0	0	0
61	28	4	0	0	1	0
61	29	1	0	0	0	0
61	2A	1094	0	0	79	0
61	2B	18	0	0	0	0
61	2D	22	0	0	0	0
61	2E	9	0	0	0	0
61	2F	11	0	0	0	0
61	2I	3	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2Q	1	0	0	0	0
61	2R	1	0	0	0	0
61	2T	5	0	0	0	0
61	2U	3	0	0	0	0
61	2W	3	0	0	0	0
61	2X	2	0	0	0	0
61	2w	1	0	0	0	0
61	2x	6	0	0	1	0
61	2y	2	0	0	0	0
All	All	299618	0	196724	3553	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3553 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	1.19	1.40
1:1A:1082:U:N3	1:1A:1086:A:N6	2.05	1.05
1:1A:1082:U:O4	1:1A:1086:A:N1	1.94	1.00
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.50	0.93
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.53	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	34
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24	34
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	24	34
5	2F	200/210 (95%)	188 (94%)	11 (6%)	1 (0%)	24	34
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	29
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	7	8
7	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	21	29
7	2H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	21	29
8	1I	144/148 (97%)	128 (89%)	16 (11%)	0	100	100
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	9	11
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	18	25
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	22
11	1P	147/150 (98%)	132 (90%)	10 (7%)	5 (3%)	3	1
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	3
12	1Q	139/141 (99%)	134 (96%)	3 (2%)	2 (1%)	9	11
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	25
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	20
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	3	2
17	2V	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	12	17
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	15
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12	17
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6	7
21	1Z	148/206 (72%)	132 (89%)	14 (10%)	2 (1%)	9	11
21	2Z	156/206 (76%)	124 (80%)	25 (16%)	7 (4%)	2	1
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	15
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	54 (81%)	6 (9%)	7 (10%)	0	0
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	197 (86%)	26 (11%)	6 (3%)	4	3
33	2b	229/256 (90%)	185 (81%)	37 (16%)	7 (3%)	3	2
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	24	34
34	2c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	24	34
35	1d	206/209 (99%)	193 (94%)	9 (4%)	4 (2%)	6	7
35	2d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	1e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	9	11
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	11
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	18	25
38	2g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	18	25
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	18	25
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	12 (10%)	3 (2%)	4	4
40	2i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	22
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5	5
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	3	2
42	1k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	14	20
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	20
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	108 (89%)	10 (8%)	3 (2%)	4	4
44	2m	120/126 (95%)	109 (91%)	9 (8%)	2 (2%)	7	8
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	13
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	6 (6%)	2 (2%)	5	5
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	5	5
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10	13
50	2s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11368/12128 (94%)	10523 (93%)	737 (6%)	108 (1%)	12	17

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	29	LYS
11	1P	38	GLN
11	1P	44	GLY
17	1V	79	VAL

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	40
3	2D	215/218 (99%)	203 (94%)	12 (6%)	19	29
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	21
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	29
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	7
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	10
6	1G	143/156 (92%)	128 (90%)	15 (10%)	6	8
6	2G	143/156 (92%)	131 (92%)	12 (8%)	10	14
7	1H	144/148 (97%)	132 (92%)	12 (8%)	10	14
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	6
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	2
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10	13
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14	20
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	80
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14	19
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17	25
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	16
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39	58
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	38
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22	33
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	42
14	1S	86/88 (98%)	81 (94%)	5 (6%)	18	27
14	2S	85/88 (97%)	80 (94%)	5 (6%)	18	27
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	32
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	15
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	39
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	30
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	60
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12	17
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	38
18	2W	90/92 (98%)	87 (97%)	3 (3%)	33	50
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	32
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	59
20	1Y	85/91 (93%)	73 (86%)	12 (14%)	3	3
20	2Y	85/91 (93%)	75 (88%)	10 (12%)	5	5
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	15
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	3	2
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	53
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	53
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	60
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	17
24	12	65/67 (97%)	64 (98%)	1 (2%)	57	74
24	22	65/67 (97%)	63 (97%)	2 (3%)	35	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	5
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	5
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	3
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	2
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	42
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	42
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	5
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	26
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	9
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	4
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	45
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	29
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	55
33	1b	192/220 (87%)	170 (88%)	22 (12%)	5	6
33	2b	187/220 (85%)	148 (79%)	39 (21%)	1	1
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	7
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	7
35	1d	169/181 (93%)	159 (94%)	10 (6%)	18	27
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4	4
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	24
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14	19
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	7
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	36
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	5
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	7
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17	25
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	16
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3	2
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	6
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	2j	69/92 (75%)	57 (83%)	12 (17%)	2	1
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17	25
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	18
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	14
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	40
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	7
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	5
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	4
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	59
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	23
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	18
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18	27
48	1q	94/97 (97%)	88 (94%)	6 (6%)	16	23
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	31
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	20
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	33
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	13
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	11
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26	39
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8569 (92%)	734 (8%)	11	16

5 of 734 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	2T	72	VAL
33	2b	107	THR
17	2V	61	VAL
15	2T	63	VAL
23	2I	78	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	148	ASN
41	2j	33	GLN
51	2t	9	ASN
42	1k	116	HIS
42	1k	99	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	416 (14%)	31 (1%)
1	2A	2791/2915 (95%)	458 (16%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	20 (16%)	0
32	1a	1497/1521 (98%)	223 (14%)	0
32	2a	1501/1521 (98%)	255 (16%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	2w	68/76 (89%)	24 (35%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	72/76 (94%)	28 (38%)	0
56	2y	70/76 (92%)	30 (42%)	0
All	All	9345/9620 (97%)	1501 (16%)	56 (0%)

5 of 1501 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	55	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2611	U
1	2A	2689	U
1	2A	266	G

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Mol	Chain	Res	Type
1	2A	2126	A
1	2A	1530	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	1a	1402	32	20,23,24	0.79	0	25,32,35	0.86	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	2.23	3 (14%)
55	5MC	1x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.21	3 (11%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	4.99	3 (50%)
54	PSU	2w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.94	3 (14%)
56	5MU	2y	54	56	19,22,23	1.41	4 (21%)	27,32,35	2.21	6 (22%)
56	PSU	1y	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.78	3 (14%)
55	31H	1x	76	57,55	31,34,35	1.17	3 (9%)	35,47,50	2.17	14 (40%)
56	MIA	1y	37	56	21,24,32	1.64	3 (14%)	30,35,47	2.00	7 (23%)
32	UR3	1a	1498	32	19,22,23	0.93	1 (5%)	26,32,35	1.78	3 (11%)
32	5MC	2a	967	32	19,22,23	1.65	3 (15%)	26,32,35	1.12	2 (7%)
54	5MU	1w	54	54	19,22,23	1.50	5 (26%)	27,32,35	1.72	5 (18%)
1	2MU	1A	2552	1	19,22,24	1.20	2 (10%)	25,31,36	2.00	6 (24%)
1	OMC	1A	1920	1	19,22,23	0.77	0	25,31,34	0.98	1 (4%)
55	5MU	2x	54	55	19,22,23	1.44	6 (31%)	27,32,35	1.92	7 (25%)
1	5MU	2A	1915	1	19,22,23	1.43	6 (31%)	27,32,35	2.34	7 (25%)
55	31H	2x	76	57,55	31,34,35	1.23	3 (9%)	35,47,50	2.15	12 (34%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	6.01	2 (33%)
56	G7M	1y	46	56	23,26,27	1.55	4 (17%)	34,39,42	1.78	4 (11%)
1	5MC	2A	1962	1,57	19,22,23	1.52	3 (15%)	26,32,35	1.17	2 (7%)
1	5MU	2A	1939	1,57	19,22,23	1.44	6 (31%)	27,32,35	2.19	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.89	3 (14%)
54	PSU	1w	39	54	18,21,22	1.43	3 (16%)	21,30,33	1.56	3 (14%)
56	PSU	2y	55	56	18,21,22	1.37	3 (16%)	21,30,33	2.01	5 (23%)
1	PSU	1A	2605	1,57	18,21,22	1.42	2 (11%)	21,30,33	2.25	3 (14%)
56	5MU	1y	54	56	19,22,23	1.42	4 (21%)	27,32,35	2.09	6 (22%)
1	8AH	1A	2503	1,57	22,26,27	1.47	5 (22%)	29,39,42	2.16	7 (24%)
54	F3N	2w	76	54,1	33,36,37	1.49	4 (12%)	41,51,54	1.73	9 (21%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
32	5MC	2a	1407	32,57	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
1	5MC	1A	1942	1,57	19,22,23	1.60	3 (15%)	26,32,35	1.21	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	1 (5%)	25,31,34	1.02	1 (4%)
56	PSU	2y	32	56	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
32	2MG	1a	1207	32,57	23,26,27	1.24	2 (8%)	33,38,41	2.22	8 (24%)
55	4SU	1x	8	55	18,21,22	2.37	6 (33%)	25,30,33	1.92	7 (28%)
32	MA6	2a	1519	32	23,26,27	0.48	0	33,38,41	2.10	9 (27%)
54	MIA	1w	37	54	28,31,32	2.30	7 (25%)	38,44,47	2.94	14 (36%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.06	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.58	3 (15%)	26,32,35	1.13	3 (11%)
1	5MU	1A	1939	1,57	19,22,23	1.47	6 (31%)	27,32,35	2.16	6 (22%)
54	MIA	2w	37	54	24,27,32	2.14	5 (20%)	32,39,47	2.51	11 (34%)
32	5MC	1a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.15	2 (7%)
32	G7M	2a	527	32	23,26,27	1.49	4 (17%)	34,39,42	1.67	5 (14%)
32	5MC	1a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.08	2 (7%)
32	G7M	1a	527	32	23,26,27	1.48	3 (13%)	34,39,42	1.70	5 (14%)
56	4SU	2y	8	56	18,21,22	1.82	5 (27%)	25,30,33	1.80	4 (16%)
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	27,32,35	1.81	7 (25%)
56	PSU	1y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	21,30,33	2.15	4 (19%)
55	4SU	2x	8	55	18,21,22	2.07	6 (33%)	25,30,33	1.25	4 (16%)
56	PSU	2y	39	56	18,21,22	1.40	2 (11%)	21,30,33	1.74	4 (19%)
54	F3N	1w	76	54,1	33,36,37	1.49	4 (12%)	41,51,54	1.85	9 (21%)
1	PSU	2A	2605	1	18,21,22	1.24	2 (11%)	21,30,33	2.07	3 (14%)
56	G7M	2y	46	56	23,26,27	1.59	3 (13%)	34,39,42	1.79	4 (11%)
1	OMG	2A	2251	1,55	23,26,27	1.19	3 (13%)	32,38,41	2.04	6 (18%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	1.98	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MC	2x	32	55	19,22,23	1.57	3 (15%)	26,32,35	1.24	4 (15%)
1	8AH	2A	2503	1,57	22,26,27	1.66	5 (22%)	29,39,42	2.24	5 (17%)
1	PSU	1A	1911	1	18,21,22	1.42	2 (11%)	21,30,33	1.98	3 (14%)
54	G7M	1w	46	54	23,26,27	1.57	4 (17%)	34,39,42	1.65	4 (11%)
55	5MU	1x	54	57,55	19,22,23	1.45	5 (26%)	27,32,35	1.92	7 (25%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.16	2 (7%)
54	PSU	1w	32	54,57	18,21,22	1.33	2 (11%)	21,30,33	1.99	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.79	0	25,32,35	1.00	1 (4%)
54	G7M	2w	46	54	23,26,27	1.52	4 (17%)	34,39,42	1.61	4 (11%)
32	MA6	1a	1519	32	23,26,27	0.47	0	33,38,41	2.14	9 (27%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	21,30,33	1.92	4 (19%)
54	4SU	2w	8	54	18,21,22	1.83	5 (27%)	25,30,33	2.43	5 (20%)
56	PSU	1y	55	56	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
1	5MC	1A	1962	1,57	19,22,23	1.90	3 (15%)	26,32,35	1.24	4 (15%)
32	2MG	2a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.23	8 (24%)
56	4SU	1y	8	56	18,21,22	1.78	5 (27%)	25,30,33	1.71	4 (16%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.12	3 (11%)
54	4SU	1w	8	54	18,21,22	1.88	5 (27%)	25,30,33	2.14	5 (20%)
1	OMG	1A	2251	1,55,57	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)
32	MA6	1a	1518	32	23,26,27	0.44	0	33,38,41	1.95	10 (30%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.72	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.16	2 (7%)
32	M2G	2a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.88	6 (18%)
1	2MU	2A	2552	1,57	19,22,24	1.20	2 (10%)	25,31,36	1.84	6 (24%)
32	M2G	1a	966	32	24,27,28	1.31	3 (12%)	33,40,43	1.84	6 (18%)
55	PSU	1x	55	57,55	18,21,22	1.30	2 (11%)	21,30,33	1.99	4 (19%)
56	MIA	2y	37	56	21,24,32	1.59	4 (19%)	30,35,47	2.00	7 (23%)
32	PSU	2a	516	32	18,21,22	1.30	2 (11%)	21,30,33	2.05	4 (19%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.95	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.65	2 (10%)	26,32,35	1.11	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.38	4 (21%)	27,32,35	2.18	7 (25%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.95	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	5/7/12/14	-
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
55	31H	1x	76	57,55	-	4/22/40/41	0/3/3/3
56	MIA	1y	37	56	-	0/7/25/34	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1	-	0/9/27/28	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	57,55	-	4/22/40/41	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
56	G7M	1y	46	56	-	3/7/25/26	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	5/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	1/7/25/26	0/2/2/2
1	8AH	1A	2503	1,57	-	1/7/25/26	0/3/3/3
54	F3N	2w	76	54,1	-	0/19/37/38	0/4/4/4
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,57	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,57	-	1/9/27/28	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	1,57	-	0/7/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
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
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	2MU	2A	2552	1,57	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	PSU	1x	55	57,55	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	2/7/25/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

The worst 5 of 262 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.29	1.69	1.82
43	1l	92	0TD	CB-SB	-12.24	1.69	1.82
1	1A	1962	5MC	C5-C4	7.33	1.49	1.44
54	1w	37	MIA	C2-S10	-7.16	1.69	1.75
54	2w	37	MIA	C2-S10	-6.92	1.70	1.75

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-14.25	76.74	102.36
43	2l	92	0TD	CSB-SB-CB	-11.44	81.80	102.36
54	1w	37	MIA	C12-C13-C14	-10.07	108.93	127.01
54	2w	37	MIA	C5-C4-N3	-8.70	118.01	127.18
1	2A	2503	8AH	C5-C4-N3	-8.65	118.07	127.18

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N6-C12-C13-C14

There are no ring outliers.

38 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1402	4OC	1	0
43	2l	92	0TD	1	0
56	2y	54	5MU	1	0
56	1y	39	PSU	1	0
32	2a	967	5MC	1	0
1	1A	2552	2MU	1	0
55	2x	54	5MU	2	0
1	2A	1915	5MU	1	0
55	2x	76	31H	2	0
1	2A	1939	5MU	1	0
54	1w	39	PSU	1	0
56	2y	55	PSU	6	0
54	2w	76	F3N	3	0
54	2w	39	PSU	1	0
55	1x	8	4SU	1	0
32	2a	1519	MA6	1	0
54	1w	37	MIA	2	0
1	1A	1939	5MU	1	0
54	2w	37	MIA	1	0
56	2y	8	4SU	1	0
1	1A	1917	PSU	1	0
55	2x	8	4SU	1	0
54	1w	76	F3N	1	0
56	2y	46	G7M	2	0
1	2A	2251	OMG	1	0
32	2a	1518	MA6	2	0
54	2w	46	G7M	1	0
32	1a	1519	MA6	1	0
54	2w	8	4SU	1	0
56	1y	55	PSU	2	0
56	1y	8	4SU	2	0
54	1w	8	4SU	2	0
32	1a	1518	MA6	2	0
1	2A	2552	2MU	2	0
32	1a	966	M2G	2	0
56	2y	37	MIA	2	0
32	1a	516	PSU	1	0
1	2A	1917	PSU	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2472 ligands modelled in this entry, 2470 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	2d	501	35	0,12,12	-	-	-		
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.35	189 (6%) 24 24	22, 39, 97, 108	0
1	2A	2789/2915 (95%)	0.15	156 (5%) 30 29	38, 59, 96, 109	0
2	1B	120/121 (99%)	-0.23	0 100 100	34, 53, 65, 87	0
2	2B	120/121 (99%)	0.46	3 (2%) 58 59	62, 73, 84, 97	0
3	1D	275/276 (99%)	0.02	3 (1%) 78 79	24, 39, 53, 84	0
3	2D	275/276 (99%)	0.23	3 (1%) 78 79	34, 50, 62, 78	0
4	1E	204/206 (99%)	-0.08	1 (0%) 87 89	21, 41, 60, 73	0
4	2E	204/206 (99%)	0.83	5 (2%) 58 59	41, 64, 76, 83	0
5	1F	202/210 (96%)	0.08	4 (1%) 65 65	21, 44, 68, 82	0
5	2F	202/210 (96%)	0.58	6 (2%) 52 54	38, 64, 78, 85	0
6	1G	181/182 (99%)	0.59	9 (4%) 34 33	46, 58, 72, 86	0
6	2G	181/182 (99%)	1.14	19 (10%) 11 11	63, 74, 82, 88	0
7	1H	174/180 (96%)	0.39	4 (2%) 61 62	39, 54, 67, 72	0
7	2H	174/180 (96%)	2.03	88 (50%) 0 0	73, 86, 92, 97	0
8	1I	146/148 (98%)	0.97	9 (6%) 26 26	51, 73, 80, 84	0
8	2I	146/148 (98%)	1.23	22 (15%) 5 5	52, 73, 84, 91	0
9	1N	140/140 (100%)	-0.07	1 (0%) 84 86	26, 38, 59, 75	0
9	2N	140/140 (100%)	1.10	9 (6%) 25 24	51, 69, 80, 84	0
10	1O	122/122 (100%)	0.02	1 (0%) 82 84	30, 42, 59, 62	0
10	2O	122/122 (100%)	0.81	1 (0%) 82 84	50, 63, 73, 78	0
11	1P	149/150 (99%)	0.30	4 (2%) 56 57	24, 52, 69, 77	0
11	2P	149/150 (99%)	0.72	5 (3%) 48 49	42, 64, 79, 88	0
12	1Q	141/141 (100%)	0.08	1 (0%) 84 86	26, 42, 57, 71	0
12	2Q	141/141 (100%)	1.15	15 (10%) 11 11	46, 68, 78, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.18	0 100 100	28, 37, 51, 57	0
13	2R	118/118 (100%)	0.64	2 (1%) 69 69	48, 58, 66, 76	0
14	1S	110/112 (98%)	0.26	1 (0%) 81 83	40, 53, 64, 69	0
14	2S	110/112 (98%)	0.86	4 (3%) 46 47	59, 70, 78, 84	0
15	1T	131/146 (89%)	0.37	5 (3%) 44 45	37, 46, 72, 84	0
15	2T	131/146 (89%)	1.02	12 (9%) 14 14	56, 66, 81, 84	0
16	1U	116/118 (98%)	-0.30	1 (0%) 81 83	22, 31, 44, 62	0
16	2U	116/118 (98%)	0.88	7 (6%) 27 27	45, 66, 76, 81	0
17	1V	101/101 (100%)	-0.22	0 100 100	24, 38, 55, 65	0
17	2V	101/101 (100%)	0.98	6 (5%) 28 27	47, 72, 79, 84	0
18	1W	112/113 (99%)	-0.21	1 (0%) 81 83	25, 33, 56, 80	0
18	2W	112/113 (99%)	0.42	3 (2%) 56 57	43, 52, 67, 90	0
19	1X	95/96 (98%)	0.07	3 (3%) 50 51	30, 42, 65, 75	0
19	2X	95/96 (98%)	0.70	7 (7%) 20 19	49, 58, 76, 82	0
20	1Y	107/110 (97%)	0.50	3 (2%) 55 56	39, 52, 69, 82	0
20	2Y	107/110 (97%)	1.47	23 (21%) 2 2	58, 70, 84, 89	0
21	1Z	154/206 (74%)	0.95	17 (11%) 10 10	41, 66, 84, 89	0
21	2Z	160/206 (77%)	1.69	44 (27%) 1 1	72, 82, 90, 92	0
22	10	83/85 (97%)	-0.03	1 (1%) 76 77	27, 40, 52, 63	0
22	20	83/85 (97%)	0.84	6 (7%) 21 20	45, 62, 70, 77	0
23	11	97/98 (98%)	0.51	3 (3%) 51 52	31, 50, 71, 76	0
23	21	97/98 (98%)	0.67	4 (4%) 41 42	42, 56, 75, 84	0
24	12	70/72 (97%)	0.44	2 (2%) 53 55	38, 50, 61, 76	0
24	22	70/72 (97%)	0.90	4 (5%) 29 29	56, 68, 76, 86	0
25	13	59/60 (98%)	0.00	2 (3%) 48 49	27, 37, 63, 82	0
25	23	59/60 (98%)	0.76	3 (5%) 33 33	53, 67, 78, 85	0
26	14	69/71 (97%)	1.19	14 (20%) 3 2	59, 75, 87, 90	0
26	24	69/71 (97%)	1.45	14 (20%) 3 2	71, 84, 91, 93	0
27	15	59/60 (98%)	-0.14	0 100 100	22, 34, 49, 57	0
27	25	59/60 (98%)	0.49	1 (1%) 69 69	41, 57, 69, 78	0
28	16	53/54 (98%)	0.20	1 (1%) 66 66	36, 45, 57, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.59	1 (1%) 66 66	47, 59, 67, 77	0
29	17	48/49 (97%)	0.06	4 (8%) 17 17	26, 31, 56, 66	0
29	27	48/49 (97%)	0.52	5 (10%) 11 11	38, 42, 67, 71	0
30	18	64/65 (98%)	-0.09	0 100 100	29, 37, 44, 56	0
30	28	64/65 (98%)	0.46	0 100 100	46, 56, 61, 68	0
31	19	37/37 (100%)	-0.06	0 100 100	32, 40, 61, 62	0
31	29	37/37 (100%)	1.39	7 (18%) 3 2	64, 73, 84, 88	0
32	1a	1488/1521 (97%)	0.31	58 (3%) 43 44	35, 67, 94, 109	0
32	2a	1491/1521 (98%)	0.54	78 (5%) 33 32	45, 72, 94, 108	0
33	1b	231/256 (90%)	1.51	62 (26%) 1 1	62, 78, 87, 93	0
33	2b	231/256 (90%)	1.74	81 (35%) 1 0	69, 83, 89, 93	0
34	1c	206/239 (86%)	1.15	22 (10%) 11 10	63, 73, 83, 90	0
34	2c	206/239 (86%)	1.72	69 (33%) 1 0	70, 79, 86, 90	0
35	1d	208/209 (99%)	1.12	20 (9%) 13 13	57, 69, 78, 89	0
35	2d	208/209 (99%)	0.89	11 (5%) 32 31	56, 66, 75, 85	0
36	1e	148/162 (91%)	0.85	7 (4%) 36 36	48, 64, 75, 81	0
36	2e	148/162 (91%)	1.02	6 (4%) 41 42	54, 71, 80, 87	0
37	1f	100/101 (99%)	0.85	5 (5%) 34 33	55, 68, 76, 80	0
37	2f	100/101 (99%)	0.65	2 (2%) 65 65	55, 66, 74, 81	0
38	1g	155/156 (99%)	1.02	19 (12%) 8 7	61, 71, 85, 91	0
38	2g	155/156 (99%)	1.25	23 (14%) 5 5	68, 75, 85, 96	0
39	1h	137/138 (99%)	0.74	2 (1%) 72 73	55, 65, 72, 76	0
39	2h	137/138 (99%)	0.93	7 (5%) 33 33	64, 72, 78, 81	0
40	1i	127/128 (99%)	1.60	30 (23%) 2 1	51, 78, 85, 88	0
40	2i	127/128 (99%)	1.98	61 (48%) 0 0	68, 83, 88, 91	0
41	1j	97/105 (92%)	1.85	43 (44%) 0 0	57, 78, 87, 93	0
41	2j	96/105 (91%)	2.38	59 (61%) 0 0	72, 83, 89, 96	0
42	1k	114/129 (88%)	0.86	9 (7%) 18 18	44, 64, 76, 80	0
42	2k	114/129 (88%)	1.05	13 (11%) 10 9	54, 71, 80, 84	0
43	1l	121/132 (91%)	0.38	3 (2%) 58 59	48, 54, 65, 71	0
43	2l	121/132 (91%)	0.87	7 (5%) 29 28	58, 65, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.13	17 (13%) 6 5	54, 70, 77, 86	0
44	2m	122/126 (96%)	1.51	27 (22%) 2 2	67, 78, 84, 90	0
45	1n	60/61 (98%)	1.13	6 (10%) 12 12	61, 69, 77, 78	0
45	2n	60/61 (98%)	2.23	30 (50%) 0 0	72, 79, 87, 89	0
46	1o	88/89 (98%)	0.85	7 (7%) 18 18	45, 65, 73, 77	0
46	2o	88/89 (98%)	0.86	4 (4%) 38 38	54, 66, 78, 86	0
47	1p	82/88 (93%)	1.43	19 (23%) 2 1	59, 71, 79, 84	0
47	2p	82/88 (93%)	1.02	9 (10%) 10 10	58, 68, 77, 79	0
48	1q	99/105 (94%)	1.03	5 (5%) 33 33	53, 66, 74, 76	0
48	2q	99/105 (94%)	1.02	6 (6%) 27 26	58, 70, 79, 80	0
49	1r	68/88 (77%)	0.61	4 (5%) 28 27	56, 64, 77, 79	0
49	2r	68/88 (77%)	0.75	2 (2%) 53 55	58, 67, 76, 79	0
50	1s	83/93 (89%)	1.09	11 (13%) 7 6	62, 73, 81, 86	0
50	2s	83/93 (89%)	1.76	29 (34%) 1 0	72, 82, 88, 90	0
51	1t	96/106 (90%)	1.14	14 (14%) 6 5	61, 71, 80, 85	0
51	2t	96/106 (90%)	1.33	15 (15%) 5 4	60, 72, 82, 85	0
52	1u	23/27 (85%)	1.69	7 (30%) 1 0	62, 66, 72, 78	0
52	2u	23/27 (85%)	1.84	9 (39%) 1 0	67, 75, 81, 84	0
53	1v	13/24 (54%)	0.81	3 (23%) 2 1	48, 55, 91, 97	0
53	2v	13/24 (54%)	1.10	3 (23%) 2 1	60, 70, 96, 103	0
54	1w	66/76 (86%)	1.34	15 (22%) 2 2	31, 86, 98, 102	0
54	2w	64/76 (84%)	1.48	17 (26%) 1 1	50, 95, 100, 104	0
55	1x	72/77 (93%)	0.24	2 (2%) 55 56	28, 60, 79, 90	0
55	2x	72/77 (93%)	0.36	1 (1%) 73 74	45, 72, 84, 100	0
56	1y	67/76 (88%)	1.96	31 (46%) 0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	2.24	41 (62%) 0 0	69, 101, 104, 107	0
All	All	20871/21748 (95%)	0.52	1800 (8%) 16 15	21, 64, 89, 109	0

The worst 5 of 1800 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	10.3
1	2A	652(U)	G	10.3

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Mol	Chain	Res	Type	RSRZ
1	2A	653	A	9.4
1	2A	654	A	7.5
1	1A	653	A	7.3

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
56	4SU	2y	8	20/21	0.37	0.19	98,102,113,128	0
56	5MU	2y	54	21/22	0.45	0.21	94,100,111,124	0
56	PSU	2y	55	20/21	0.45	0.16	92,99,110,115	0
56	MIA	2y	37	22/30	0.47	0.17	88,94,108,126	0
56	G7M	2y	46	24/25	0.48	0.17	86,101,106,121	0
56	PSU	1y	55	20/21	0.52	0.17	96,101,103,114	0
56	G7M	1y	46	24/25	0.52	0.16	90,98,107,113	0
56	4SU	1y	8	20/21	0.54	0.15	97,101,109,117	0
56	MIA	1y	37	22/30	0.56	0.18	88,95,103,115	0
56	PSU	1y	39	20/21	0.59	0.16	88,94,105,106	0
56	5MU	1y	54	21/22	0.61	0.16	89,98,103,112	0
56	PSU	2y	39	20/21	0.62	0.17	88,94,105,111	0
56	PSU	2y	32	20/21	0.67	0.16	89,96,103,113	0
54	G7M	2w	46	24/25	0.68	0.16	87,94,105,120	0
56	PSU	1y	32	20/21	0.74	0.16	90,96,105,109	0
54	G7M	1w	46	24/25	0.75	0.15	79,86,99,118	0
54	4SU	2w	8	20/21	0.77	0.14	89,94,104,105	0
54	PSU	2w	55	20/21	0.83	0.11	85,89,96,99	0
54	MIA	2w	37	25/30	0.84	0.17	56,74,82,100	0
54	4SU	1w	8	20/21	0.84	0.14	83,88,93,95	0
54	PSU	1w	55	20/21	0.85	0.12	59,73,84,87	0
54	5MU	2w	54	21/22	0.86	0.12	79,84,89,93	0
55	PSU	2x	55	20/21	0.87	0.12	69,75,87,90	0
55	PSU	1x	55	20/21	0.89	0.12	57,63,72,72	0
54	PSU	2w	32	20/21	0.90	0.12	73,78,86,86	0
55	4SU	2x	8	20/21	0.90	0.12	71,78,82,83	0
55	5MU	1x	54	21/22	0.90	0.11	58,63,72,74	0
32	2MG	2a	1207	24/25	0.90	0.11	71,81,83,85	0
54	MIA	1w	37	29/30	0.90	0.17	51,59,73,87	0
55	5MU	2x	54	21/22	0.91	0.12	72,77,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
43	0TD	2l	92	10/11	0.91	0.11	63,65,68,72	0
32	G7M	2a	527	24/25	0.91	0.14	56,64,71,72	0
54	5MU	1w	54	21/22	0.92	0.09	52,63,66,70	0
32	PSU	2a	516	20/21	0.92	0.10	53,67,71,74	0
43	0TD	1l	92	10/11	0.92	0.12	47,52,55,67	0
32	5MC	2a	1400	21/22	0.93	0.14	61,66,74,74	0
54	PSU	1w	32	20/21	0.93	0.11	56,62,69,71	0
55	4SU	1x	8	20/21	0.93	0.10	55,62,66,67	0
32	5MC	2a	967	21/22	0.93	0.13	59,66,72,75	0
55	5MC	2x	32	21/22	0.93	0.13	63,68,73,78	0
55	5MC	1x	32	21/22	0.93	0.12	51,56,60,64	0
54	PSU	2w	39	20/21	0.93	0.11	68,78,84,85	0
1	5MU	2A	1915	21/22	0.93	0.10	53,61,65,67	0
32	M2G	2a	966	25/26	0.94	0.14	53,62,68,73	0
32	2MG	1a	1207	24/25	0.94	0.09	66,70,74,75	0
32	G7M	1a	527	24/25	0.94	0.10	36,49,56,60	0
32	M2G	1a	966	25/26	0.94	0.11	39,49,60,63	0
32	MA6	2a	1518	24/25	0.95	0.11	52,59,64,67	0
32	MA6	2a	1519	24/25	0.95	0.11	48,59,64,66	0
32	5MC	1a	967	21/22	0.95	0.10	45,50,59,62	0
55	31H	1x	76	32/33	0.95	0.09	21,27,33,45	10
32	PSU	1a	516	20/21	0.95	0.07	51,57,62,62	0
32	4OC	2a	1402	22/23	0.95	0.10	53,59,63,66	0
32	UR3	2a	1498	21/22	0.95	0.10	51,56,59,62	0
1	5MU	1A	1915	21/22	0.95	0.09	44,49,57,57	0
55	31H	2x	76	32/33	0.95	0.10	39,47,57,57	0
1	PSU	2A	1917	20/21	0.95	0.08	50,57,63,64	0
1	OMC	2A	1920	21/22	0.95	0.10	51,56,60,62	0
32	5MC	1a	1407	21/22	0.96	0.09	35,44,46,50	0
32	5MC	2a	1404	21/22	0.96	0.09	49,52,56,58	0
1	PSU	2A	1911	20/21	0.96	0.08	49,53,58,64	0
32	5MC	2a	1407	21/22	0.96	0.09	49,56,60,62	0
32	5MC	1a	1400	21/22	0.96	0.10	45,51,56,56	0
1	PSU	1A	1917	20/21	0.96	0.07	47,51,55,55	0
54	PSU	1w	39	20/21	0.96	0.09	47,61,66,69	0
32	4OC	1a	1402	22/23	0.96	0.09	36,43,46,50	0
1	5MC	2A	1942	21/22	0.96	0.08	50,57,63,73	0
1	5MC	2A	1962	21/22	0.96	0.09	43,48,53,61	0
1	OMG	2A	2251	24/25	0.96	0.09	40,45,50,52	0
1	2MU	2A	2552	21/23	0.96	0.09	44,49,52,58	0
1	PSU	2A	2605	20/21	0.96	0.08	36,42,47,51	0
1	5MC	1A	1942	21/22	0.97	0.08	35,41,46,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	F3N	2w	76	33/34	0.97	0.08	36,43,47,50	0
1	PSU	1A	1911	20/21	0.97	0.07	40,51,54,55	0
32	MA6	1a	1518	24/25	0.97	0.08	34,40,47,47	0
1	8AH	2A	2503	24/25	0.97	0.10	35,40,43,49	0
32	MA6	1a	1519	24/25	0.97	0.08	33,41,45,49	0
1	PSU	1A	2605	20/21	0.97	0.07	23,29,32,35	0
1	5MU	2A	1939	21/22	0.97	0.07	33,41,46,51	0
32	5MC	1a	1404	21/22	0.98	0.06	34,40,45,47	0
1	5MU	1A	1939	21/22	0.98	0.07	25,31,35,42	0
1	8AH	1A	2503	24/25	0.98	0.07	16,25,30,32	0
32	UR3	1a	1498	21/22	0.98	0.07	37,42,45,48	0
1	2MU	1A	2552	21/23	0.98	0.07	24,29,34,35	0
54	F3N	1w	76	33/34	0.98	0.07	19,27,32,33	0
1	OMC	1A	1920	21/22	0.98	0.07	38,47,50,52	0
1	5MC	1A	1962	21/22	0.98	0.06	28,34,37,41	0
1	OMG	1A	2251	24/25	0.99	0.05	22,26,30,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	230	1/1	-0.02	0.25	84,84,84,84	0
57	MG	1A	4003	1/1	0.38	0.19	75,75,75,75	0
57	MG	2A	3264	1/1	0.49	0.36	82,82,82,82	0
57	MG	2A	3384	1/1	0.49	0.32	91,91,91,91	0
57	MG	2A	3674	1/1	0.54	0.29	57,57,57,57	0
57	MG	2A	3592	1/1	0.55	0.32	73,73,73,73	0
57	MG	10	106	1/1	0.58	0.28	68,68,68,68	0
57	MG	1A	4041	1/1	0.59	0.33	70,70,70,70	0
57	MG	1x	111	1/1	0.60	0.20	78,78,78,78	0
57	MG	1A	3562	1/1	0.61	0.32	70,70,70,70	0
57	MG	2A	3451	1/1	0.61	0.25	68,68,68,68	0
57	MG	2E	302	1/1	0.63	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2y	105	1/1	0.63	0.28	89,89,89,89	0
57	MG	2A	3491	1/1	0.65	0.17	82,82,82,82	0
57	MG	2A	3772	1/1	0.65	0.30	77,77,77,77	0
57	MG	1O	204	1/1	0.66	0.29	67,67,67,67	0
57	MG	1A	3884	1/1	0.66	0.30	47,47,47,47	0
57	MG	2w	103	1/1	0.66	0.21	93,93,93,93	0
57	MG	1B	237	1/1	0.66	0.17	62,62,62,62	0
57	MG	2A	3791	1/1	0.68	0.19	71,71,71,71	0
57	MG	1A	4035	1/1	0.68	0.17	65,65,65,65	0
57	MG	2A	3235	1/1	0.69	0.21	80,80,80,80	0
57	MG	2A	3639	1/1	0.69	0.19	88,88,88,88	0
57	MG	1A	4101	1/1	0.69	0.21	65,65,65,65	0
57	MG	2A	3316	1/1	0.69	0.39	76,76,76,76	0
57	MG	2A	3525	1/1	0.70	0.16	65,65,65,65	0
57	MG	2A	3790	1/1	0.70	0.19	75,75,75,75	0
57	MG	1A	3356	1/1	0.70	0.24	68,68,68,68	0
57	MG	2A	3792	1/1	0.70	0.27	78,78,78,78	0
57	MG	2A	3634	1/1	0.70	0.21	66,66,66,66	0
57	MG	18	105	1/1	0.70	0.27	78,78,78,78	0
57	MG	1A	4022	1/1	0.70	0.24	55,55,55,55	0
57	MG	1a	1629	1/1	0.71	0.18	77,77,77,77	0
57	MG	2A	3387	1/1	0.71	0.33	79,79,79,79	0
57	MG	2A	3062	1/1	0.71	0.20	73,73,73,73	0
57	MG	2A	3097	1/1	0.71	0.28	75,75,75,75	0
57	MG	2A	3749	1/1	0.72	0.20	65,65,65,65	0
57	MG	2A	3502	1/1	0.72	0.13	70,70,70,70	0
57	MG	2A	3161	1/1	0.72	0.12	87,87,87,87	0
57	MG	2A	3031	1/1	0.72	0.29	70,70,70,70	0
57	MG	1A	3641	1/1	0.72	0.21	53,53,53,53	0
57	MG	1A	3983	1/1	0.72	0.18	43,43,43,43	0
57	MG	2A	3500	1/1	0.72	0.25	84,84,84,84	0
57	MG	2y	104	1/1	0.72	0.15	71,71,71,71	0
57	MG	2A	3721	1/1	0.72	0.16	69,69,69,69	0
57	MG	1A	3795	1/1	0.73	0.17	51,51,51,51	0
57	MG	1A	3819	1/1	0.73	0.22	70,70,70,70	0
57	MG	1A	3506	1/1	0.73	0.24	65,65,65,65	0
57	MG	2A	3499	1/1	0.73	0.23	75,75,75,75	0
57	MG	1A	3925	1/1	0.73	0.18	73,73,73,73	0
57	MG	1A	3939	1/1	0.73	0.23	74,74,74,74	0
57	MG	1A	4050	1/1	0.73	0.18	56,56,56,56	0
57	MG	1A	4073	1/1	0.73	0.15	73,73,73,73	0
57	MG	1a	1655	1/1	0.73	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2y	102	1/1	0.73	0.22	87,87,87,87	0
57	MG	1a	1786	1/1	0.73	0.17	71,71,71,71	0
57	MG	2A	3657	1/1	0.73	0.19	68,68,68,68	0
57	MG	2A	3733	1/1	0.74	0.19	57,57,57,57	0
57	MG	1A	3092	1/1	0.74	0.14	79,79,79,79	0
57	MG	2A	3562	1/1	0.74	0.22	56,56,56,56	0
57	MG	2A	3141	1/1	0.74	0.25	74,74,74,74	0
57	MG	2A	3620	1/1	0.74	0.16	77,77,77,77	0
57	MG	2A	3633	1/1	0.74	0.26	74,74,74,74	0
57	MG	1A	3499	1/1	0.74	0.23	51,51,51,51	0
57	MG	2A	3016	1/1	0.74	0.30	67,67,67,67	0
57	MG	15	108	1/1	0.74	0.44	60,60,60,60	0
57	MG	2A	3269	1/1	0.74	0.21	73,73,73,73	0
57	MG	1a	1685	1/1	0.74	0.21	61,61,61,61	0
57	MG	1a	1645	1/1	0.75	0.26	78,78,78,78	0
57	MG	2A	3318	1/1	0.75	0.41	72,72,72,72	0
57	MG	1S	201	1/1	0.75	0.35	60,60,60,60	0
57	MG	1A	4070	1/1	0.75	0.17	71,71,71,71	0
57	MG	1a	1785	1/1	0.75	0.19	76,76,76,76	0
57	MG	1A	3479	1/1	0.75	0.23	65,65,65,65	0
57	MG	2A	3494	1/1	0.75	0.19	56,56,56,56	0
57	MG	2A	3644	1/1	0.75	0.14	63,63,63,63	0
57	MG	1b	301	1/1	0.75	0.22	86,86,86,86	0
57	MG	1D	311	1/1	0.75	0.20	65,65,65,65	0
57	MG	1A	3814	1/1	0.75	0.16	41,41,41,41	0
57	MG	1a	1659	1/1	0.76	0.45	80,80,80,80	0
57	MG	1S	203	1/1	0.76	0.15	72,72,72,72	0
57	MG	2A	3673	1/1	0.76	0.19	64,64,64,64	0
57	MG	1a	1725	1/1	0.76	0.15	75,75,75,75	0
57	MG	2A	3686	1/1	0.76	0.34	58,58,58,58	0
57	MG	1A	3072	1/1	0.76	0.30	69,69,69,69	0
57	MG	1A	3757	1/1	0.76	0.12	22,22,22,22	0
57	MG	1a	1818	1/1	0.76	0.19	54,54,54,54	0
57	MG	1A	4042	1/1	0.76	0.28	40,40,40,40	0
57	MG	1q	201	1/1	0.76	0.18	64,64,64,64	0
57	MG	2A	3567	1/1	0.76	0.37	73,73,73,73	0
57	MG	1A	3503	1/1	0.76	0.18	57,57,57,57	0
57	MG	2B	201	1/1	0.76	0.32	75,75,75,75	0
57	MG	2B	203	1/1	0.76	0.14	68,68,68,68	0
57	MG	2A	3617	1/1	0.76	0.25	76,76,76,76	0
57	MG	1A	3908	1/1	0.76	0.14	52,52,52,52	0
57	MG	1A	3909	1/1	0.76	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3403	1/1	0.76	0.35	76,76,76,76	0
57	MG	2A	3404	1/1	0.76	0.22	72,72,72,72	0
57	MG	2y	107	1/1	0.76	0.19	84,84,84,84	0
57	MG	1a	1648	1/1	0.77	0.25	79,79,79,79	0
57	MG	1A	4103	1/1	0.77	0.12	63,63,63,63	0
57	MG	2A	3704	1/1	0.77	0.18	68,68,68,68	0
57	MG	2A	3708	1/1	0.77	0.19	73,73,73,73	0
57	MG	1A	3978	1/1	0.77	0.16	66,66,66,66	0
57	MG	1B	231	1/1	0.77	0.24	67,67,67,67	0
57	MG	2A	3532	1/1	0.77	0.17	52,52,52,52	0
57	MG	1A	3776	1/1	0.77	0.25	84,84,84,84	0
57	MG	1A	3291	1/1	0.77	0.18	64,64,64,64	0
57	MG	1A	3428	1/1	0.77	0.22	61,61,61,61	0
57	MG	1A	3533	1/1	0.77	0.20	60,60,60,60	0
57	MG	1A	3824	1/1	0.77	0.22	64,64,64,64	0
57	MG	1A	3293	1/1	0.77	0.33	64,64,64,64	0
57	MG	1A	3485	1/1	0.77	0.17	69,69,69,69	0
57	MG	1A	3673	1/1	0.77	0.13	61,61,61,61	0
57	MG	1A	3734	1/1	0.77	0.16	62,62,62,62	0
57	MG	2A	3649	1/1	0.77	0.15	67,67,67,67	0
57	MG	2A	3041	1/1	0.77	0.36	71,71,71,71	0
57	MG	1A	3352	1/1	0.77	0.30	64,64,64,64	0
57	MG	2A	3564	1/1	0.78	0.14	70,70,70,70	0
57	MG	2A	3271	1/1	0.78	0.21	80,80,80,80	0
57	MG	2A	3669	1/1	0.78	0.17	44,44,44,44	0
57	MG	2A	3580	1/1	0.78	0.24	75,75,75,75	0
57	MG	2A	3106	1/1	0.78	0.28	69,69,69,69	0
57	MG	1A	3669	1/1	0.78	0.24	70,70,70,70	0
57	MG	1A	4010	1/1	0.78	0.12	83,83,83,83	0
57	MG	2Z	301	1/1	0.78	0.14	80,80,80,80	0
57	MG	2A	3057	1/1	0.78	0.21	72,72,72,72	0
57	MG	2A	3709	1/1	0.78	0.17	52,52,52,52	0
57	MG	2A	3238	1/1	0.78	0.17	65,65,65,65	0
57	MG	1A	4018	1/1	0.78	0.23	56,56,56,56	0
57	MG	1A	3945	1/1	0.78	0.12	57,57,57,57	0
57	MG	1a	1604	1/1	0.79	0.20	68,68,68,68	0
57	MG	1A	3711	1/1	0.79	0.26	61,61,61,61	0
57	MG	1a	1632	1/1	0.79	0.35	70,70,70,70	0
57	MG	1A	4008	1/1	0.79	0.15	73,73,73,73	0
57	MG	1A	3721	1/1	0.79	0.16	66,66,66,66	0
57	MG	1a	1650	1/1	0.79	0.25	74,74,74,74	0
57	MG	1A	4014	1/1	0.79	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3895	1/1	0.79	0.22	67,67,67,67	0
57	MG	2A	3518	1/1	0.79	0.20	69,69,69,69	0
57	MG	2A	3144	1/1	0.79	0.36	62,62,62,62	0
57	MG	1A	3729	1/1	0.79	0.25	47,47,47,47	0
57	MG	2A	3762	1/1	0.79	0.14	78,78,78,78	0
57	MG	2A	3221	1/1	0.79	0.28	77,77,77,77	0
57	MG	1E	311	1/1	0.79	0.14	53,53,53,53	0
57	MG	1a	1727	1/1	0.79	0.16	82,82,82,82	0
57	MG	1A	3329	1/1	0.79	0.20	59,59,59,59	0
57	MG	2A	3591	1/1	0.79	0.20	61,61,61,61	0
57	MG	1A	3222	1/1	0.79	0.18	61,61,61,61	0
57	MG	1A	3051	1/1	0.79	0.17	54,54,54,54	0
57	MG	2A	3298	1/1	0.79	0.26	69,69,69,69	0
57	MG	2A	3301	1/1	0.79	0.34	55,55,55,55	0
57	MG	2w	105	1/1	0.79	0.21	79,79,79,79	0
57	MG	1A	3198	1/1	0.79	0.19	58,58,58,58	0
57	MG	1A	3447	1/1	0.79	0.15	57,57,57,57	0
57	MG	1v	101	1/1	0.79	0.24	74,74,74,74	0
57	MG	1A	3696	1/1	0.79	0.21	54,54,54,54	0
57	MG	2A	3456	1/1	0.80	0.19	64,64,64,64	0
57	MG	2A	3247	1/1	0.80	0.16	76,76,76,76	0
57	MG	2A	3252	1/1	0.80	0.27	76,76,76,76	0
57	MG	1A	3699	1/1	0.80	0.19	55,55,55,55	0
57	MG	1a	1814	1/1	0.80	0.21	64,64,64,64	0
57	MG	1A	3521	1/1	0.80	0.25	77,77,77,77	0
57	MG	2A	3099	1/1	0.80	0.26	59,59,59,59	0
57	MG	1A	3831	1/1	0.80	0.14	57,57,57,57	0
57	MG	2A	3310	1/1	0.80	0.33	61,61,61,61	0
57	MG	2A	3312	1/1	0.80	0.24	75,75,75,75	0
57	MG	2A	3753	1/1	0.80	0.18	48,48,48,48	0
57	MG	1A	3975	1/1	0.80	0.11	32,32,32,32	0
57	MG	1A	3712	1/1	0.80	0.18	74,74,74,74	0
57	MG	2A	3789	1/1	0.80	0.20	69,69,69,69	0
57	MG	2A	3329	1/1	0.80	0.23	73,73,73,73	0
57	MG	2A	3338	1/1	0.80	0.28	51,51,51,51	0
57	MG	2A	3355	1/1	0.80	0.12	63,63,63,63	0
57	MG	2A	3598	1/1	0.80	0.16	57,57,57,57	0
57	MG	1A	3786	1/1	0.80	0.13	56,56,56,56	0
57	MG	2B	208	1/1	0.80	0.18	66,66,66,66	0
57	MG	2A	3182	1/1	0.80	0.20	69,69,69,69	0
57	MG	1A	3199	1/1	0.80	0.18	70,70,70,70	0
57	MG	1A	3666	1/1	0.80	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3410	1/1	0.80	0.12	73,73,73,73	0
57	MG	2x	103	1/1	0.80	0.14	76,76,76,76	0
57	MG	2x	107	1/1	0.80	0.13	49,49,49,49	0
57	MG	2A	3426	1/1	0.80	0.18	57,57,57,57	0
57	MG	2y	103	1/1	0.80	0.14	80,80,80,80	0
57	MG	2A	3648	1/1	0.80	0.21	68,68,68,68	0
57	MG	2A	3427	1/1	0.80	0.17	63,63,63,63	0
57	MG	1A	4058	1/1	0.80	0.22	61,61,61,61	0
57	MG	1A	3302	1/1	0.81	0.19	50,50,50,50	0
57	MG	2A	3142	1/1	0.81	0.19	64,64,64,64	0
57	MG	1A	3882	1/1	0.81	0.15	64,64,64,64	0
57	MG	2A	3160	1/1	0.81	0.19	68,68,68,68	0
57	MG	1a	1742	1/1	0.81	0.15	71,71,71,71	0
57	MG	1a	1782	1/1	0.81	0.28	85,85,85,85	0
57	MG	2A	3188	1/1	0.81	0.16	68,68,68,68	0
57	MG	1A	4061	1/1	0.81	0.12	28,28,28,28	0
57	MG	1A	3281	1/1	0.81	0.34	77,77,77,77	0
57	MG	2A	3715	1/1	0.81	0.14	62,62,62,62	0
57	MG	1A	3693	1/1	0.81	0.15	35,35,35,35	0
57	MG	2A	3731	1/1	0.81	0.20	52,52,52,52	0
57	MG	1A	3331	1/1	0.81	0.21	67,67,67,67	0
57	MG	1a	1623	1/1	0.81	0.14	57,57,57,57	0
57	MG	2A	3514	1/1	0.81	0.17	69,69,69,69	0
57	MG	1A	3560	1/1	0.81	0.12	47,47,47,47	0
57	MG	1A	4104	1/1	0.81	0.22	64,64,64,64	0
57	MG	1a	1634	1/1	0.81	0.28	74,74,74,74	0
57	MG	2A	3538	1/1	0.81	0.26	75,75,75,75	0
57	MG	2A	3546	1/1	0.81	0.18	60,60,60,60	0
57	MG	1A	3350	1/1	0.81	0.38	67,67,67,67	0
57	MG	2A	3023	1/1	0.81	0.28	71,71,71,71	0
57	MG	1A	3160	1/1	0.81	0.32	68,68,68,68	0
57	MG	1A	4024	1/1	0.81	0.31	74,74,74,74	0
57	MG	2B	210	1/1	0.81	0.13	68,68,68,68	0
57	MG	1A	3713	1/1	0.81	0.18	54,54,54,54	0
57	MG	1a	1656	1/1	0.81	0.22	68,68,68,68	0
57	MG	25	103	1/1	0.81	0.15	76,76,76,76	0
57	MG	2w	102	1/1	0.81	0.28	86,86,86,86	0
57	MG	2A	3328	1/1	0.81	0.17	73,73,73,73	0
57	MG	2A	3605	1/1	0.81	0.28	67,67,67,67	0
57	MG	2A	3082	1/1	0.81	0.28	69,69,69,69	0
57	MG	1A	3949	1/1	0.81	0.12	49,49,49,49	0
57	MG	1A	3246	1/1	0.81	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3356	1/1	0.81	0.25	53,53,53,53	0
57	MG	2A	3369	1/1	0.81	0.22	73,73,73,73	0
57	MG	2A	3102	1/1	0.81	0.14	72,72,72,72	0
57	MG	1a	1711	1/1	0.81	0.13	71,71,71,71	0
57	MG	1A	3788	1/1	0.82	0.12	54,54,54,54	0
57	MG	1a	1710	1/1	0.82	0.28	68,68,68,68	0
57	MG	2A	3571	1/1	0.82	0.25	84,84,84,84	0
57	MG	2A	3408	1/1	0.82	0.10	81,81,81,81	0
57	MG	2A	3757	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3294	1/1	0.82	0.24	63,63,63,63	0
57	MG	2A	3422	1/1	0.82	0.12	67,67,67,67	0
57	MG	2A	3423	1/1	0.82	0.17	69,69,69,69	0
57	MG	1A	3840	1/1	0.82	0.13	68,68,68,68	0
57	MG	2A	3607	1/1	0.82	0.13	66,66,66,66	0
57	MG	1w	104	1/1	0.82	0.17	65,65,65,65	0
57	MG	1a	1722	1/1	0.82	0.18	71,71,71,71	0
57	MG	1A	3653	1/1	0.82	0.18	40,40,40,40	0
57	MG	2B	205	1/1	0.82	0.25	67,67,67,67	0
57	MG	2A	3477	1/1	0.82	0.15	54,54,54,54	0
57	MG	1A	3968	1/1	0.82	0.14	65,65,65,65	0
57	MG	2B	214	1/1	0.82	0.24	69,69,69,69	0
57	MG	2A	3493	1/1	0.82	0.20	77,77,77,77	0
57	MG	1a	1741	1/1	0.82	0.15	65,65,65,65	0
57	MG	2A	3322	1/1	0.82	0.16	70,70,70,70	0
57	MG	1A	3520	1/1	0.82	0.12	71,71,71,71	0
57	MG	2A	3050	1/1	0.82	0.28	73,73,73,73	0
57	MG	1A	3818	1/1	0.82	0.16	62,62,62,62	0
57	MG	2w	106	1/1	0.82	0.37	82,82,82,82	0
57	MG	2A	3352	1/1	0.82	0.24	65,65,65,65	0
57	MG	2x	106	1/1	0.82	0.19	66,66,66,66	0
57	MG	2A	3237	1/1	0.82	0.23	79,79,79,79	0
57	MG	1A	3456	1/1	0.82	0.14	61,61,61,61	0
57	MG	1B	222	1/1	0.82	0.12	61,61,61,61	0
57	MG	1A	3823	1/1	0.82	0.18	67,67,67,67	0
57	MG	2A	3560	1/1	0.82	0.17	44,44,44,44	0
57	MG	1A	3381	1/1	0.82	0.20	65,65,65,65	0
57	MG	1A	3680	1/1	0.83	0.13	65,65,65,65	0
57	MG	1A	4113	1/1	0.83	0.15	56,56,56,56	0
57	MG	1a	1810	1/1	0.83	0.19	69,69,69,69	0
57	MG	1a	1635	1/1	0.83	0.23	62,62,62,62	0
57	MG	2A	3662	1/1	0.83	0.20	71,71,71,71	0
57	MG	1a	1816	1/1	0.83	0.35	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3229	1/1	0.83	0.12	76,76,76,76	0
57	MG	1a	1817	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3444	1/1	0.83	0.13	69,69,69,69	0
57	MG	2A	3700	1/1	0.83	0.16	62,62,62,62	0
57	MG	1a	1646	1/1	0.83	0.16	66,66,66,66	0
57	MG	2A	3240	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3296	1/1	0.83	0.22	58,58,58,58	0
57	MG	1A	3697	1/1	0.83	0.12	59,59,59,59	0
57	MG	1A	3239	1/1	0.83	0.21	59,59,59,59	0
57	MG	1A	3475	1/1	0.83	0.17	65,65,65,65	0
57	MG	1A	3117	1/1	0.83	0.22	59,59,59,59	0
57	MG	2A	3275	1/1	0.83	0.29	71,71,71,71	0
57	MG	2A	3511	1/1	0.83	0.24	74,74,74,74	0
57	MG	1a	1664	1/1	0.83	0.29	73,73,73,73	0
57	MG	1a	1666	1/1	0.83	0.19	73,73,73,73	0
57	MG	1A	3631	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3783	1/1	0.83	0.20	75,75,75,75	0
57	MG	2A	3529	1/1	0.83	0.24	70,70,70,70	0
57	MG	1a	1686	1/1	0.83	0.18	76,76,76,76	0
57	MG	1A	4051	1/1	0.83	0.13	54,54,54,54	0
57	MG	2A	3543	1/1	0.83	0.26	65,65,65,65	0
57	MG	2A	3804	1/1	0.83	0.26	79,79,79,79	0
57	MG	1A	4056	1/1	0.83	0.09	51,51,51,51	0
57	MG	2B	202	1/1	0.83	0.24	67,67,67,67	0
57	MG	1A	3247	1/1	0.83	0.19	74,74,74,74	0
57	MG	2A	3320	1/1	0.83	0.20	70,70,70,70	0
57	MG	2A	3084	1/1	0.83	0.27	57,57,57,57	0
57	MG	1A	3496	1/1	0.83	0.16	87,87,87,87	0
57	MG	1A	3989	1/1	0.83	0.11	68,68,68,68	0
57	MG	2A	3332	1/1	0.83	0.22	72,72,72,72	0
57	MG	2E	307	1/1	0.83	0.17	71,71,71,71	0
57	MG	2A	3581	1/1	0.83	0.16	64,64,64,64	0
57	MG	1A	3387	1/1	0.83	0.20	75,75,75,75	0
57	MG	27	102	1/1	0.83	0.32	67,67,67,67	0
57	MG	1A	3399	1/1	0.83	0.27	64,64,64,64	0
57	MG	2A	3108	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3125	1/1	0.83	0.12	65,65,65,65	0
57	MG	2A	3365	1/1	0.83	0.23	62,62,62,62	0
57	MG	2A	3608	1/1	0.83	0.14	62,62,62,62	0
57	MG	2A	3610	1/1	0.83	0.23	49,49,49,49	0
57	MG	2A	3615	1/1	0.83	0.20	63,63,63,63	0
57	MG	1a	1746	1/1	0.83	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1755	1/1	0.83	0.14	70,70,70,70	0
57	MG	2A	3386	1/1	0.83	0.14	68,68,68,68	0
57	MG	1A	3338	1/1	0.83	0.21	62,62,62,62	0
57	MG	2A	3158	1/1	0.83	0.34	79,79,79,79	0
57	MG	2A	3018	1/1	0.84	0.20	66,66,66,66	0
57	MG	1A	3905	1/1	0.84	0.10	40,40,40,40	0
57	MG	2A	3375	1/1	0.84	0.23	72,72,72,72	0
57	MG	1A	3596	1/1	0.84	0.13	57,57,57,57	0
57	MG	1A	3238	1/1	0.84	0.21	66,66,66,66	0
57	MG	1A	3476	1/1	0.84	0.17	61,61,61,61	0
57	MG	2A	3245	1/1	0.84	0.34	72,72,72,72	0
57	MG	2A	3590	1/1	0.84	0.32	78,78,78,78	0
57	MG	1A	3927	1/1	0.84	0.12	30,30,30,30	0
57	MG	1A	3408	1/1	0.84	0.23	55,55,55,55	0
57	MG	2A	3076	1/1	0.84	0.18	58,58,58,58	0
57	MG	1a	1787	1/1	0.84	0.11	74,74,74,74	0
57	MG	1a	1795	1/1	0.84	0.19	68,68,68,68	0
57	MG	1a	1807	1/1	0.84	0.15	61,61,61,61	0
57	MG	1a	1809	1/1	0.84	0.16	66,66,66,66	0
57	MG	2A	3297	1/1	0.84	0.37	74,74,74,74	0
57	MG	1A	3367	1/1	0.84	0.17	60,60,60,60	0
57	MG	1A	3514	1/1	0.84	0.25	62,62,62,62	0
57	MG	2A	3480	1/1	0.84	0.19	55,55,55,55	0
57	MG	1B	233	1/1	0.84	0.21	61,61,61,61	0
57	MG	1a	1691	1/1	0.84	0.28	68,68,68,68	0
57	MG	2D	306	1/1	0.84	0.16	62,62,62,62	0
57	MG	1A	4059	1/1	0.84	0.14	55,55,55,55	0
57	MG	1A	3951	1/1	0.84	0.19	55,55,55,55	0
57	MG	2O	201	1/1	0.84	0.13	55,55,55,55	0
57	MG	2A	3143	1/1	0.84	0.22	72,72,72,72	0
57	MG	1l	201	1/1	0.84	0.17	82,82,82,82	0
57	MG	2A	3510	1/1	0.84	0.13	71,71,71,71	0
57	MG	2w	101	1/1	0.84	0.12	75,75,75,75	0
57	MG	2A	3327	1/1	0.84	0.17	73,73,73,73	0
57	MG	2A	3151	1/1	0.84	0.38	67,67,67,67	0
57	MG	2w	104	1/1	0.84	0.11	80,80,80,80	0
57	MG	1D	312	1/1	0.84	0.27	47,47,47,47	0
57	MG	2A	3331	1/1	0.84	0.14	75,75,75,75	0
57	MG	2A	3696	1/1	0.84	0.17	82,82,82,82	0
57	MG	1a	1643	1/1	0.84	0.28	60,60,60,60	0
57	MG	2A	3701	1/1	0.84	0.11	68,68,68,68	0
57	MG	1A	3708	1/1	0.84	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3705	1/1	0.84	0.11	68,68,68,68	0
57	MG	1x	108	1/1	0.84	0.31	72,72,72,72	0
57	MG	1a	1736	1/1	0.84	0.23	76,76,76,76	0
57	MG	1O	203	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3398	1/1	0.85	0.17	67,67,67,67	0
57	MG	2A	3400	1/1	0.85	0.17	65,65,65,65	0
57	MG	2A	3653	1/1	0.85	0.20	76,76,76,76	0
57	MG	1A	3027	1/1	0.85	0.14	51,51,51,51	0
57	MG	2A	3661	1/1	0.85	0.17	72,72,72,72	0
57	MG	2A	3181	1/1	0.85	0.25	64,64,64,64	0
57	MG	1A	3853	1/1	0.85	0.16	47,47,47,47	0
57	MG	2A	3184	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3187	1/1	0.85	0.13	49,49,49,49	0
57	MG	2A	3679	1/1	0.85	0.20	71,71,71,71	0
57	MG	1m	3001	1/1	0.85	0.15	61,61,61,61	0
57	MG	2A	3189	1/1	0.85	0.17	67,67,67,67	0
57	MG	2A	3198	1/1	0.85	0.30	73,73,73,73	0
57	MG	1A	4060	1/1	0.85	0.17	43,43,43,43	0
57	MG	2A	3455	1/1	0.85	0.45	72,72,72,72	0
57	MG	2A	3226	1/1	0.85	0.16	69,69,69,69	0
57	MG	1a	1692	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3231	1/1	0.85	0.28	73,73,73,73	0
57	MG	2A	3710	1/1	0.85	0.24	85,85,85,85	0
57	MG	1w	101	1/1	0.85	0.37	74,74,74,74	0
57	MG	1a	1694	1/1	0.85	0.24	62,62,62,62	0
57	MG	1w	108	1/1	0.85	0.29	66,66,66,66	0
57	MG	1A	3870	1/1	0.85	0.14	25,25,25,25	0
57	MG	1l	105	1/1	0.85	0.20	78,78,78,78	0
57	MG	1a	1718	1/1	0.85	0.17	68,68,68,68	0
57	MG	1A	3703	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3284	1/1	0.85	0.31	66,66,66,66	0
57	MG	1A	4007	1/1	0.85	0.13	77,77,77,77	0
57	MG	1A	3889	1/1	0.85	0.16	55,55,55,55	0
57	MG	2A	3523	1/1	0.85	0.11	73,73,73,73	0
57	MG	2A	3272	1/1	0.85	0.13	59,59,59,59	0
57	MG	2A	3274	1/1	0.85	0.25	76,76,76,76	0
57	MG	2A	3042	1/1	0.85	0.18	74,74,74,74	0
57	MG	2A	3794	1/1	0.85	0.19	63,63,63,63	0
57	MG	1A	3002	1/1	0.85	0.16	55,55,55,55	0
57	MG	2A	3054	1/1	0.85	0.18	66,66,66,66	0
57	MG	1A	3794	1/1	0.85	0.22	69,69,69,69	0
57	MG	2A	3547	1/1	0.85	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1743	1/1	0.85	0.12	87,87,87,87	0
57	MG	1B	212	1/1	0.85	0.17	58,58,58,58	0
57	MG	1A	3425	1/1	0.85	0.21	63,63,63,63	0
57	MG	1a	1771	1/1	0.85	0.17	69,69,69,69	0
57	MG	2A	3090	1/1	0.85	0.20	69,69,69,69	0
57	MG	2A	3575	1/1	0.85	0.17	61,61,61,61	0
57	MG	1B	224	1/1	0.85	0.16	59,59,59,59	0
57	MG	2A	3098	1/1	0.85	0.17	82,82,82,82	0
57	MG	1B	227	1/1	0.85	0.20	67,67,67,67	0
57	MG	23	101	1/1	0.85	0.19	70,70,70,70	0
57	MG	1A	3507	1/1	0.85	0.21	47,47,47,47	0
57	MG	1A	3604	1/1	0.85	0.16	16,16,16,16	0
57	MG	1a	1649	1/1	0.85	0.12	61,61,61,61	0
57	MG	2A	3604	1/1	0.85	0.23	61,61,61,61	0
57	MG	2A	3110	1/1	0.85	0.15	73,73,73,73	0
57	MG	1A	3101	1/1	0.85	0.31	44,44,44,44	0
57	MG	2A	3138	1/1	0.85	0.18	58,58,58,58	0
57	MG	2A	3139	1/1	0.85	0.31	61,61,61,61	0
57	MG	1a	1654	1/1	0.85	0.20	61,61,61,61	0
57	MG	1A	3295	1/1	0.85	0.12	47,47,47,47	0
57	MG	1a	1813	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3625	1/1	0.85	0.19	72,72,72,72	0
57	MG	1A	3735	1/1	0.85	0.14	45,45,45,45	0
57	MG	1A	3825	1/1	0.85	0.14	51,51,51,51	0
57	MG	1A	3830	1/1	0.85	0.09	61,61,61,61	0
57	MG	2y	106	1/1	0.85	0.21	71,71,71,71	0
57	MG	1A	3741	1/1	0.85	0.10	30,30,30,30	0
57	MG	1A	3832	1/1	0.86	0.11	60,60,60,60	0
57	MG	2A	3585	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3567	1/1	0.86	0.19	46,46,46,46	0
57	MG	2A	3270	1/1	0.86	0.28	76,76,76,76	0
57	MG	1A	3588	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3595	1/1	0.86	0.11	52,52,52,52	0
57	MG	1A	3858	1/1	0.86	0.07	38,38,38,38	0
57	MG	2A	3599	1/1	0.86	0.31	75,75,75,75	0
57	MG	1A	3859	1/1	0.86	0.14	42,42,42,42	0
57	MG	1A	3716	1/1	0.86	0.10	49,49,49,49	0
57	MG	2A	3281	1/1	0.86	0.22	70,70,70,70	0
57	MG	1A	3874	1/1	0.86	0.12	39,39,39,39	0
57	MG	2A	3295	1/1	0.86	0.26	59,59,59,59	0
57	MG	1x	106	1/1	0.86	0.22	58,58,58,58	0
57	MG	1x	107	1/1	0.86	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3877	1/1	0.86	0.10	29,29,29,29	0
57	MG	2A	3305	1/1	0.86	0.40	71,71,71,71	0
57	MG	1x	109	1/1	0.86	0.14	32,32,32,32	0
57	MG	1A	4052	1/1	0.86	0.14	22,22,22,22	0
57	MG	1A	3484	1/1	0.86	0.20	62,62,62,62	0
57	MG	2A	3642	1/1	0.86	0.14	69,69,69,69	0
57	MG	2A	3317	1/1	0.86	0.22	71,71,71,71	0
57	MG	1A	3725	1/1	0.86	0.11	52,52,52,52	0
57	MG	2A	3020	1/1	0.86	0.13	62,62,62,62	0
57	MG	1A	3726	1/1	0.86	0.18	68,68,68,68	0
57	MG	1A	3893	1/1	0.86	0.12	45,45,45,45	0
57	MG	2A	3658	1/1	0.86	0.24	68,68,68,68	0
57	MG	2A	3659	1/1	0.86	0.14	60,60,60,60	0
57	MG	1A	3359	1/1	0.86	0.12	70,70,70,70	0
57	MG	1a	1651	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3330	1/1	0.86	0.34	60,60,60,60	0
57	MG	2A	3672	1/1	0.86	0.15	43,43,43,43	0
57	MG	1a	1652	1/1	0.86	0.12	69,69,69,69	0
57	MG	1A	3901	1/1	0.86	0.12	23,23,23,23	0
57	MG	1A	4071	1/1	0.86	0.20	56,56,56,56	0
57	MG	2A	3343	1/1	0.86	0.34	59,59,59,59	0
57	MG	1A	3902	1/1	0.86	0.14	46,46,46,46	0
57	MG	2A	3065	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	4091	1/1	0.86	0.11	68,68,68,68	0
57	MG	2A	3357	1/1	0.86	0.26	59,59,59,59	0
57	MG	1A	3625	1/1	0.86	0.21	55,55,55,55	0
57	MG	1A	3413	1/1	0.86	0.30	66,66,66,66	0
57	MG	2A	3085	1/1	0.86	0.21	64,64,64,64	0
57	MG	2A	3380	1/1	0.86	0.16	75,75,75,75	0
57	MG	2A	3382	1/1	0.86	0.17	65,65,65,65	0
57	MG	2A	3720	1/1	0.86	0.17	69,69,69,69	0
57	MG	1a	1667	1/1	0.86	0.26	64,64,64,64	0
57	MG	2A	3724	1/1	0.86	0.13	56,56,56,56	0
57	MG	1a	1676	1/1	0.86	0.22	61,61,61,61	0
57	MG	1A	3640	1/1	0.86	0.13	50,50,50,50	0
57	MG	1A	4105	1/1	0.86	0.19	68,68,68,68	0
57	MG	1A	4109	1/1	0.86	0.20	52,52,52,52	0
57	MG	1A	3911	1/1	0.86	0.12	29,29,29,29	0
57	MG	1B	203	1/1	0.86	0.21	60,60,60,60	0
57	MG	1A	3417	1/1	0.86	0.15	48,48,48,48	0
57	MG	2A	3778	1/1	0.86	0.12	61,61,61,61	0
57	MG	1B	216	1/1	0.86	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3784	1/1	0.86	0.14	56,56,56,56	0
57	MG	2A	3786	1/1	0.86	0.20	72,72,72,72	0
57	MG	1B	219	1/1	0.86	0.15	57,57,57,57	0
57	MG	1A	3423	1/1	0.86	0.20	45,45,45,45	0
57	MG	1B	223	1/1	0.86	0.17	60,60,60,60	0
57	MG	1A	3361	1/1	0.86	0.16	58,58,58,58	0
57	MG	1a	1731	1/1	0.86	0.28	57,57,57,57	0
57	MG	2A	3796	1/1	0.86	0.18	70,70,70,70	0
57	MG	1A	3141	1/1	0.86	0.13	49,49,49,49	0
57	MG	1A	3510	1/1	0.86	0.28	64,64,64,64	0
57	MG	2A	3465	1/1	0.86	0.16	59,59,59,59	0
57	MG	2A	3154	1/1	0.86	0.25	68,68,68,68	0
57	MG	1A	3377	1/1	0.86	0.15	45,45,45,45	0
57	MG	1A	3519	1/1	0.86	0.18	61,61,61,61	0
57	MG	1A	3325	1/1	0.86	0.15	44,44,44,44	0
57	MG	2A	3171	1/1	0.86	0.22	61,61,61,61	0
57	MG	2D	303	1/1	0.86	0.36	54,54,54,54	0
57	MG	1a	1753	1/1	0.86	0.09	48,48,48,48	0
57	MG	1A	3042	1/1	0.86	0.13	47,47,47,47	0
57	MG	1a	1756	1/1	0.86	0.17	55,55,55,55	0
57	MG	2G	201	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3979	1/1	0.86	0.10	52,52,52,52	0
57	MG	1E	306	1/1	0.86	0.16	58,58,58,58	0
57	MG	2I	101	1/1	0.86	0.14	68,68,68,68	0
57	MG	1A	3391	1/1	0.86	0.17	58,58,58,58	0
57	MG	25	101	1/1	0.86	0.11	59,59,59,59	0
57	MG	1A	3396	1/1	0.86	0.27	62,62,62,62	0
57	MG	2A	3202	1/1	0.86	0.16	53,53,53,53	0
57	MG	1A	3292	1/1	0.86	0.19	55,55,55,55	0
57	MG	1Q	204	1/1	0.86	0.20	73,73,73,73	0
57	MG	1Q	207	1/1	0.86	0.18	54,54,54,54	0
57	MG	1R	204	1/1	0.86	0.19	53,53,53,53	0
57	MG	2A	3540	1/1	0.86	0.10	77,77,77,77	0
57	MG	1A	3827	1/1	0.86	0.30	68,68,68,68	0
57	MG	1A	3829	1/1	0.86	0.11	69,69,69,69	0
57	MG	1T	203	1/1	0.86	0.19	64,64,64,64	0
57	MG	1V	207	1/1	0.86	0.13	53,53,53,53	0
57	MG	1W	202	1/1	0.86	0.11	58,58,58,58	0
57	MG	1A	3710	1/1	0.86	0.15	59,59,59,59	0
57	MG	2A	3250	1/1	0.86	0.25	74,74,74,74	0
57	MG	1A	3565	1/1	0.86	0.27	68,68,68,68	0
57	MG	2A	3253	1/1	0.86	0.30	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3256	1/1	0.86	0.24	68,68,68,68	0
57	MG	2A	3244	1/1	0.87	0.14	72,72,72,72	0
57	MG	1B	214	1/1	0.87	0.28	69,69,69,69	0
57	MG	2A	3413	1/1	0.87	0.35	68,68,68,68	0
57	MG	1A	3752	1/1	0.87	0.10	26,26,26,26	0
57	MG	1A	3162	1/1	0.87	0.23	41,41,41,41	0
57	MG	1a	1764	1/1	0.87	0.14	77,77,77,77	0
57	MG	1A	3762	1/1	0.87	0.12	66,66,66,66	0
57	MG	2A	3440	1/1	0.87	0.14	69,69,69,69	0
57	MG	2A	3079	1/1	0.87	0.27	58,58,58,58	0
57	MG	2A	3081	1/1	0.87	0.16	58,58,58,58	0
57	MG	1A	3467	1/1	0.87	0.17	65,65,65,65	0
57	MG	2A	3461	1/1	0.87	0.17	62,62,62,62	0
57	MG	2A	3683	1/1	0.87	0.17	66,66,66,66	0
57	MG	1A	4038	1/1	0.87	0.24	69,69,69,69	0
57	MG	2A	3687	1/1	0.87	0.25	69,69,69,69	0
57	MG	2A	3688	1/1	0.87	0.17	69,69,69,69	0
57	MG	2A	3466	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3467	1/1	0.87	0.18	55,55,55,55	0
57	MG	2A	3474	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3914	1/1	0.87	0.12	57,57,57,57	0
57	MG	1A	3243	1/1	0.87	0.21	65,65,65,65	0
57	MG	1a	1790	1/1	0.87	0.17	56,56,56,56	0
57	MG	1A	4044	1/1	0.87	0.09	42,42,42,42	0
57	MG	2A	3279	1/1	0.87	0.23	61,61,61,61	0
57	MG	1A	3851	1/1	0.87	0.24	68,68,68,68	0
57	MG	2A	3285	1/1	0.87	0.16	65,65,65,65	0
57	MG	1A	3373	1/1	0.87	0.19	69,69,69,69	0
57	MG	2A	3506	1/1	0.87	0.22	69,69,69,69	0
57	MG	2A	3728	1/1	0.87	0.15	62,62,62,62	0
57	MG	2A	3730	1/1	0.87	0.10	79,79,79,79	0
57	MG	1A	3854	1/1	0.87	0.10	40,40,40,40	0
57	MG	1A	4053	1/1	0.87	0.16	74,74,74,74	0
57	MG	2A	3736	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3109	1/1	0.87	0.21	58,58,58,58	0
57	MG	1A	3580	1/1	0.87	0.15	51,51,51,51	0
57	MG	1A	3581	1/1	0.87	0.21	64,64,64,64	0
57	MG	2A	3761	1/1	0.87	0.14	85,85,85,85	0
57	MG	2A	3524	1/1	0.87	0.19	75,75,75,75	0
57	MG	1F	311	1/1	0.87	0.13	64,64,64,64	0
57	MG	2A	3311	1/1	0.87	0.23	69,69,69,69	0
57	MG	2A	3780	1/1	0.87	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3781	1/1	0.87	0.21	75,75,75,75	0
57	MG	1A	3953	1/1	0.87	0.24	53,53,53,53	0
57	MG	1A	3800	1/1	0.87	0.16	64,64,64,64	0
57	MG	1a	1674	1/1	0.87	0.32	64,64,64,64	0
57	MG	2A	3788	1/1	0.87	0.14	65,65,65,65	0
57	MG	1l	202	1/1	0.87	0.12	65,65,65,65	0
57	MG	1A	3970	1/1	0.87	0.11	33,33,33,33	0
57	MG	1Q	206	1/1	0.87	0.10	51,51,51,51	0
57	MG	1A	3811	1/1	0.87	0.10	39,39,39,39	0
57	MG	2A	3561	1/1	0.87	0.14	55,55,55,55	0
57	MG	2A	3795	1/1	0.87	0.22	62,62,62,62	0
57	MG	1A	3174	1/1	0.87	0.18	63,63,63,63	0
57	MG	2A	3799	1/1	0.87	0.18	58,58,58,58	0
57	MG	2A	3803	1/1	0.87	0.18	59,59,59,59	0
57	MG	1w	102	1/1	0.87	0.11	60,60,60,60	0
57	MG	1R	206	1/1	0.87	0.23	44,44,44,44	0
57	MG	2A	3569	1/1	0.87	0.20	55,55,55,55	0
57	MG	2A	3165	1/1	0.87	0.25	66,66,66,66	0
57	MG	1w	106	1/1	0.87	0.16	82,82,82,82	0
57	MG	2B	207	1/1	0.87	0.22	61,61,61,61	0
57	MG	2A	3577	1/1	0.87	0.16	60,60,60,60	0
57	MG	2A	3334	1/1	0.87	0.23	50,50,50,50	0
57	MG	2B	211	1/1	0.87	0.19	71,71,71,71	0
57	MG	2A	3177	1/1	0.87	0.27	70,70,70,70	0
57	MG	2B	215	1/1	0.87	0.12	73,73,73,73	0
57	MG	2A	3582	1/1	0.87	0.10	59,59,59,59	0
57	MG	1w	107	1/1	0.87	0.27	68,68,68,68	0
57	MG	2A	3587	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3817	1/1	0.87	0.18	66,66,66,66	0
57	MG	1w	109	1/1	0.87	0.21	79,79,79,79	0
57	MG	1A	4083	1/1	0.87	0.19	58,58,58,58	0
57	MG	1A	3443	1/1	0.87	0.13	55,55,55,55	0
57	MG	2A	3597	1/1	0.87	0.35	65,65,65,65	0
57	MG	2A	3362	1/1	0.87	0.44	71,71,71,71	0
57	MG	1a	1714	1/1	0.87	0.21	78,78,78,78	0
57	MG	1A	3378	1/1	0.87	0.18	49,49,49,49	0
57	MG	2A	3372	1/1	0.87	0.22	52,52,52,52	0
57	MG	1A	4102	1/1	0.87	0.14	64,64,64,64	0
57	MG	2A	3212	1/1	0.87	0.17	52,52,52,52	0
57	MG	1A	3995	1/1	0.87	0.13	41,41,41,41	0
57	MG	1A	3891	1/1	0.87	0.13	42,42,42,42	0
57	MG	1A	3136	1/1	0.87	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3618	1/1	0.87	0.11	59,59,59,59	0
57	MG	1A	3522	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3388	1/1	0.87	0.32	70,70,70,70	0
57	MG	2A	3632	1/1	0.87	0.15	69,69,69,69	0
57	MG	2A	3397	1/1	0.87	0.16	57,57,57,57	0
57	MG	1A	3448	1/1	0.87	0.10	50,50,50,50	0
57	MG	1a	1611	1/1	0.87	0.23	74,74,74,74	0
57	MG	2A	3402	1/1	0.87	0.27	56,56,56,56	0
57	MG	1A	4012	1/1	0.87	0.12	49,49,49,49	0
57	MG	1A	3743	1/1	0.87	0.16	44,44,44,44	0
57	MG	1A	3493	1/1	0.88	0.15	68,68,68,68	0
57	MG	1A	3314	1/1	0.88	0.28	57,57,57,57	0
57	MG	2A	3660	1/1	0.88	0.07	75,75,75,75	0
57	MG	1A	3317	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3415	1/1	0.88	0.29	66,66,66,66	0
57	MG	2A	3667	1/1	0.88	0.11	69,69,69,69	0
57	MG	1A	4072	1/1	0.88	0.14	49,49,49,49	0
57	MG	1A	3838	1/1	0.88	0.20	52,52,52,52	0
57	MG	2A	3028	1/1	0.88	0.36	62,62,62,62	0
57	MG	1V	206	1/1	0.88	0.18	57,57,57,57	0
57	MG	2A	3676	1/1	0.88	0.18	60,60,60,60	0
57	MG	2A	3428	1/1	0.88	0.13	52,52,52,52	0
57	MG	2A	3438	1/1	0.88	0.10	57,57,57,57	0
57	MG	2A	3033	1/1	0.88	0.22	56,56,56,56	0
57	MG	1A	3080	1/1	0.88	0.21	50,50,50,50	0
57	MG	2A	3453	1/1	0.88	0.15	55,55,55,55	0
57	MG	2A	3691	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	3736	1/1	0.88	0.11	45,45,45,45	0
57	MG	2A	3699	1/1	0.88	0.13	56,56,56,56	0
57	MG	2A	3044	1/1	0.88	0.28	71,71,71,71	0
57	MG	2A	3459	1/1	0.88	0.13	69,69,69,69	0
57	MG	1W	206	1/1	0.88	0.18	27,27,27,27	0
57	MG	2A	3462	1/1	0.88	0.14	41,41,41,41	0
57	MG	1A	4095	1/1	0.88	0.10	65,65,65,65	0
57	MG	1A	3976	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3257	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3261	1/1	0.88	0.22	69,69,69,69	0
57	MG	1l	106	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3267	1/1	0.88	0.17	61,61,61,61	0
57	MG	1a	1748	1/1	0.88	0.13	57,57,57,57	0
57	MG	2A	3067	1/1	0.88	0.22	65,65,65,65	0
57	MG	1A	3244	1/1	0.88	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3436	1/1	0.88	0.26	65,65,65,65	0
57	MG	1a	1602	1/1	0.88	0.19	62,62,62,62	0
57	MG	1A	3085	1/1	0.88	0.16	37,37,37,37	0
57	MG	1A	3332	1/1	0.88	0.12	64,64,64,64	0
57	MG	1A	3867	1/1	0.88	0.10	39,39,39,39	0
57	MG	1a	1625	1/1	0.88	0.27	63,63,63,63	0
57	MG	2A	3096	1/1	0.88	0.11	57,57,57,57	0
57	MG	2A	3517	1/1	0.88	0.15	62,62,62,62	0
57	MG	2A	3763	1/1	0.88	0.10	42,42,42,42	0
57	MG	1A	3335	1/1	0.88	0.29	65,65,65,65	0
57	MG	2A	3296	1/1	0.88	0.19	65,65,65,65	0
57	MG	1A	4006	1/1	0.88	0.11	70,70,70,70	0
57	MG	1a	1633	1/1	0.88	0.30	66,66,66,66	0
57	MG	2A	3782	1/1	0.88	0.11	50,50,50,50	0
57	MG	1a	1793	1/1	0.88	0.15	66,66,66,66	0
57	MG	1B	211	1/1	0.88	0.23	50,50,50,50	0
57	MG	2A	3537	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3308	1/1	0.88	0.18	65,65,65,65	0
57	MG	1A	3382	1/1	0.88	0.14	50,50,50,50	0
57	MG	1a	1808	1/1	0.88	0.24	67,67,67,67	0
57	MG	1a	1636	1/1	0.88	0.21	69,69,69,69	0
57	MG	2A	3113	1/1	0.88	0.35	73,73,73,73	0
57	MG	1A	3785	1/1	0.88	0.11	44,44,44,44	0
57	MG	2A	3126	1/1	0.88	0.19	47,47,47,47	0
57	MG	1A	3878	1/1	0.88	0.11	30,30,30,30	0
57	MG	1A	3452	1/1	0.88	0.20	55,55,55,55	0
57	MG	1A	3337	1/1	0.88	0.13	59,59,59,59	0
57	MG	1A	3461	1/1	0.88	0.24	61,61,61,61	0
57	MG	1A	3535	1/1	0.88	0.32	56,56,56,56	0
57	MG	1A	3796	1/1	0.88	0.10	44,44,44,44	0
57	MG	1d	301	1/1	0.88	0.34	61,61,61,61	0
57	MG	1A	3554	1/1	0.88	0.35	65,65,65,65	0
57	MG	2A	3155	1/1	0.88	0.27	64,64,64,64	0
57	MG	2A	3336	1/1	0.88	0.28	55,55,55,55	0
57	MG	1A	4037	1/1	0.88	0.08	17,17,17,17	0
57	MG	1A	3068	1/1	0.88	0.16	54,54,54,54	0
57	MG	2A	3347	1/1	0.88	0.32	61,61,61,61	0
57	MG	2A	3349	1/1	0.88	0.19	69,69,69,69	0
57	MG	2B	216	1/1	0.88	0.28	74,74,74,74	0
57	MG	2A	3350	1/1	0.88	0.21	58,58,58,58	0
57	MG	1B	236	1/1	0.88	0.17	71,71,71,71	0
57	MG	2E	301	1/1	0.88	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3813	1/1	0.88	0.17	50,50,50,50	0
57	MG	2A	3166	1/1	0.88	0.23	74,74,74,74	0
57	MG	2A	3167	1/1	0.88	0.17	65,65,65,65	0
57	MG	1A	3253	1/1	0.88	0.14	69,69,69,69	0
57	MG	2W	203	1/1	0.88	0.26	65,65,65,65	0
57	MG	1A	3260	1/1	0.88	0.15	56,56,56,56	0
57	MG	20	101	1/1	0.88	0.18	67,67,67,67	0
57	MG	1w	103	1/1	0.88	0.21	75,75,75,75	0
57	MG	2A	3370	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	3407	1/1	0.88	0.11	52,52,52,52	0
57	MG	1A	3480	1/1	0.88	0.13	45,45,45,45	0
57	MG	1F	310	1/1	0.88	0.16	38,38,38,38	0
57	MG	1A	3353	1/1	0.88	0.14	51,51,51,51	0
57	MG	1A	3719	1/1	0.88	0.12	69,69,69,69	0
57	MG	1A	3720	1/1	0.88	0.08	69,69,69,69	0
57	MG	2A	3200	1/1	0.88	0.23	66,66,66,66	0
57	MG	1A	3929	1/1	0.88	0.11	62,62,62,62	0
57	MG	2A	3390	1/1	0.88	0.09	75,75,75,75	0
57	MG	2x	101	1/1	0.88	0.14	71,71,71,71	0
57	MG	2A	3204	1/1	0.88	0.38	55,55,55,55	0
57	MG	2x	104	1/1	0.88	0.38	73,73,73,73	0
57	MG	2A	3205	1/1	0.88	0.21	58,58,58,58	0
57	MG	1A	3099	1/1	0.88	0.14	68,68,68,68	0
57	MG	2y	101	1/1	0.88	0.09	57,57,57,57	0
57	MG	2A	3645	1/1	0.88	0.12	68,68,68,68	0
57	MG	2A	3401	1/1	0.88	0.13	67,67,67,67	0
57	MG	2A	3218	1/1	0.88	0.24	68,68,68,68	0
57	MG	2A	3651	1/1	0.88	0.25	62,62,62,62	0
57	MG	1A	3488	1/1	0.88	0.42	43,43,43,43	0
57	MG	2A	3222	1/1	0.88	0.10	72,72,72,72	0
57	MG	2A	3239	1/1	0.89	0.27	73,73,73,73	0
57	MG	1A	3783	1/1	0.89	0.08	23,23,23,23	0
57	MG	1A	3058	1/1	0.89	0.18	59,59,59,59	0
57	MG	1A	4026	1/1	0.89	0.07	43,43,43,43	0
57	MG	2A	3668	1/1	0.89	0.20	61,61,61,61	0
57	MG	1A	3542	1/1	0.89	0.11	62,62,62,62	0
57	MG	1A	3433	1/1	0.89	0.26	57,57,57,57	0
57	MG	1A	3888	1/1	0.89	0.14	48,48,48,48	0
57	MG	1A	3789	1/1	0.89	0.08	24,24,24,24	0
57	MG	2A	3434	1/1	0.89	0.31	55,55,55,55	0
57	MG	2A	3061	1/1	0.89	0.12	51,51,51,51	0
57	MG	1A	3176	1/1	0.89	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3258	1/1	0.89	0.17	67,67,67,67	0
57	MG	1Q	205	1/1	0.89	0.29	55,55,55,55	0
57	MG	1A	3438	1/1	0.89	0.09	69,69,69,69	0
57	MG	2A	3071	1/1	0.89	0.23	71,71,71,71	0
57	MG	2A	3457	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	4045	1/1	0.89	0.13	64,64,64,64	0
57	MG	1A	3564	1/1	0.89	0.26	54,54,54,54	0
57	MG	1A	3701	1/1	0.89	0.24	69,69,69,69	0
57	MG	1A	3801	1/1	0.89	0.12	32,32,32,32	0
57	MG	1A	3393	1/1	0.89	0.13	64,64,64,64	0
57	MG	1A	3566	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3087	1/1	0.89	0.15	55,55,55,55	0
57	MG	1A	3186	1/1	0.89	0.37	66,66,66,66	0
57	MG	2A	3714	1/1	0.89	0.19	66,66,66,66	0
57	MG	2A	3093	1/1	0.89	0.20	71,71,71,71	0
57	MG	2A	3716	1/1	0.89	0.11	70,70,70,70	0
57	MG	2A	3490	1/1	0.89	0.19	55,55,55,55	0
57	MG	2A	3287	1/1	0.89	0.18	77,77,77,77	0
57	MG	1a	1752	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3815	1/1	0.89	0.24	53,53,53,53	0
57	MG	1A	3816	1/1	0.89	0.27	64,64,64,64	0
57	MG	1A	3196	1/1	0.89	0.12	50,50,50,50	0
57	MG	1X	105	1/1	0.89	0.16	51,51,51,51	0
57	MG	2A	3105	1/1	0.89	0.22	65,65,65,65	0
57	MG	2A	3740	1/1	0.89	0.12	56,56,56,56	0
57	MG	2A	3302	1/1	0.89	0.24	55,55,55,55	0
57	MG	2A	3750	1/1	0.89	0.13	63,63,63,63	0
57	MG	10	104	1/1	0.89	0.18	57,57,57,57	0
57	MG	1A	4064	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3404	1/1	0.89	0.11	49,49,49,49	0
57	MG	1A	3928	1/1	0.89	0.10	26,26,26,26	0
57	MG	2A	3112	1/1	0.89	0.18	49,49,49,49	0
57	MG	2A	3764	1/1	0.89	0.13	57,57,57,57	0
57	MG	1A	3582	1/1	0.89	0.22	47,47,47,47	0
57	MG	1A	3822	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3449	1/1	0.89	0.20	51,51,51,51	0
57	MG	1A	3946	1/1	0.89	0.10	32,32,32,32	0
57	MG	2A	3534	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3321	1/1	0.89	0.29	62,62,62,62	0
57	MG	1a	1608	1/1	0.89	0.35	70,70,70,70	0
57	MG	2A	3325	1/1	0.89	0.09	77,77,77,77	0
57	MG	1A	3948	1/1	0.89	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1621	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3592	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3558	1/1	0.89	0.18	59,59,59,59	0
57	MG	1A	3041	1/1	0.89	0.16	68,68,68,68	0
57	MG	1a	1628	1/1	0.89	0.22	58,58,58,58	0
57	MG	1A	3826	1/1	0.89	0.08	40,40,40,40	0
57	MG	1A	3966	1/1	0.89	0.16	73,73,73,73	0
57	MG	2A	3335	1/1	0.89	0.24	46,46,46,46	0
57	MG	1A	3149	1/1	0.89	0.25	48,48,48,48	0
57	MG	1A	3969	1/1	0.89	0.19	67,67,67,67	0
57	MG	2A	3573	1/1	0.89	0.16	65,65,65,65	0
57	MG	2A	3574	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3339	1/1	0.89	0.15	51,51,51,51	0
57	MG	2A	3340	1/1	0.89	0.29	58,58,58,58	0
57	MG	1A	3513	1/1	0.89	0.34	54,54,54,54	0
57	MG	1A	4114	1/1	0.89	0.15	61,61,61,61	0
57	MG	2B	209	1/1	0.89	0.10	78,78,78,78	0
57	MG	1A	3102	1/1	0.89	0.30	50,50,50,50	0
57	MG	2A	3583	1/1	0.89	0.11	64,64,64,64	0
57	MG	2B	212	1/1	0.89	0.22	73,73,73,73	0
57	MG	1B	204	1/1	0.89	0.19	62,62,62,62	0
57	MG	1p	101	1/1	0.89	0.17	57,57,57,57	0
57	MG	1B	208	1/1	0.89	0.13	63,63,63,63	0
57	MG	1t	201	1/1	0.89	0.13	55,55,55,55	0
57	MG	1B	209	1/1	0.89	0.17	54,54,54,54	0
57	MG	2A	3359	1/1	0.89	0.14	67,67,67,67	0
57	MG	2A	3360	1/1	0.89	0.28	66,66,66,66	0
57	MG	1A	3634	1/1	0.89	0.08	37,37,37,37	0
57	MG	2A	3363	1/1	0.89	0.21	63,63,63,63	0
57	MG	2A	3364	1/1	0.89	0.23	46,46,46,46	0
57	MG	1A	3349	1/1	0.89	0.23	47,47,47,47	0
57	MG	1A	3473	1/1	0.89	0.08	53,53,53,53	0
57	MG	1A	3650	1/1	0.89	0.11	44,44,44,44	0
57	MG	2A	3195	1/1	0.89	0.33	68,68,68,68	0
57	MG	2A	3374	1/1	0.89	0.15	69,69,69,69	0
57	MG	1A	3847	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3990	1/1	0.89	0.12	75,75,75,75	0
57	MG	2A	3619	1/1	0.89	0.10	81,81,81,81	0
57	MG	1A	3651	1/1	0.89	0.11	49,49,49,49	0
57	MG	2A	3624	1/1	0.89	0.09	37,37,37,37	0
57	MG	2A	3383	1/1	0.89	0.34	58,58,58,58	0
57	MG	1a	1658	1/1	0.89	0.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3385	1/1	0.89	0.40	59,59,59,59	0
57	MG	1A	3418	1/1	0.89	0.18	50,50,50,50	0
57	MG	2A	3636	1/1	0.89	0.15	53,53,53,53	0
57	MG	1a	1661	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3748	1/1	0.89	0.11	23,23,23,23	0
57	MG	2x	105	1/1	0.89	0.10	56,56,56,56	0
57	MG	2A	3219	1/1	0.89	0.22	71,71,71,71	0
57	MG	1A	3855	1/1	0.89	0.17	39,39,39,39	0
57	MG	1A	3656	1/1	0.89	0.12	37,37,37,37	0
57	MG	1A	3278	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3097	1/1	0.89	0.15	62,62,62,62	0
57	MG	1a	1682	1/1	0.89	0.23	64,64,64,64	0
57	MG	1a	1684	1/1	0.89	0.26	61,61,61,61	0
57	MG	1A	3775	1/1	0.89	0.11	23,23,23,23	0
57	MG	1A	3671	1/1	0.89	0.10	43,43,43,43	0
57	MG	1a	1703	1/1	0.90	0.14	67,67,67,67	0
57	MG	1a	1705	1/1	0.90	0.11	57,57,57,57	0
57	MG	1a	1706	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3249	1/1	0.90	0.08	43,43,43,43	0
57	MG	1A	3330	1/1	0.90	0.15	60,60,60,60	0
57	MG	1A	3251	1/1	0.90	0.16	49,49,49,49	0
57	MG	2A	3348	1/1	0.90	0.20	64,64,64,64	0
57	MG	1A	3147	1/1	0.90	0.18	45,45,45,45	0
57	MG	1A	3494	1/1	0.90	0.17	59,59,59,59	0
57	MG	2A	3627	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3351	1/1	0.90	0.33	62,62,62,62	0
57	MG	1A	3254	1/1	0.90	0.24	65,65,65,65	0
57	MG	2A	3353	1/1	0.90	0.22	54,54,54,54	0
57	MG	2A	3635	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3086	1/1	0.90	0.12	42,42,42,42	0
57	MG	2A	3117	1/1	0.90	0.10	58,58,58,58	0
57	MG	2A	3640	1/1	0.90	0.10	42,42,42,42	0
57	MG	1A	3276	1/1	0.90	0.15	56,56,56,56	0
57	MG	1a	1734	1/1	0.90	0.17	66,66,66,66	0
57	MG	1A	3277	1/1	0.90	0.13	43,43,43,43	0
57	MG	1E	308	1/1	0.90	0.20	55,55,55,55	0
57	MG	1A	3684	1/1	0.90	0.11	41,41,41,41	0
57	MG	1A	3688	1/1	0.90	0.11	28,28,28,28	0
57	MG	1A	3155	1/1	0.90	0.16	64,64,64,64	0
57	MG	2A	3656	1/1	0.90	0.16	49,49,49,49	0
57	MG	1N	205	1/1	0.90	0.36	53,53,53,53	0
57	MG	1N	206	1/1	0.90	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3371	1/1	0.90	0.14	59,59,59,59	0
57	MG	2A	3153	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	3351	1/1	0.90	0.18	60,60,60,60	0
57	MG	1A	4001	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3665	1/1	0.90	0.22	61,61,61,61	0
57	MG	1P	204	1/1	0.90	0.06	40,40,40,40	0
57	MG	1P	205	1/1	0.90	0.16	45,45,45,45	0
57	MG	1Q	203	1/1	0.90	0.11	50,50,50,50	0
57	MG	1a	1772	1/1	0.90	0.09	86,86,86,86	0
57	MG	1a	1780	1/1	0.90	0.23	66,66,66,66	0
57	MG	1A	3512	1/1	0.90	0.18	46,46,46,46	0
57	MG	2A	3168	1/1	0.90	0.30	64,64,64,64	0
57	MG	1A	3430	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3175	1/1	0.90	0.14	68,68,68,68	0
57	MG	2A	3392	1/1	0.90	0.19	65,65,65,65	0
57	MG	2A	3395	1/1	0.90	0.11	65,65,65,65	0
57	MG	1A	3214	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3282	1/1	0.90	0.10	45,45,45,45	0
57	MG	1A	3437	1/1	0.90	0.24	44,44,44,44	0
57	MG	1a	1791	1/1	0.90	0.10	62,62,62,62	0
57	MG	1A	3283	1/1	0.90	0.20	40,40,40,40	0
57	MG	1A	3833	1/1	0.90	0.13	68,68,68,68	0
57	MG	1A	3357	1/1	0.90	0.14	58,58,58,58	0
57	MG	1A	3839	1/1	0.90	0.16	61,61,61,61	0
57	MG	2A	3706	1/1	0.90	0.09	54,54,54,54	0
57	MG	2A	3409	1/1	0.90	0.17	55,55,55,55	0
57	MG	1A	3216	1/1	0.90	0.18	57,57,57,57	0
57	MG	1A	3843	1/1	0.90	0.07	29,29,29,29	0
57	MG	1A	3845	1/1	0.90	0.23	33,33,33,33	0
57	MG	2A	3420	1/1	0.90	0.21	60,60,60,60	0
57	MG	1A	3445	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3537	1/1	0.90	0.12	54,54,54,54	0
57	MG	2A	3211	1/1	0.90	0.16	67,67,67,67	0
57	MG	2A	3722	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3723	1/1	0.90	0.12	80,80,80,80	0
57	MG	1A	3446	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3216	1/1	0.90	0.20	56,56,56,56	0
57	MG	1A	3550	1/1	0.90	0.14	48,48,48,48	0
57	MG	11	102	1/1	0.90	0.10	54,54,54,54	0
57	MG	1A	3125	1/1	0.90	0.18	59,59,59,59	0
57	MG	1A	3857	1/1	0.90	0.19	38,38,38,38	0
57	MG	2A	3225	1/1	0.90	0.35	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3746	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3747	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3724	1/1	0.90	0.09	54,54,54,54	0
57	MG	1A	3235	1/1	0.90	0.19	52,52,52,52	0
57	MG	1A	3863	1/1	0.90	0.13	42,42,42,42	0
57	MG	1A	3866	1/1	0.90	0.15	66,66,66,66	0
57	MG	2A	3760	1/1	0.90	0.12	39,39,39,39	0
57	MG	2A	3460	1/1	0.90	0.13	46,46,46,46	0
57	MG	1a	1607	1/1	0.90	0.20	60,60,60,60	0
57	MG	1A	3135	1/1	0.90	0.18	47,47,47,47	0
57	MG	1A	3869	1/1	0.90	0.09	48,48,48,48	0
57	MG	1a	1614	1/1	0.90	0.09	73,73,73,73	0
57	MG	1A	3727	1/1	0.90	0.09	58,58,58,58	0
57	MG	1A	3374	1/1	0.90	0.27	40,40,40,40	0
57	MG	1A	3163	1/1	0.90	0.21	63,63,63,63	0
57	MG	1A	3457	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3484	1/1	0.90	0.18	62,62,62,62	0
57	MG	2A	3487	1/1	0.90	0.14	35,35,35,35	0
57	MG	1A	3460	1/1	0.90	0.15	64,64,64,64	0
57	MG	1A	3241	1/1	0.90	0.08	61,61,61,61	0
57	MG	1x	101	1/1	0.90	0.32	69,69,69,69	0
57	MG	1x	102	1/1	0.90	0.30	73,73,73,73	0
57	MG	2A	3495	1/1	0.90	0.11	43,43,43,43	0
57	MG	1A	3887	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3463	1/1	0.90	0.20	46,46,46,46	0
57	MG	1A	4074	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3266	1/1	0.90	0.36	49,49,49,49	0
57	MG	1A	4081	1/1	0.90	0.22	53,53,53,53	0
57	MG	1a	1637	1/1	0.90	0.29	63,63,63,63	0
57	MG	2A	3001	1/1	0.90	0.39	68,68,68,68	0
57	MG	2A	3515	1/1	0.90	0.21	56,56,56,56	0
57	MG	1A	3744	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3745	1/1	0.90	0.09	24,24,24,24	0
57	MG	2B	204	1/1	0.90	0.23	71,71,71,71	0
57	MG	1A	3466	1/1	0.90	0.11	60,60,60,60	0
57	MG	1A	4096	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3278	1/1	0.90	0.18	58,58,58,58	0
57	MG	1A	3018	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3280	1/1	0.90	0.15	57,57,57,57	0
57	MG	1A	3471	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3283	1/1	0.90	0.19	59,59,59,59	0
57	MG	1A	3595	1/1	0.90	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3040	1/1	0.90	0.11	58,58,58,58	0
57	MG	2A	3541	1/1	0.90	0.12	46,46,46,46	0
57	MG	1A	3766	1/1	0.90	0.10	28,28,28,28	0
57	MG	1A	3769	1/1	0.90	0.09	31,31,31,31	0
57	MG	1A	3770	1/1	0.90	0.08	72,72,72,72	0
57	MG	2A	3553	1/1	0.90	0.24	55,55,55,55	0
57	MG	2E	305	1/1	0.90	0.18	60,60,60,60	0
57	MG	2E	306	1/1	0.90	0.16	56,56,56,56	0
57	MG	2A	3047	1/1	0.90	0.36	68,68,68,68	0
57	MG	2F	302	1/1	0.90	0.26	65,65,65,65	0
57	MG	1A	3910	1/1	0.90	0.12	56,56,56,56	0
57	MG	1A	3312	1/1	0.90	0.24	59,59,59,59	0
57	MG	2U	201	1/1	0.90	0.15	54,54,54,54	0
57	MG	2W	201	1/1	0.90	0.27	72,72,72,72	0
57	MG	2A	3055	1/1	0.90	0.32	64,64,64,64	0
57	MG	2A	3303	1/1	0.90	0.17	68,68,68,68	0
57	MG	1B	201	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3058	1/1	0.90	0.17	61,61,61,61	0
57	MG	1a	1660	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3597	1/1	0.90	0.11	36,36,36,36	0
57	MG	1A	3782	1/1	0.90	0.10	32,32,32,32	0
57	MG	2A	3314	1/1	0.90	0.11	77,77,77,77	0
57	MG	2A	3315	1/1	0.90	0.23	67,67,67,67	0
57	MG	2A	3578	1/1	0.90	0.15	65,65,65,65	0
57	MG	1A	3598	1/1	0.90	0.15	62,62,62,62	0
57	MG	2A	3070	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3474	1/1	0.90	0.08	52,52,52,52	0
57	MG	1a	1669	1/1	0.90	0.20	47,47,47,47	0
57	MG	1A	3619	1/1	0.90	0.10	30,30,30,30	0
57	MG	2x	102	1/1	0.90	0.28	76,76,76,76	0
57	MG	1A	3937	1/1	0.90	0.15	75,75,75,75	0
57	MG	2A	3589	1/1	0.90	0.11	47,47,47,47	0
57	MG	2A	3323	1/1	0.90	0.12	62,62,62,62	0
57	MG	1a	1681	1/1	0.90	0.29	70,70,70,70	0
57	MG	1A	3621	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3060	1/1	0.90	0.13	34,34,34,34	0
57	MG	1A	3315	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3089	1/1	0.90	0.18	72,72,72,72	0
57	MG	1B	220	1/1	0.90	0.23	53,53,53,53	0
57	MG	1A	3477	1/1	0.90	0.13	53,53,53,53	0
57	MG	1A	3145	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3193	1/1	0.90	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3616	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	1789	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3354	1/1	0.91	0.20	61,61,61,61	0
57	MG	15	104	1/1	0.91	0.22	44,44,44,44	0
57	MG	15	106	1/1	0.91	0.32	46,46,46,46	0
57	MG	2A	3156	1/1	0.91	0.14	52,52,52,52	0
57	MG	1a	1792	1/1	0.91	0.11	66,66,66,66	0
57	MG	2A	3159	1/1	0.91	0.23	71,71,71,71	0
57	MG	1A	3424	1/1	0.91	0.09	67,67,67,67	0
57	MG	1a	1794	1/1	0.91	0.23	64,64,64,64	0
57	MG	1A	4075	1/1	0.91	0.16	60,60,60,60	0
57	MG	1a	1804	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3366	1/1	0.91	0.41	66,66,66,66	0
57	MG	2A	3368	1/1	0.91	0.33	57,57,57,57	0
57	MG	1A	4076	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3704	1/1	0.91	0.13	47,47,47,47	0
57	MG	1A	3318	1/1	0.91	0.11	62,62,62,62	0
57	MG	1A	3237	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	4093	1/1	0.91	0.07	43,43,43,43	0
57	MG	1A	3573	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1618	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3381	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3655	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3938	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	4099	1/1	0.91	0.10	64,64,64,64	0
57	MG	1a	1820	1/1	0.91	0.11	45,45,45,45	0
57	MG	1a	1624	1/1	0.91	0.17	60,60,60,60	0
57	MG	2A	3192	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3193	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3429	1/1	0.91	0.33	47,47,47,47	0
57	MG	1e	202	1/1	0.91	0.25	64,64,64,64	0
57	MG	2A	3199	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3393	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3328	1/1	0.91	0.24	40,40,40,40	0
57	MG	1A	3127	1/1	0.91	0.11	66,66,66,66	0
57	MG	1a	1631	1/1	0.91	0.09	51,51,51,51	0
57	MG	1A	3947	1/1	0.91	0.07	45,45,45,45	0
57	MG	1A	3583	1/1	0.91	0.09	36,36,36,36	0
57	MG	1A	3287	1/1	0.91	0.32	62,62,62,62	0
57	MG	2A	3680	1/1	0.91	0.14	66,66,66,66	0
57	MG	2A	3682	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3591	1/1	0.91	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3173	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3593	1/1	0.91	0.10	30,30,30,30	0
57	MG	2A	3220	1/1	0.91	0.31	62,62,62,62	0
57	MG	2A	3689	1/1	0.91	0.22	73,73,73,73	0
57	MG	1a	1639	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3693	1/1	0.91	0.19	64,64,64,64	0
57	MG	1B	202	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3224	1/1	0.91	0.24	53,53,53,53	0
57	MG	1A	3256	1/1	0.91	0.15	61,61,61,61	0
57	MG	1A	3441	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3257	1/1	0.91	0.12	63,63,63,63	0
57	MG	2A	3425	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3230	1/1	0.91	0.21	57,57,57,57	0
57	MG	1A	3973	1/1	0.91	0.10	21,21,21,21	0
57	MG	1A	3836	1/1	0.91	0.23	41,41,41,41	0
57	MG	2A	3432	1/1	0.91	0.24	57,57,57,57	0
57	MG	1A	3730	1/1	0.91	0.09	28,28,28,28	0
57	MG	2A	3435	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3502	1/1	0.91	0.26	38,38,38,38	0
57	MG	1B	215	1/1	0.91	0.13	71,71,71,71	0
57	MG	2A	3447	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3599	1/1	0.91	0.13	37,37,37,37	0
57	MG	1A	3113	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3454	1/1	0.91	0.12	62,62,62,62	0
57	MG	1a	1657	1/1	0.91	0.33	67,67,67,67	0
57	MG	1A	3737	1/1	0.91	0.07	48,48,48,48	0
57	MG	2A	3248	1/1	0.91	0.09	60,60,60,60	0
57	MG	2A	3732	1/1	0.91	0.09	36,36,36,36	0
57	MG	2A	3458	1/1	0.91	0.19	57,57,57,57	0
57	MG	2A	3005	1/1	0.91	0.38	71,71,71,71	0
57	MG	2A	3737	1/1	0.91	0.23	66,66,66,66	0
57	MG	2A	3007	1/1	0.91	0.14	54,54,54,54	0
57	MG	2A	3010	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3011	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3463	1/1	0.91	0.17	59,59,59,59	0
57	MG	1A	3505	1/1	0.91	0.20	57,57,57,57	0
57	MG	1A	3993	1/1	0.91	0.08	25,25,25,25	0
57	MG	2A	3756	1/1	0.91	0.09	67,67,67,67	0
57	MG	1A	3211	1/1	0.91	0.10	45,45,45,45	0
57	MG	1a	1663	1/1	0.91	0.24	77,77,77,77	0
57	MG	1B	226	1/1	0.91	0.14	62,62,62,62	0
57	MG	1A	3997	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
57	MG	2A	3032	1/1	0.91	0.19	47,47,47,47	0
57	MG	1B	228	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3765	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3767	1/1	0.91	0.08	51,51,51,51	0
57	MG	2A	3771	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3488	1/1	0.91	0.11	49,49,49,49	0
57	MG	2A	3776	1/1	0.91	0.17	63,63,63,63	0
57	MG	2A	3489	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3036	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3339	1/1	0.91	0.10	54,54,54,54	0
57	MG	2A	3273	1/1	0.91	0.14	59,59,59,59	0
57	MG	1a	1670	1/1	0.91	0.31	49,49,49,49	0
57	MG	1A	3627	1/1	0.91	0.16	47,47,47,47	0
57	MG	2A	3785	1/1	0.91	0.20	51,51,51,51	0
57	MG	1a	1675	1/1	0.91	0.17	61,61,61,61	0
57	MG	1A	4005	1/1	0.91	0.11	64,64,64,64	0
57	MG	1a	1677	1/1	0.91	0.23	63,63,63,63	0
57	MG	2A	3052	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3508	1/1	0.91	0.12	54,54,54,54	0
57	MG	1B	234	1/1	0.91	0.14	56,56,56,56	0
57	MG	1A	3509	1/1	0.91	0.27	58,58,58,58	0
57	MG	2A	3286	1/1	0.91	0.26	69,69,69,69	0
57	MG	1A	3750	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3797	1/1	0.91	0.17	72,72,72,72	0
57	MG	1A	3394	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3344	1/1	0.91	0.16	42,42,42,42	0
57	MG	2A	3520	1/1	0.91	0.22	67,67,67,67	0
57	MG	2A	3521	1/1	0.91	0.18	67,67,67,67	0
57	MG	1A	3297	1/1	0.91	0.14	50,50,50,50	0
57	MG	1A	3400	1/1	0.91	0.27	56,56,56,56	0
57	MG	1a	1693	1/1	0.91	0.26	58,58,58,58	0
57	MG	2A	3527	1/1	0.91	0.12	48,48,48,48	0
57	MG	2A	3528	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3299	1/1	0.91	0.22	64,64,64,64	0
57	MG	2A	3300	1/1	0.91	0.19	67,67,67,67	0
57	MG	1A	3516	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	4021	1/1	0.91	0.18	57,57,57,57	0
57	MG	1A	3298	1/1	0.91	0.16	58,58,58,58	0
57	MG	2A	3304	1/1	0.91	0.26	65,65,65,65	0
57	MG	1A	3774	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	3872	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	4032	1/1	0.91	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3406	1/1	0.91	0.17	61,61,61,61	0
57	MG	1A	3175	1/1	0.91	0.18	73,73,73,73	0
57	MG	2A	3313	1/1	0.91	0.10	73,73,73,73	0
57	MG	1A	3311	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1724	1/1	0.91	0.21	59,59,59,59	0
57	MG	1A	4040	1/1	0.91	0.13	52,52,52,52	0
57	MG	1A	3411	1/1	0.91	0.24	39,39,39,39	0
57	MG	1A	3089	1/1	0.91	0.30	65,65,65,65	0
57	MG	2A	3319	1/1	0.91	0.09	75,75,75,75	0
57	MG	2R	201	1/1	0.91	0.11	64,64,64,64	0
57	MG	1a	1733	1/1	0.91	0.12	57,57,57,57	0
57	MG	2V	201	1/1	0.91	0.12	65,65,65,65	0
57	MG	1A	3679	1/1	0.91	0.10	31,31,31,31	0
57	MG	1A	3415	1/1	0.91	0.23	45,45,45,45	0
57	MG	1a	1739	1/1	0.91	0.17	58,58,58,58	0
57	MG	2A	3576	1/1	0.91	0.19	76,76,76,76	0
57	MG	2A	3324	1/1	0.91	0.15	78,78,78,78	0
57	MG	2I	102	1/1	0.91	0.52	59,59,59,59	0
57	MG	1A	3541	1/1	0.91	0.21	59,59,59,59	0
57	MG	2A	3326	1/1	0.91	0.12	61,61,61,61	0
57	MG	1A	3685	1/1	0.91	0.13	36,36,36,36	0
57	MG	2A	3107	1/1	0.91	0.36	69,69,69,69	0
57	MG	2a	1602	1/1	0.91	0.33	70,70,70,70	0
57	MG	1A	3892	1/1	0.91	0.21	64,64,64,64	0
57	MG	1A	3469	1/1	0.91	0.20	31,31,31,31	0
57	MG	1A	3280	1/1	0.91	0.10	44,44,44,44	0
57	MG	1A	3798	1/1	0.91	0.11	73,73,73,73	0
57	MG	1A	3472	1/1	0.91	0.22	39,39,39,39	0
57	MG	1A	3118	1/1	0.91	0.14	37,37,37,37	0
57	MG	1A	3907	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3802	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3135	1/1	0.91	0.26	64,64,64,64	0
57	MG	2A	3136	1/1	0.91	0.20	45,45,45,45	0
57	MG	1Z	302	1/1	0.91	0.21	54,54,54,54	0
57	MG	2A	3601	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3603	1/1	0.91	0.11	65,65,65,65	0
57	MG	1A	4066	1/1	0.91	0.20	56,56,56,56	0
57	MG	1A	3809	1/1	0.91	0.11	43,43,43,43	0
57	MG	10	107	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3698	1/1	0.91	0.11	64,64,64,64	0
57	MG	1A	3422	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3611	1/1	0.91	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3006	1/1	0.91	0.09	38,38,38,38	0
57	MG	2A	3176	1/1	0.92	0.17	67,67,67,67	0
57	MG	1A	3123	1/1	0.92	0.30	41,41,41,41	0
57	MG	2A	3376	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3915	1/1	0.92	0.07	43,43,43,43	0
57	MG	1a	1811	1/1	0.92	0.15	53,53,53,53	0
57	MG	1A	3922	1/1	0.92	0.15	55,55,55,55	0
57	MG	1A	3530	1/1	0.92	0.45	50,50,50,50	0
57	MG	1A	4087	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3691	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3190	1/1	0.92	0.29	57,57,57,57	0
57	MG	1A	3806	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3228	1/1	0.92	0.14	46,46,46,46	0
57	MG	1A	3695	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3391	1/1	0.92	0.18	48,48,48,48	0
57	MG	1A	4098	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3091	1/1	0.92	0.21	56,56,56,56	0
57	MG	2A	3394	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	4100	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3396	1/1	0.92	0.11	39,39,39,39	0
57	MG	1a	1630	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3384	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3940	1/1	0.92	0.13	64,64,64,64	0
57	MG	2A	3663	1/1	0.92	0.17	54,54,54,54	0
57	MG	2A	3207	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3385	1/1	0.92	0.28	49,49,49,49	0
57	MG	1A	3321	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3213	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3671	1/1	0.92	0.12	65,65,65,65	0
57	MG	1A	3458	1/1	0.92	0.32	53,53,53,53	0
57	MG	1A	4106	1/1	0.92	0.16	53,53,53,53	0
57	MG	1A	4107	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3388	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3559	1/1	0.92	0.20	40,40,40,40	0
57	MG	2A	3418	1/1	0.92	0.24	60,60,60,60	0
57	MG	2A	3681	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3390	1/1	0.92	0.17	49,49,49,49	0
57	MG	1A	3172	1/1	0.92	0.13	39,39,39,39	0
57	MG	1a	1647	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3955	1/1	0.92	0.14	49,49,49,49	0
57	MG	1A	3961	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3963	1/1	0.92	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
57	MG	2A	3690	1/1	0.92	0.14	71,71,71,71	0
57	MG	1A	3965	1/1	0.92	0.09	69,69,69,69	0
57	MG	1A	3465	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3694	1/1	0.92	0.13	68,68,68,68	0
57	MG	1a	1653	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3070	1/1	0.92	0.18	35,35,35,35	0
57	MG	2A	3437	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3130	1/1	0.92	0.14	46,46,46,46	0
57	MG	1x	113	1/1	0.92	0.14	66,66,66,66	0
57	MG	2A	3442	1/1	0.92	0.16	65,65,65,65	0
57	MG	1B	213	1/1	0.92	0.26	61,61,61,61	0
57	MG	2A	3449	1/1	0.92	0.12	43,43,43,43	0
57	MG	2A	3002	1/1	0.92	0.28	63,63,63,63	0
57	MG	2A	3246	1/1	0.92	0.09	72,72,72,72	0
57	MG	1A	3004	1/1	0.92	0.10	34,34,34,34	0
57	MG	2A	3006	1/1	0.92	0.25	59,59,59,59	0
57	MG	1A	3036	1/1	0.92	0.07	51,51,51,51	0
57	MG	2A	3008	1/1	0.92	0.08	59,59,59,59	0
57	MG	1A	3575	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3286	1/1	0.92	0.35	60,60,60,60	0
57	MG	1A	3403	1/1	0.92	0.16	46,46,46,46	0
57	MG	1A	3081	1/1	0.92	0.08	41,41,41,41	0
57	MG	2A	3259	1/1	0.92	0.20	58,58,58,58	0
57	MG	1A	3289	1/1	0.92	0.11	52,52,52,52	0
57	MG	1a	1665	1/1	0.92	0.22	64,64,64,64	0
57	MG	1A	3984	1/1	0.92	0.08	15,15,15,15	0
57	MG	1A	3985	1/1	0.92	0.30	43,43,43,43	0
57	MG	1A	3587	1/1	0.92	0.12	49,49,49,49	0
57	MG	1A	3189	1/1	0.92	0.09	39,39,39,39	0
57	MG	2A	3478	1/1	0.92	0.15	55,55,55,55	0
57	MG	1a	1671	1/1	0.92	0.26	54,54,54,54	0
57	MG	2A	3482	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3047	1/1	0.92	0.06	31,31,31,31	0
57	MG	1A	3731	1/1	0.92	0.08	24,24,24,24	0
57	MG	1A	3410	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3340	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3046	1/1	0.92	0.31	63,63,63,63	0
57	MG	1B	235	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	4002	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3849	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3053	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3284	1/1	0.92	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3341	1/1	0.92	0.08	55,55,55,55	0
57	MG	1A	3342	1/1	0.92	0.23	54,54,54,54	0
57	MG	2A	3769	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3248	1/1	0.92	0.19	32,32,32,32	0
57	MG	2A	3289	1/1	0.92	0.10	64,64,64,64	0
57	MG	1A	3490	1/1	0.92	0.16	53,53,53,53	0
57	MG	1E	309	1/1	0.92	0.10	29,29,29,29	0
57	MG	1A	3856	1/1	0.92	0.09	38,38,38,38	0
57	MG	2A	3063	1/1	0.92	0.30	67,67,67,67	0
57	MG	1a	1696	1/1	0.92	0.19	58,58,58,58	0
57	MG	1a	1699	1/1	0.92	0.23	59,59,59,59	0
57	MG	1a	1700	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3294	1/1	0.92	0.31	60,60,60,60	0
57	MG	2A	3074	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3146	1/1	0.92	0.26	37,37,37,37	0
57	MG	1N	202	1/1	0.92	0.19	52,52,52,52	0
57	MG	1N	204	1/1	0.92	0.17	40,40,40,40	0
57	MG	2A	3306	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3112	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3793	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3531	1/1	0.92	0.09	42,42,42,42	0
57	MG	1A	3749	1/1	0.92	0.10	47,47,47,47	0
57	MG	1O	201	1/1	0.92	0.25	51,51,51,51	0
57	MG	2A	3536	1/1	0.92	0.14	55,55,55,55	0
57	MG	1O	202	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	3148	1/1	0.92	0.17	40,40,40,40	0
57	MG	1A	3201	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3091	1/1	0.92	0.10	63,63,63,63	0
57	MG	1A	4025	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3094	1/1	0.92	0.11	76,76,76,76	0
57	MG	1a	1730	1/1	0.92	0.12	61,61,61,61	0
57	MG	1A	3754	1/1	0.92	0.10	39,39,39,39	0
57	MG	1Q	202	1/1	0.92	0.14	34,34,34,34	0
57	MG	1A	4028	1/1	0.92	0.12	32,32,32,32	0
57	MG	1A	3301	1/1	0.92	0.22	36,36,36,36	0
57	MG	1A	3504	1/1	0.92	0.27	55,55,55,55	0
57	MG	1A	3062	1/1	0.92	0.24	54,54,54,54	0
57	MG	2A	3566	1/1	0.92	0.12	60,60,60,60	0
57	MG	2B	213	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3767	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3568	1/1	0.92	0.21	50,50,50,50	0
57	MG	1A	3304	1/1	0.92	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1R	205	1/1	0.92	0.11	34,34,34,34	0
57	MG	1a	1747	1/1	0.92	0.12	66,66,66,66	0
57	MG	1A	3360	1/1	0.92	0.13	53,53,53,53	0
57	MG	1A	3772	1/1	0.92	0.07	42,42,42,42	0
57	MG	2E	304	1/1	0.92	0.12	40,40,40,40	0
57	MG	1A	3435	1/1	0.92	0.09	60,60,60,60	0
57	MG	2A	3119	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3122	1/1	0.92	0.10	73,73,73,73	0
57	MG	1A	3306	1/1	0.92	0.14	46,46,46,46	0
57	MG	1A	3511	1/1	0.92	0.07	24,24,24,24	0
57	MG	2A	3129	1/1	0.92	0.23	59,59,59,59	0
57	MG	2Q	201	1/1	0.92	0.09	64,64,64,64	0
57	MG	2Q	202	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3780	1/1	0.92	0.08	22,22,22,22	0
57	MG	1A	3362	1/1	0.92	0.23	71,71,71,71	0
57	MG	2U	202	1/1	0.92	0.20	62,62,62,62	0
57	MG	2A	3586	1/1	0.92	0.13	63,63,63,63	0
57	MG	1A	3365	1/1	0.92	0.18	25,25,25,25	0
57	MG	2A	3344	1/1	0.92	0.26	53,53,53,53	0
57	MG	1a	1777	1/1	0.92	0.13	58,58,58,58	0
57	MG	2A	3140	1/1	0.92	0.28	60,60,60,60	0
57	MG	20	102	1/1	0.92	0.17	72,72,72,72	0
57	MG	1A	3310	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	4057	1/1	0.92	0.11	47,47,47,47	0
57	MG	1Z	303	1/1	0.92	0.23	59,59,59,59	0
57	MG	1A	3898	1/1	0.92	0.22	37,37,37,37	0
57	MG	1A	3372	1/1	0.92	0.30	68,68,68,68	0
57	MG	1a	1788	1/1	0.92	0.13	68,68,68,68	0
57	MG	28	101	1/1	0.92	0.31	64,64,64,64	0
57	MG	1A	3787	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3903	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3517	1/1	0.92	0.25	58,58,58,58	0
57	MG	1A	3677	1/1	0.92	0.15	30,30,30,30	0
57	MG	1A	3678	1/1	0.92	0.10	28,28,28,28	0
57	MG	2A	3609	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3087	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3050	1/1	0.92	0.08	24,24,24,24	0
57	MG	2A	3613	1/1	0.92	0.10	60,60,60,60	0
57	MG	1a	1798	1/1	0.92	0.10	63,63,63,63	0
57	MG	1a	1802	1/1	0.92	0.12	75,75,75,75	0
57	MG	1A	3261	1/1	0.92	0.18	49,49,49,49	0
57	MG	1a	1806	1/1	0.92	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3169	1/1	0.92	0.19	54,54,54,54	0
57	MG	1a	1601	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3621	1/1	0.92	0.17	65,65,65,65	0
57	MG	2A	3172	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3913	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3626	1/1	0.92	0.22	56,56,56,56	0
57	MG	2A	3373	1/1	0.92	0.12	71,71,71,71	0
57	MG	2A	3631	1/1	0.92	0.12	49,49,49,49	0
57	MG	1a	1776	1/1	0.93	0.09	50,50,50,50	0
57	MG	2A	3358	1/1	0.93	0.25	48,48,48,48	0
57	MG	1A	3778	1/1	0.93	0.17	50,50,50,50	0
57	MG	1A	3316	1/1	0.93	0.18	50,50,50,50	0
57	MG	1a	1781	1/1	0.93	0.12	60,60,60,60	0
57	MG	1Y	201	1/1	0.93	0.25	69,69,69,69	0
57	MG	1a	1783	1/1	0.93	0.30	70,70,70,70	0
57	MG	2A	3149	1/1	0.93	0.14	61,61,61,61	0
57	MG	1Y	202	1/1	0.93	0.32	53,53,53,53	0
57	MG	1A	3518	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3459	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3658	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3131	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3638	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3048	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3259	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3526	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3790	1/1	0.93	0.09	25,25,25,25	0
57	MG	2A	3164	1/1	0.93	0.13	50,50,50,50	0
57	MG	1A	3912	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3676	1/1	0.93	0.17	35,35,35,35	0
57	MG	1A	3322	1/1	0.93	0.22	60,60,60,60	0
57	MG	16	102	1/1	0.93	0.20	51,51,51,51	0
57	MG	1A	3324	1/1	0.93	0.18	45,45,45,45	0
57	MG	2A	3170	1/1	0.93	0.15	44,44,44,44	0
57	MG	1a	1805	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3918	1/1	0.93	0.10	78,78,78,78	0
57	MG	2A	3173	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3920	1/1	0.93	0.07	39,39,39,39	0
57	MG	1A	3409	1/1	0.93	0.10	41,41,41,41	0
57	MG	1a	1606	1/1	0.93	0.08	67,67,67,67	0
57	MG	2A	3178	1/1	0.93	0.16	59,59,59,59	0
57	MG	1A	4088	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3666	1/1	0.93	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3161	1/1	0.93	0.18	43,43,43,43	0
57	MG	1a	1812	1/1	0.93	0.17	73,73,73,73	0
57	MG	2A	3185	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3186	1/1	0.93	0.07	57,57,57,57	0
57	MG	1A	3096	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3265	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3804	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	1619	1/1	0.93	0.07	56,56,56,56	0
57	MG	1a	1620	1/1	0.93	0.08	61,61,61,61	0
57	MG	2A	3407	1/1	0.93	0.09	54,54,54,54	0
57	MG	1a	1819	1/1	0.93	0.09	76,76,76,76	0
57	MG	2A	3194	1/1	0.93	0.12	65,65,65,65	0
57	MG	1A	3930	1/1	0.93	0.11	67,67,67,67	0
57	MG	2A	3197	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3934	1/1	0.93	0.07	72,72,72,72	0
57	MG	2A	3416	1/1	0.93	0.09	53,53,53,53	0
57	MG	1A	3936	1/1	0.93	0.11	66,66,66,66	0
57	MG	1A	3546	1/1	0.93	0.17	41,41,41,41	0
57	MG	1f	202	1/1	0.93	0.07	70,70,70,70	0
57	MG	2A	3692	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3203	1/1	0.93	0.09	52,52,52,52	0
57	MG	1a	1626	1/1	0.93	0.22	51,51,51,51	0
57	MG	1A	3808	1/1	0.93	0.08	29,29,29,29	0
57	MG	1A	3369	1/1	0.93	0.50	44,44,44,44	0
57	MG	1A	3552	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3371	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3556	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3103	1/1	0.93	0.12	42,42,42,42	0
57	MG	2A	3217	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3124	1/1	0.93	0.32	37,37,37,37	0
57	MG	1A	4110	1/1	0.93	0.10	36,36,36,36	0
57	MG	1A	3299	1/1	0.93	0.24	70,70,70,70	0
57	MG	2A	3712	1/1	0.93	0.12	66,66,66,66	0
57	MG	2A	3713	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3445	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3375	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3376	1/1	0.93	0.17	37,37,37,37	0
57	MG	2A	3718	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3719	1/1	0.93	0.08	65,65,65,65	0
57	MG	1a	1641	1/1	0.93	0.26	53,53,53,53	0
57	MG	2A	3452	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3482	1/1	0.93	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3960	1/1	0.93	0.19	76,76,76,76	0
57	MG	1A	3426	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3962	1/1	0.93	0.14	74,74,74,74	0
57	MG	2A	3729	1/1	0.93	0.14	62,62,62,62	0
57	MG	1x	104	1/1	0.93	0.20	67,67,67,67	0
57	MG	2A	3233	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3569	1/1	0.93	0.29	48,48,48,48	0
57	MG	2A	3236	1/1	0.93	0.16	61,61,61,61	0
57	MG	1B	210	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3105	1/1	0.93	0.34	44,44,44,44	0
57	MG	1A	3486	1/1	0.93	0.22	37,37,37,37	0
57	MG	2A	3743	1/1	0.93	0.09	64,64,64,64	0
57	MG	1x	110	1/1	0.93	0.18	67,67,67,67	0
57	MG	2A	3242	1/1	0.93	0.26	56,56,56,56	0
57	MG	2A	3748	1/1	0.93	0.09	69,69,69,69	0
57	MG	1A	3487	1/1	0.93	0.20	42,42,42,42	0
57	MG	1x	112	1/1	0.93	0.25	67,67,67,67	0
57	MG	2A	3752	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3336	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3379	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3491	1/1	0.93	0.20	36,36,36,36	0
57	MG	2A	3481	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3584	1/1	0.93	0.06	41,41,41,41	0
57	MG	1A	3722	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3977	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3254	1/1	0.93	0.14	66,66,66,66	0
57	MG	1A	3835	1/1	0.93	0.18	68,68,68,68	0
57	MG	1A	3492	1/1	0.93	0.11	56,56,56,56	0
57	MG	1B	225	1/1	0.93	0.16	57,57,57,57	0
57	MG	1A	3980	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3017	1/1	0.93	0.26	54,54,54,54	0
57	MG	1A	3090	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3498	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3019	1/1	0.93	0.07	44,44,44,44	0
57	MG	1A	3303	1/1	0.93	0.24	40,40,40,40	0
57	MG	1B	229	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3026	1/1	0.93	0.22	56,56,56,56	0
57	MG	1A	3383	1/1	0.93	0.16	56,56,56,56	0
57	MG	1A	3497	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3129	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3846	1/1	0.93	0.07	53,53,53,53	0
57	MG	1a	1672	1/1	0.93	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1673	1/1	0.93	0.32	60,60,60,60	0
57	MG	1A	3305	1/1	0.93	0.22	60,60,60,60	0
57	MG	2A	3519	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3732	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3015	1/1	0.93	0.30	51,51,51,51	0
57	MG	2A	3045	1/1	0.93	0.18	48,48,48,48	0
57	MG	1D	303	1/1	0.93	0.13	40,40,40,40	0
57	MG	1a	1678	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3309	1/1	0.93	0.15	48,48,48,48	0
57	MG	2A	3051	1/1	0.93	0.05	51,51,51,51	0
57	MG	1A	3220	1/1	0.93	0.18	54,54,54,54	0
57	MG	1A	3348	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3612	1/1	0.93	0.15	55,55,55,55	0
57	MG	1A	3618	1/1	0.93	0.08	21,21,21,21	0
57	MG	2A	3535	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3056	1/1	0.93	0.15	66,66,66,66	0
57	MG	2B	206	1/1	0.93	0.10	71,71,71,71	0
57	MG	1E	310	1/1	0.93	0.12	33,33,33,33	0
57	MG	1A	3180	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3060	1/1	0.93	0.16	51,51,51,51	0
57	MG	1F	302	1/1	0.93	0.17	35,35,35,35	0
57	MG	1F	304	1/1	0.93	0.13	42,42,42,42	0
57	MG	1F	308	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3620	1/1	0.93	0.10	22,22,22,22	0
57	MG	2A	3550	1/1	0.93	0.12	61,61,61,61	0
57	MG	1A	3861	1/1	0.93	0.23	39,39,39,39	0
57	MG	2A	3554	1/1	0.93	0.17	54,54,54,54	0
57	MG	2D	302	1/1	0.93	0.33	72,72,72,72	0
57	MG	2A	3069	1/1	0.93	0.08	57,57,57,57	0
57	MG	1G	202	1/1	0.93	0.15	64,64,64,64	0
57	MG	1H	201	1/1	0.93	0.17	54,54,54,54	0
57	MG	1A	4013	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3746	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	4015	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3508	1/1	0.93	0.19	44,44,44,44	0
57	MG	1a	1717	1/1	0.93	0.09	61,61,61,61	0
57	MG	2F	301	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3083	1/1	0.93	0.14	63,63,63,63	0
57	MG	2F	303	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3570	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3224	1/1	0.93	0.25	48,48,48,48	0
57	MG	1A	3395	1/1	0.93	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3628	1/1	0.93	0.11	23,23,23,23	0
57	MG	1A	3753	1/1	0.93	0.13	32,32,32,32	0
57	MG	2T	201	1/1	0.93	0.10	62,62,62,62	0
57	MG	2T	202	1/1	0.93	0.13	52,52,52,52	0
57	MG	2T	203	1/1	0.93	0.11	72,72,72,72	0
57	MG	1A	3873	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3630	1/1	0.93	0.10	66,66,66,66	0
57	MG	1Q	201	1/1	0.93	0.21	41,41,41,41	0
57	MG	1a	1732	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	4031	1/1	0.93	0.08	49,49,49,49	0
57	MG	2X	101	1/1	0.93	0.18	61,61,61,61	0
57	MG	1A	3182	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3633	1/1	0.93	0.08	36,36,36,36	0
57	MG	2A	3584	1/1	0.93	0.08	37,37,37,37	0
57	MG	1a	1738	1/1	0.93	0.09	63,63,63,63	0
57	MG	2A	3101	1/1	0.93	0.17	48,48,48,48	0
57	MG	2I	103	1/1	0.93	0.13	54,54,54,54	0
57	MG	1A	3879	1/1	0.93	0.08	26,26,26,26	0
57	MG	1A	3880	1/1	0.93	0.07	25,25,25,25	0
57	MG	1A	3397	1/1	0.93	0.22	48,48,48,48	0
57	MG	2A	3333	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3637	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3593	1/1	0.93	0.12	78,78,78,78	0
57	MG	2A	3594	1/1	0.93	0.23	49,49,49,49	0
57	MG	1a	1744	1/1	0.93	0.08	64,64,64,64	0
57	MG	1A	3768	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3455	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3398	1/1	0.93	0.11	55,55,55,55	0
57	MG	1a	1750	1/1	0.93	0.15	78,78,78,78	0
57	MG	2A	3115	1/1	0.93	0.24	67,67,67,67	0
57	MG	1a	1751	1/1	0.93	0.09	71,71,71,71	0
57	MG	2A	3346	1/1	0.93	0.31	63,63,63,63	0
57	MG	2A	3606	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3118	1/1	0.93	0.29	68,68,68,68	0
57	MG	1S	202	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3643	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3124	1/1	0.93	0.13	52,52,52,52	0
57	MG	1A	3645	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3649	1/1	0.93	0.07	27,27,27,27	0
57	MG	1A	3255	1/1	0.93	0.14	57,57,57,57	0
57	MG	1a	1769	1/1	0.93	0.09	81,81,81,81	0
57	MG	1W	201	1/1	0.93	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3896	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3215	1/1	0.94	0.14	56,56,56,56	0
57	MG	2A	3630	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3820	1/1	0.94	0.31	45,45,45,45	0
57	MG	1A	3821	1/1	0.94	0.06	38,38,38,38	0
57	MG	2A	3162	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3106	1/1	0.94	0.28	33,33,33,33	0
57	MG	1A	3950	1/1	0.94	0.05	33,33,33,33	0
57	MG	1A	3023	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3017	1/1	0.94	0.09	33,33,33,33	0
57	MG	1A	4112	1/1	0.94	0.14	55,55,55,55	0
57	MG	1A	3954	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3641	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3715	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3223	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3307	1/1	0.94	0.20	63,63,63,63	0
57	MG	1A	3354	1/1	0.94	0.24	37,37,37,37	0
57	MG	1A	3600	1/1	0.94	0.10	46,46,46,46	0
57	MG	1B	205	1/1	0.94	0.29	62,62,62,62	0
57	MG	1B	207	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3654	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3601	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3179	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3308	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	3607	1/1	0.94	0.20	60,60,60,60	0
57	MG	2A	3183	1/1	0.94	0.26	54,54,54,54	0
57	MG	1A	3834	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3608	1/1	0.94	0.10	31,31,31,31	0
57	MG	1a	1640	1/1	0.94	0.13	54,54,54,54	0
57	MG	1A	3462	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3399	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3114	1/1	0.94	0.28	51,51,51,51	0
57	MG	1A	3464	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3225	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3191	1/1	0.94	0.30	66,66,66,66	0
57	MG	1A	3266	1/1	0.94	0.16	42,42,42,42	0
57	MG	1A	3844	1/1	0.94	0.14	63,63,63,63	0
57	MG	1B	221	1/1	0.94	0.10	46,46,46,46	0
57	MG	1w	105	1/1	0.94	0.14	63,63,63,63	0
57	MG	2A	3675	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3622	1/1	0.94	0.09	34,34,34,34	0
57	MG	2A	3677	1/1	0.94	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3624	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	3268	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3626	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3417	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3739	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3684	1/1	0.94	0.08	46,46,46,46	0
57	MG	2A	3685	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3468	1/1	0.94	0.23	48,48,48,48	0
57	MG	1x	103	1/1	0.94	0.11	55,55,55,55	0
57	MG	1A	3991	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3742	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3208	1/1	0.94	0.13	66,66,66,66	0
57	MG	2A	3210	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3994	1/1	0.94	0.05	32,32,32,32	0
57	MG	2A	3430	1/1	0.94	0.19	71,71,71,71	0
57	MG	1A	3177	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3695	1/1	0.94	0.11	49,49,49,49	0
57	MG	1B	232	1/1	0.94	0.09	72,72,72,72	0
57	MG	2A	3697	1/1	0.94	0.18	74,74,74,74	0
57	MG	2A	3698	1/1	0.94	0.07	60,60,60,60	0
57	MG	1A	3528	1/1	0.94	0.13	40,40,40,40	0
57	MG	1A	3529	1/1	0.94	0.18	38,38,38,38	0
57	MG	1A	3470	1/1	0.94	0.20	30,30,30,30	0
57	MG	2A	3702	1/1	0.94	0.10	46,46,46,46	0
57	MG	2A	3703	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3531	1/1	0.94	0.13	46,46,46,46	0
57	MG	1x	114	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3444	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3860	1/1	0.94	0.14	37,37,37,37	0
57	MG	1D	302	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3004	1/1	0.94	0.29	67,67,67,67	0
57	MG	2A	3450	1/1	0.94	0.13	62,62,62,62	0
57	MG	1a	1668	1/1	0.94	0.07	70,70,70,70	0
57	MG	1A	3232	1/1	0.94	0.24	37,37,37,37	0
57	MG	2A	3227	1/1	0.94	0.09	60,60,60,60	0
57	MG	1D	307	1/1	0.94	0.29	45,45,45,45	0
57	MG	1A	3534	1/1	0.94	0.22	60,60,60,60	0
57	MG	1A	3751	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	4009	1/1	0.94	0.10	61,61,61,61	0
57	MG	2A	3012	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3014	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3233	1/1	0.94	0.27	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4011	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3868	1/1	0.94	0.06	30,30,30,30	0
57	MG	1A	3279	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3464	1/1	0.94	0.10	39,39,39,39	0
57	MG	1E	312	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3022	1/1	0.94	0.24	47,47,47,47	0
57	MG	1a	1679	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3735	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3024	1/1	0.94	0.10	60,60,60,60	0
57	MG	2A	3475	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3025	1/1	0.94	0.13	54,54,54,54	0
57	MG	1E	314	1/1	0.94	0.05	36,36,36,36	0
57	MG	1A	3054	1/1	0.94	0.26	49,49,49,49	0
57	MG	2A	3251	1/1	0.94	0.22	54,54,54,54	0
57	MG	2A	3029	1/1	0.94	0.09	68,68,68,68	0
57	MG	2A	3483	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3648	1/1	0.94	0.07	23,23,23,23	0
57	MG	1F	305	1/1	0.94	0.13	43,43,43,43	0
57	MG	2A	3255	1/1	0.94	0.27	62,62,62,62	0
57	MG	1A	3760	1/1	0.94	0.07	26,26,26,26	0
57	MG	1a	1687	1/1	0.94	0.17	55,55,55,55	0
57	MG	1a	1690	1/1	0.94	0.27	58,58,58,58	0
57	MG	1A	3421	1/1	0.94	0.24	40,40,40,40	0
57	MG	1A	3764	1/1	0.94	0.08	33,33,33,33	0
57	MG	1F	312	1/1	0.94	0.19	56,56,56,56	0
57	MG	1A	3543	1/1	0.94	0.17	38,38,38,38	0
57	MG	1G	203	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3766	1/1	0.94	0.06	49,49,49,49	0
57	MG	1a	1697	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3501	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3770	1/1	0.94	0.17	62,62,62,62	0
57	MG	1a	1698	1/1	0.94	0.08	46,46,46,46	0
57	MG	1A	3236	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3774	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3775	1/1	0.94	0.09	65,65,65,65	0
57	MG	1A	3075	1/1	0.94	0.25	44,44,44,44	0
57	MG	2A	3509	1/1	0.94	0.20	65,65,65,65	0
57	MG	1a	1701	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3654	1/1	0.94	0.06	30,30,30,30	0
57	MG	1A	3551	1/1	0.94	0.29	42,42,42,42	0
57	MG	2A	3276	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3516	1/1	0.94	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3277	1/1	0.94	0.26	69,69,69,69	0
57	MG	1A	3657	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3787	1/1	0.94	0.16	60,60,60,60	0
57	MG	1A	4033	1/1	0.94	0.07	50,50,50,50	0
57	MG	1A	3076	1/1	0.94	0.20	53,53,53,53	0
57	MG	1a	1712	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3056	1/1	0.94	0.07	50,50,50,50	0
57	MG	1a	1716	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3667	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3192	1/1	0.94	0.22	39,39,39,39	0
57	MG	1A	3242	1/1	0.94	0.19	59,59,59,59	0
57	MG	2A	3288	1/1	0.94	0.13	78,78,78,78	0
57	MG	2A	3068	1/1	0.94	0.16	52,52,52,52	0
57	MG	2A	3293	1/1	0.94	0.12	63,63,63,63	0
57	MG	2A	3801	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3802	1/1	0.94	0.08	59,59,59,59	0
57	MG	1a	1723	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3043	1/1	0.94	0.27	31,31,31,31	0
57	MG	2A	3805	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	4043	1/1	0.94	0.05	25,25,25,25	0
57	MG	1A	3561	1/1	0.94	0.16	35,35,35,35	0
57	MG	1a	1729	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3077	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3078	1/1	0.94	0.21	57,57,57,57	0
57	MG	1A	3897	1/1	0.94	0.21	40,40,40,40	0
57	MG	2A	3545	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	4047	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3784	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3548	1/1	0.94	0.20	68,68,68,68	0
57	MG	1A	3290	1/1	0.94	0.20	48,48,48,48	0
57	MG	1R	201	1/1	0.94	0.16	45,45,45,45	0
57	MG	1a	1735	1/1	0.94	0.12	68,68,68,68	0
57	MG	2A	3557	1/1	0.94	0.11	46,46,46,46	0
57	MG	1A	3084	1/1	0.94	0.21	44,44,44,44	0
57	MG	2A	3559	1/1	0.94	0.11	72,72,72,72	0
57	MG	2D	301	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3030	1/1	0.94	0.10	33,33,33,33	0
57	MG	1A	3016	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3906	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3682	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3200	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3568	1/1	0.94	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1U	204	1/1	0.94	0.33	46,46,46,46	0
57	MG	1A	3686	1/1	0.94	0.05	24,24,24,24	0
57	MG	1A	3065	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3570	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3799	1/1	0.94	0.08	56,56,56,56	0
57	MG	1W	205	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3692	1/1	0.94	0.07	33,33,33,33	0
57	MG	1X	104	1/1	0.94	0.20	45,45,45,45	0
57	MG	2P	201	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	3386	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1757	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3579	1/1	0.94	0.19	68,68,68,68	0
57	MG	1A	3442	1/1	0.94	0.24	59,59,59,59	0
57	MG	1A	3803	1/1	0.94	0.20	26,26,26,26	0
57	MG	1Z	301	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3114	1/1	0.94	0.21	61,61,61,61	0
57	MG	1A	3250	1/1	0.94	0.08	44,44,44,44	0
57	MG	2U	203	1/1	0.94	0.15	68,68,68,68	0
57	MG	1a	1773	1/1	0.94	0.07	71,71,71,71	0
57	MG	1a	1775	1/1	0.94	0.07	70,70,70,70	0
57	MG	1A	3805	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3120	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	4077	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3204	1/1	0.94	0.18	52,52,52,52	0
57	MG	2A	3337	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	4082	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3252	1/1	0.94	0.12	66,66,66,66	0
57	MG	2A	3127	1/1	0.94	0.27	68,68,68,68	0
57	MG	11	104	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3130	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3131	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3600	1/1	0.94	0.08	71,71,71,71	0
57	MG	2A	3134	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3165	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3700	1/1	0.94	0.07	48,48,48,48	0
57	MG	12	101	1/1	0.94	0.17	51,51,51,51	0
57	MG	13	103	1/1	0.94	0.07	51,51,51,51	0
57	MG	1A	3812	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3343	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	4094	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3133	1/1	0.94	0.25	35,35,35,35	0
57	MG	1A	3347	1/1	0.94	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3612	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3145	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3146	1/1	0.94	0.22	58,58,58,58	0
57	MG	2A	3147	1/1	0.94	0.14	69,69,69,69	0
57	MG	1A	4097	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3706	1/1	0.94	0.22	48,48,48,48	0
57	MG	1a	1796	1/1	0.94	0.10	66,66,66,66	0
57	MG	1A	3707	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3943	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3944	1/1	0.94	0.07	44,44,44,44	0
57	MG	2A	3367	1/1	0.94	0.39	65,65,65,65	0
57	MG	1A	3451	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3103	1/1	0.95	0.17	55,55,55,55	0
57	MG	1A	3933	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3756	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3282	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3935	1/1	0.95	0.07	61,61,61,61	0
57	MG	2A	3678	1/1	0.95	0.06	61,61,61,61	0
57	MG	2A	3470	1/1	0.95	0.15	39,39,39,39	0
57	MG	1a	1803	1/1	0.95	0.13	62,62,62,62	0
57	MG	1A	3432	1/1	0.95	0.10	39,39,39,39	0
57	MG	1a	1642	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	4046	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3758	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3589	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3290	1/1	0.95	0.21	65,65,65,65	0
57	MG	1A	3219	1/1	0.95	0.19	37,37,37,37	0
57	MG	2A	3116	1/1	0.95	0.08	56,56,56,56	0
57	MG	1F	301	1/1	0.95	0.16	30,30,30,30	0
57	MG	1A	3137	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3942	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	4054	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3681	1/1	0.95	0.10	29,29,29,29	0
57	MG	1a	1815	1/1	0.95	0.09	74,74,74,74	0
57	MG	1F	309	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3008	1/1	0.95	0.05	23,23,23,23	0
57	MG	2A	3497	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3848	1/1	0.95	0.05	42,42,42,42	0
57	MG	2A	3128	1/1	0.95	0.24	47,47,47,47	0
57	MG	1A	3683	1/1	0.95	0.08	33,33,33,33	0
57	MG	1F	313	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3594	1/1	0.95	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3504	1/1	0.95	0.24	64,64,64,64	0
57	MG	2A	3133	1/1	0.95	0.19	70,70,70,70	0
57	MG	2A	3507	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3523	1/1	0.95	0.20	42,42,42,42	0
57	MG	1e	201	1/1	0.95	0.11	69,69,69,69	0
57	MG	1G	205	1/1	0.95	0.15	57,57,57,57	0
57	MG	1f	201	1/1	0.95	0.19	52,52,52,52	0
57	MG	1A	3525	1/1	0.95	0.10	55,55,55,55	0
57	MG	1a	1662	1/1	0.95	0.10	48,48,48,48	0
57	MG	1N	201	1/1	0.95	0.15	40,40,40,40	0
57	MG	1A	3179	1/1	0.95	0.18	50,50,50,50	0
57	MG	1n	101	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3717	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	4067	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3689	1/1	0.95	0.05	31,31,31,31	0
57	MG	1A	3952	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3522	1/1	0.95	0.08	66,66,66,66	0
57	MG	1A	3478	1/1	0.95	0.16	40,40,40,40	0
57	MG	2A	3148	1/1	0.95	0.08	61,61,61,61	0
57	MG	1A	3028	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3526	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3115	1/1	0.95	0.19	27,27,27,27	0
57	MG	1A	3956	1/1	0.95	0.16	69,69,69,69	0
57	MG	1A	3183	1/1	0.95	0.25	39,39,39,39	0
57	MG	1A	3532	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	4079	1/1	0.95	0.06	29,29,29,29	0
57	MG	2A	3533	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	4080	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3862	1/1	0.95	0.25	35,35,35,35	0
57	MG	1A	3327	1/1	0.95	0.27	46,46,46,46	0
57	MG	1A	3865	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	4086	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3010	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3967	1/1	0.95	0.14	71,71,71,71	0
57	MG	2A	3542	1/1	0.95	0.06	39,39,39,39	0
57	MG	1x	105	1/1	0.95	0.21	53,53,53,53	0
57	MG	2A	3544	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3609	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3755	1/1	0.95	0.11	83,83,83,83	0
57	MG	1A	3611	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3031	1/1	0.95	0.17	26,26,26,26	0
57	MG	2A	3758	1/1	0.95	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3971	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3549	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3345	1/1	0.95	0.40	65,65,65,65	0
57	MG	2A	3551	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3613	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3121	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3555	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3405	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3489	1/1	0.95	0.30	38,38,38,38	0
57	MG	1V	203	1/1	0.95	0.14	30,30,30,30	0
57	MG	1A	3055	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3194	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3773	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3450	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3563	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3180	1/1	0.95	0.24	56,56,56,56	0
57	MG	2A	3565	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3982	1/1	0.95	0.11	47,47,47,47	0
57	MG	1W	204	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3333	1/1	0.95	0.09	35,35,35,35	0
57	MG	1a	1702	1/1	0.95	0.19	61,61,61,61	0
57	MG	1A	3881	1/1	0.95	0.08	19,19,19,19	0
57	MG	1a	1704	1/1	0.95	0.06	51,51,51,51	0
57	MG	2A	3572	1/1	0.95	0.26	56,56,56,56	0
57	MG	2A	3361	1/1	0.95	0.10	44,44,44,44	0
57	MG	1X	101	1/1	0.95	0.25	41,41,41,41	0
57	MG	1A	3014	1/1	0.95	0.20	44,44,44,44	0
57	MG	1A	3986	1/1	0.95	0.09	24,24,24,24	0
57	MG	1X	106	1/1	0.95	0.08	42,42,42,42	0
57	MG	1X	107	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3495	1/1	0.95	0.06	68,68,68,68	0
57	MG	1a	1715	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3555	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3454	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3557	1/1	0.95	0.23	47,47,47,47	0
57	MG	1a	1721	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3272	1/1	0.95	0.25	35,35,35,35	0
57	MG	10	101	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3273	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3588	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3030	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3996	1/1	0.95	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1726	1/1	0.95	0.15	60,60,60,60	0
57	MG	2A	3206	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3412	1/1	0.95	0.10	42,42,42,42	0
57	MG	2A	3034	1/1	0.95	0.13	53,53,53,53	0
57	MG	11	101	1/1	0.95	0.25	42,42,42,42	0
57	MG	2A	3596	1/1	0.95	0.09	64,64,64,64	0
57	MG	2A	3039	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3998	1/1	0.95	0.06	40,40,40,40	0
57	MG	11	103	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3810	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3639	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3602	1/1	0.95	0.19	57,57,57,57	0
57	MG	1A	3019	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	4004	1/1	0.95	0.09	76,76,76,76	0
57	MG	13	102	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3049	1/1	0.95	0.20	50,50,50,50	0
57	MG	1A	3563	1/1	0.95	0.19	45,45,45,45	0
57	MG	14	101	1/1	0.95	0.09	74,74,74,74	0
57	MG	2D	304	1/1	0.95	0.12	35,35,35,35	0
57	MG	2D	305	1/1	0.95	0.26	42,42,42,42	0
57	MG	1a	1740	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3642	1/1	0.95	0.08	46,46,46,46	0
57	MG	15	105	1/1	0.95	0.13	40,40,40,40	0
57	MG	2E	303	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3228	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	3414	1/1	0.95	0.10	62,62,62,62	0
57	MG	2A	3614	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3003	1/1	0.95	0.06	25,25,25,25	0
57	MG	16	101	1/1	0.95	0.09	56,56,56,56	0
57	MG	2A	3232	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3904	1/1	0.95	0.14	55,55,55,55	0
57	MG	2A	3234	1/1	0.95	0.13	72,72,72,72	0
57	MG	17	103	1/1	0.95	0.16	37,37,37,37	0
57	MG	18	101	1/1	0.95	0.16	59,59,59,59	0
57	MG	2A	3622	1/1	0.95	0.11	66,66,66,66	0
57	MG	2A	3623	1/1	0.95	0.13	62,62,62,62	0
57	MG	2Q	204	1/1	0.95	0.16	59,59,59,59	0
57	MG	1A	3025	1/1	0.95	0.32	59,59,59,59	0
57	MG	1A	3045	1/1	0.95	0.09	46,46,46,46	0
57	MG	2A	3064	1/1	0.95	0.30	62,62,62,62	0
57	MG	1B	217	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3241	1/1	0.95	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3421	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3066	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3170	1/1	0.95	0.06	22,22,22,22	0
57	MG	1a	1605	1/1	0.95	0.11	60,60,60,60	0
57	MG	2W	202	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3205	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3088	1/1	0.95	0.24	57,57,57,57	0
57	MG	1A	3346	1/1	0.95	0.11	57,57,57,57	0
57	MG	2A	3072	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3431	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3655	1/1	0.95	0.06	23,23,23,23	0
57	MG	1a	1613	1/1	0.95	0.15	63,63,63,63	0
57	MG	1A	4019	1/1	0.95	0.14	52,52,52,52	0
57	MG	1a	1616	1/1	0.95	0.09	67,67,67,67	0
57	MG	2A	3647	1/1	0.95	0.18	54,54,54,54	0
57	MG	1A	3110	1/1	0.95	0.14	39,39,39,39	0
57	MG	27	101	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3576	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3650	1/1	0.95	0.28	61,61,61,61	0
57	MG	2a	1601	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3441	1/1	0.95	0.12	46,46,46,46	0
57	MG	2A	3652	1/1	0.95	0.09	70,70,70,70	0
57	MG	1a	1778	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	4023	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3579	1/1	0.95	0.15	48,48,48,48	0
57	MG	2A	3260	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3661	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3086	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3917	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	4027	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3662	1/1	0.95	0.14	22,22,22,22	0
57	MG	1A	3111	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3427	1/1	0.95	0.11	60,60,60,60	0
57	MG	2A	3664	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3923	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3515	1/1	0.95	0.22	60,60,60,60	0
57	MG	1A	4036	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3313	1/1	0.95	0.17	49,49,49,49	0
57	MG	1A	3285	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3674	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3026	1/1	0.95	0.17	42,42,42,42	0
58	K	2A	3377	1/1	0.95	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3021	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3007	1/1	0.96	0.06	25,25,25,25	0
57	MG	1A	3664	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3931	1/1	0.96	0.05	51,51,51,51	0
57	MG	1A	3665	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3221	1/1	0.96	0.27	47,47,47,47	0
57	MG	15	107	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3711	1/1	0.96	0.07	59,59,59,59	0
57	MG	1A	3270	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3035	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3074	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3539	1/1	0.96	0.12	54,54,54,54	0
57	MG	17	101	1/1	0.96	0.12	35,35,35,35	0
57	MG	17	102	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3841	1/1	0.96	0.11	21,21,21,21	0
57	MG	17	104	1/1	0.96	0.08	57,57,57,57	0
57	MG	1A	3274	1/1	0.96	0.17	51,51,51,51	0
57	MG	18	102	1/1	0.96	0.15	47,47,47,47	0
57	MG	18	103	1/1	0.96	0.17	44,44,44,44	0
57	MG	2A	3196	1/1	0.96	0.31	65,65,65,65	0
57	MG	1A	3044	1/1	0.96	0.13	35,35,35,35	0
57	MG	2A	3725	1/1	0.96	0.06	59,59,59,59	0
57	MG	2A	3727	1/1	0.96	0.08	56,56,56,56	0
57	MG	2A	3043	1/1	0.96	0.06	56,56,56,56	0
57	MG	19	101	1/1	0.96	0.19	42,42,42,42	0
57	MG	1A	3941	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3552	1/1	0.96	0.09	40,40,40,40	0
57	MG	2A	3201	1/1	0.96	0.11	67,67,67,67	0
57	MG	1A	3061	1/1	0.96	0.08	53,53,53,53	0
57	MG	1a	1603	1/1	0.96	0.09	62,62,62,62	0
57	MG	1D	305	1/1	0.96	0.06	39,39,39,39	0
57	MG	1D	306	1/1	0.96	0.16	41,41,41,41	0
57	MG	2A	3738	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3739	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	3139	1/1	0.96	0.10	49,49,49,49	0
57	MG	1D	309	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	4048	1/1	0.96	0.10	14,14,14,14	0
57	MG	2A	3209	1/1	0.96	0.10	59,59,59,59	0
57	MG	1a	1609	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3759	1/1	0.96	0.10	19,19,19,19	0
57	MG	1E	302	1/1	0.96	0.13	40,40,40,40	0
57	MG	2A	3751	1/1	0.96	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1E	305	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	1615	1/1	0.96	0.15	53,53,53,53	0
57	MG	2A	3059	1/1	0.96	0.13	56,56,56,56	0
57	MG	1a	1761	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	3416	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3524	1/1	0.96	0.22	34,34,34,34	0
57	MG	1A	3850	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3763	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3852	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3319	1/1	0.96	0.38	47,47,47,47	0
57	MG	1E	313	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3765	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3320	1/1	0.96	0.08	46,46,46,46	0
57	MG	1a	1627	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3419	1/1	0.96	0.21	43,43,43,43	0
57	MG	1F	303	1/1	0.96	0.17	40,40,40,40	0
57	MG	2A	3073	1/1	0.96	0.32	49,49,49,49	0
57	MG	1A	3140	1/1	0.96	0.07	58,58,58,58	0
57	MG	1a	1784	1/1	0.96	0.20	57,57,57,57	0
57	MG	1A	4063	1/1	0.96	0.14	40,40,40,40	0
57	MG	1F	306	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	3077	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3777	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3080	1/1	0.96	0.11	59,59,59,59	0
57	MG	2A	3779	1/1	0.96	0.08	59,59,59,59	0
57	MG	1A	3234	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3959	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3771	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3406	1/1	0.96	0.18	52,52,52,52	0
57	MG	1A	3602	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3687	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3184	1/1	0.96	0.28	30,30,30,30	0
57	MG	1A	3864	1/1	0.96	0.11	30,30,30,30	0
57	MG	2A	3411	1/1	0.96	0.24	54,54,54,54	0
57	MG	1G	204	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3606	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3249	1/1	0.96	0.27	75,75,75,75	0
57	MG	1a	1797	1/1	0.96	0.16	57,57,57,57	0
57	MG	2A	3092	1/1	0.96	0.09	60,60,60,60	0
57	MG	1a	1644	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3142	1/1	0.96	0.26	36,36,36,36	0
57	MG	1A	3187	1/1	0.96	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3188	1/1	0.96	0.18	34,34,34,34	0
57	MG	1A	3610	1/1	0.96	0.10	29,29,29,29	0
57	MG	1A	3079	1/1	0.96	0.17	36,36,36,36	0
57	MG	2A	3100	1/1	0.96	0.18	57,57,57,57	0
57	MG	1A	3380	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3974	1/1	0.96	0.11	30,30,30,30	0
57	MG	1A	4084	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3262	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3263	1/1	0.96	0.21	70,70,70,70	0
57	MG	2A	3104	1/1	0.96	0.18	42,42,42,42	0
57	MG	2A	3265	1/1	0.96	0.20	56,56,56,56	0
57	MG	1A	3483	1/1	0.96	0.23	56,56,56,56	0
57	MG	2A	3439	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3098	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3268	1/1	0.96	0.06	58,58,58,58	0
57	MG	1P	202	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3119	1/1	0.96	0.27	43,43,43,43	0
57	MG	1A	4090	1/1	0.96	0.07	28,28,28,28	0
57	MG	2A	3446	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3548	1/1	0.96	0.22	29,29,29,29	0
57	MG	1A	3120	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3434	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3705	1/1	0.96	0.12	58,58,58,58	0
57	MG	1A	3334	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3797	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3885	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3886	1/1	0.96	0.10	32,32,32,32	0
57	MG	1R	202	1/1	0.96	0.15	35,35,35,35	0
57	MG	1A	3553	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	3053	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3197	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3153	1/1	0.96	0.36	37,37,37,37	0
57	MG	1A	3629	1/1	0.96	0.08	17,17,17,17	0
57	MG	1A	3122	1/1	0.96	0.22	33,33,33,33	0
57	MG	1A	3714	1/1	0.96	0.09	50,50,50,50	0
57	MG	1U	202	1/1	0.96	0.29	36,36,36,36	0
57	MG	1A	3558	1/1	0.96	0.17	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.26	32,32,32,32	0
57	MG	2A	3291	1/1	0.96	0.22	65,65,65,65	0
57	MG	2F	306	1/1	0.96	0.23	53,53,53,53	0
57	MG	2A	3469	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3132	1/1	0.96	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3471	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3473	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	4108	1/1	0.96	0.07	59,59,59,59	0
57	MG	1V	204	1/1	0.96	0.20	50,50,50,50	0
57	MG	1V	205	1/1	0.96	0.12	34,34,34,34	0
57	MG	2R	202	1/1	0.96	0.19	52,52,52,52	0
57	MG	1a	1680	1/1	0.96	0.19	59,59,59,59	0
57	MG	1A	3632	1/1	0.96	0.10	26,26,26,26	0
57	MG	1A	3999	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3389	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3159	1/1	0.96	0.20	34,34,34,34	0
57	MG	1A	3100	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3485	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3392	1/1	0.96	0.15	48,48,48,48	0
57	MG	1a	1688	1/1	0.96	0.15	49,49,49,49	0
57	MG	1a	1689	1/1	0.96	0.30	57,57,57,57	0
57	MG	1A	3203	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3307	1/1	0.96	0.06	58,58,58,58	0
57	MG	1A	3063	1/1	0.96	0.25	56,56,56,56	0
57	MG	2A	3670	1/1	0.96	0.07	52,52,52,52	0
57	MG	1X	102	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3064	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3496	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3150	1/1	0.96	0.23	46,46,46,46	0
57	MG	1A	3207	1/1	0.96	0.10	41,41,41,41	0
57	MG	25	102	1/1	0.96	0.11	53,53,53,53	0
57	MG	1a	1695	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3728	1/1	0.96	0.11	21,21,21,21	0
57	MG	1A	3644	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3210	1/1	0.96	0.25	46,46,46,46	0
57	MG	28	102	1/1	0.96	0.11	62,62,62,62	0
57	MG	2A	3503	1/1	0.96	0.27	58,58,58,58	0
57	MG	1A	3646	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3505	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3126	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3213	1/1	0.96	0.09	30,30,30,30	0
57	MG	1A	3453	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3258	1/1	0.96	0.17	35,35,35,35	0
57	MG	2A	3163	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3916	1/1	0.96	0.04	16,16,16,16	0
57	MG	1A	3574	1/1	0.96	0.45	43,43,43,43	0
57	MG	1A	3402	1/1	0.96	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3740	1/1	0.96	0.05	16,16,16,16	0
57	MG	1A	3921	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3029	1/1	0.96	0.39	37,37,37,37	0
57	MG	1a	1713	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3577	1/1	0.96	0.33	62,62,62,62	0
57	MG	1A	3128	1/1	0.96	0.28	48,48,48,48	0
57	MG	2A	3015	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3174	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3066	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	4029	1/1	0.96	0.07	27,27,27,27	0
57	MG	12	102	1/1	0.96	0.08	50,50,50,50	0
58	K	1A	3536	1/1	0.96	0.07	42,42,42,42	0
57	MG	1a	1720	1/1	0.96	0.06	47,47,47,47	0
59	ZN	14	102	1/1	0.96	0.09	113,113,113,113	0
59	ZN	24	501	1/1	0.96	0.12	127,127,127,127	0
57	MG	2A	3726	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3243	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3094	1/1	0.97	0.07	38,38,38,38	0
57	MG	1U	205	1/1	0.97	0.23	40,40,40,40	0
57	MG	1A	3368	1/1	0.97	0.36	44,44,44,44	0
57	MG	1V	202	1/1	0.97	0.30	34,34,34,34	0
57	MG	1A	3132	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3370	1/1	0.97	0.10	58,58,58,58	0
57	MG	1A	3738	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3001	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3585	1/1	0.97	0.21	32,32,32,32	0
57	MG	2A	3405	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3586	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3022	1/1	0.97	0.04	18,18,18,18	0
57	MG	1A	3046	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3744	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3745	1/1	0.97	0.05	59,59,59,59	0
57	MG	1A	3663	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3111	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3323	1/1	0.97	0.22	38,38,38,38	0
57	MG	2A	3412	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	3590	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3414	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3083	1/1	0.97	0.19	31,31,31,31	0
57	MG	1X	103	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3167	1/1	0.97	0.27	34,34,34,34	0
57	MG	1A	3668	1/1	0.97	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1683	1/1	0.97	0.12	41,41,41,41	0
57	MG	1B	218	1/1	0.97	0.11	46,46,46,46	0
57	MG	1A	3527	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3121	1/1	0.97	0.09	47,47,47,47	0
57	MG	2A	3424	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3168	1/1	0.97	0.23	43,43,43,43	0
57	MG	2A	3123	1/1	0.97	0.10	52,52,52,52	0
57	MG	1A	3040	1/1	0.97	0.27	33,33,33,33	0
57	MG	1A	3005	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3755	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	4030	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3932	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3433	1/1	0.97	0.14	25,25,25,25	0
57	MG	10	103	1/1	0.97	0.15	47,47,47,47	0
57	MG	1A	3675	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3436	1/1	0.97	0.08	47,47,47,47	0
57	MG	10	105	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3842	1/1	0.97	0.15	26,26,26,26	0
57	MG	1A	4034	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3059	1/1	0.97	0.20	47,47,47,47	0
57	MG	1A	3245	1/1	0.97	0.18	29,29,29,29	0
57	MG	1A	3206	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3443	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3431	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	4039	1/1	0.97	0.15	69,69,69,69	0
57	MG	1A	3761	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3073	1/1	0.97	0.04	28,28,28,28	0
57	MG	2A	3448	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3143	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3603	1/1	0.97	0.04	34,34,34,34	0
57	MG	1B	238	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3538	1/1	0.97	0.08	33,33,33,33	0
57	MG	15	102	1/1	0.97	0.17	32,32,32,32	0
57	MG	2A	3292	1/1	0.97	0.11	62,62,62,62	0
57	MG	1A	3539	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3049	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3003	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	3011	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3107	1/1	0.97	0.34	34,34,34,34	0
57	MG	2A	3152	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3800	1/1	0.97	0.06	65,65,65,65	0
57	MG	1A	3545	1/1	0.97	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3020	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3181	1/1	0.97	0.34	39,39,39,39	0
57	MG	2A	3628	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3009	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3157	1/1	0.97	0.11	53,53,53,53	0
57	MG	1E	301	1/1	0.97	0.28	31,31,31,31	0
57	MG	1A	3773	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3468	1/1	0.97	0.07	45,45,45,45	0
57	MG	1E	303	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3013	1/1	0.97	0.09	55,55,55,55	0
57	MG	1E	304	1/1	0.97	0.12	32,32,32,32	0
57	MG	17	105	1/1	0.97	0.13	46,46,46,46	0
57	MG	17	106	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3549	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3615	1/1	0.97	0.07	51,51,51,51	0
57	MG	1E	307	1/1	0.97	0.16	32,32,32,32	0
57	MG	2A	3479	1/1	0.97	0.09	37,37,37,37	0
57	MG	18	104	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3694	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3777	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3617	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3957	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3958	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3779	1/1	0.97	0.07	39,39,39,39	0
57	MG	1a	1737	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3439	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3440	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3217	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3492	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	4068	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3218	1/1	0.97	0.11	29,29,29,29	0
57	MG	1a	1610	1/1	0.97	0.16	45,45,45,45	0
57	MG	2A	3037	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3964	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3052	1/1	0.97	0.09	26,26,26,26	0
57	MG	1F	307	1/1	0.97	0.12	31,31,31,31	0
57	MG	2F	304	1/1	0.97	0.12	55,55,55,55	0
57	MG	2F	305	1/1	0.97	0.27	50,50,50,50	0
57	MG	1A	3871	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3300	1/1	0.97	0.15	35,35,35,35	0
57	MG	1a	1617	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3151	1/1	0.97	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3345	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3875	1/1	0.97	0.10	50,50,50,50	0
57	MG	2Q	203	1/1	0.97	0.37	58,58,58,58	0
57	MG	2A	3048	1/1	0.97	0.19	39,39,39,39	0
57	MG	1A	3876	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3342	1/1	0.97	0.09	48,48,48,48	0
57	MG	1G	201	1/1	0.97	0.11	39,39,39,39	0
57	MG	1a	1758	1/1	0.97	0.07	77,77,77,77	0
57	MG	1A	3972	1/1	0.97	0.09	38,38,38,38	0
57	MG	2A	3513	1/1	0.97	0.04	51,51,51,51	0
57	MG	1a	1762	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3152	1/1	0.97	0.10	46,46,46,46	0
57	MG	1a	1767	1/1	0.97	0.10	74,74,74,74	0
57	MG	1A	3498	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3791	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3185	1/1	0.97	0.24	36,36,36,36	0
57	MG	1A	3500	1/1	0.97	0.28	38,38,38,38	0
57	MG	2X	102	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3078	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3883	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	4089	1/1	0.97	0.04	17,17,17,17	0
57	MG	1A	3093	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3262	1/1	0.97	0.20	36,36,36,36	0
57	MG	1A	4092	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3263	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3635	1/1	0.97	0.04	25,25,25,25	0
57	MG	1a	1638	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3530	1/1	0.97	0.10	61,61,61,61	0
57	MG	1P	201	1/1	0.97	0.32	29,29,29,29	0
57	MG	2A	3214	1/1	0.97	0.07	63,63,63,63	0
57	MG	2A	3215	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3636	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3264	1/1	0.97	0.23	44,44,44,44	0
57	MG	1A	3988	1/1	0.97	0.05	60,60,60,60	0
57	MG	1A	3717	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3638	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3156	1/1	0.97	0.23	31,31,31,31	0
57	MG	1A	3992	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3226	1/1	0.97	0.20	30,30,30,30	0
57	MG	2A	3707	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3157	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	3269	1/1	0.97	0.32	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3572	1/1	0.97	0.23	54,54,54,54	0
57	MG	1A	3900	1/1	0.97	0.03	33,33,33,33	0
57	MG	1A	3229	1/1	0.97	0.16	33,33,33,33	0
57	MG	1a	1801	1/1	0.97	0.19	47,47,47,47	0
57	MG	1A	3230	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3231	1/1	0.97	0.34	35,35,35,35	0
57	MG	1A	3647	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	4111	1/1	0.97	0.13	49,49,49,49	0
57	MG	1A	3158	1/1	0.97	0.17	29,29,29,29	0
57	MG	1T	201	1/1	0.97	0.14	50,50,50,50	0
57	MG	1T	202	1/1	0.97	0.15	59,59,59,59	0
57	MG	1A	3364	1/1	0.97	0.17	28,28,28,28	0
57	MG	1U	201	1/1	0.97	0.12	28,28,28,28	0
57	MG	2A	3095	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3275	1/1	0.97	0.08	34,34,34,34	0
59	ZN	2Y	501	1/1	0.97	0.05	105,105,105,105	0
57	MG	1U	203	1/1	0.97	0.11	37,37,37,37	0
59	ZN	2n	501	1/1	0.97	0.06	96,96,96,96	0
57	MG	1A	3578	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	4017	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3038	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3309	1/1	0.98	0.11	53,53,53,53	0
57	MG	1A	3108	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	4020	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3138	1/1	0.98	0.06	23,23,23,23	0
57	MG	10	102	1/1	0.98	0.10	50,50,50,50	0
57	MG	1A	3267	1/1	0.98	0.24	30,30,30,30	0
57	MG	2A	3429	1/1	0.98	0.18	46,46,46,46	0
57	MG	1A	3208	1/1	0.98	0.09	49,49,49,49	0
57	MG	1A	3209	1/1	0.98	0.27	41,41,41,41	0
57	MG	1a	1749	1/1	0.98	0.05	59,59,59,59	0
57	MG	1A	3109	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3271	1/1	0.98	0.25	38,38,38,38	0
57	MG	1A	3540	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3240	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3798	1/1	0.98	0.08	73,73,73,73	0
57	MG	1a	1754	1/1	0.98	0.05	64,64,64,64	0
57	MG	1A	3032	1/1	0.98	0.08	31,31,31,31	0
57	MG	2A	3556	1/1	0.98	0.06	48,48,48,48	0
57	MG	1A	3212	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3544	1/1	0.98	0.24	40,40,40,40	0
57	MG	1A	3067	1/1	0.98	0.09	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3890	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3501	1/1	0.98	0.26	40,40,40,40	0
57	MG	1a	1763	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3702	1/1	0.98	0.04	18,18,18,18	0
57	MG	2A	3223	1/1	0.98	0.05	65,65,65,65	0
57	MG	1a	1765	1/1	0.98	0.04	62,62,62,62	0
57	MG	1A	3547	1/1	0.98	0.19	27,27,27,27	0
57	MG	1a	1768	1/1	0.98	0.07	59,59,59,59	0
57	MG	1A	3420	1/1	0.98	0.24	32,32,32,32	0
57	MG	1a	1770	1/1	0.98	0.05	76,76,76,76	0
57	MG	1A	3033	1/1	0.98	0.18	32,32,32,32	0
57	MG	15	103	1/1	0.98	0.41	32,32,32,32	0
57	MG	1A	3069	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3144	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3341	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3164	1/1	0.98	0.06	17,17,17,17	0
57	MG	2A	3021	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3012	1/1	0.98	0.12	27,27,27,27	0
57	MG	1N	203	1/1	0.98	0.04	37,37,37,37	0
57	MG	1B	206	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3652	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	3190	1/1	0.98	0.14	29,29,29,29	0
57	MG	2A	3027	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3837	1/1	0.98	0.09	21,21,21,21	0
57	MG	1A	3191	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3166	1/1	0.98	0.14	32,32,32,32	0
57	MG	2A	3137	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3009	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3605	1/1	0.98	0.09	39,39,39,39	0
57	MG	1A	3116	1/1	0.98	0.19	33,33,33,33	0
57	MG	2A	3472	1/1	0.98	0.07	34,34,34,34	0
57	MG	1P	203	1/1	0.98	0.29	33,33,33,33	0
57	MG	2A	3035	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3718	1/1	0.98	0.03	24,24,24,24	0
57	MG	2A	3476	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3659	1/1	0.98	0.05	27,27,27,27	0
57	MG	1A	3660	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	4055	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3781	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3195	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3082	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3723	1/1	0.98	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3355	1/1	0.98	0.04	41,41,41,41	0
57	MG	1a	1799	1/1	0.98	0.05	65,65,65,65	0
57	MG	1a	1800	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3288	1/1	0.98	0.11	40,40,40,40	0
57	MG	1A	4062	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3919	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3104	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	4065	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3358	1/1	0.98	0.29	27,27,27,27	0
57	MG	1a	1612	1/1	0.98	0.07	26,26,26,26	0
57	MG	2A	3378	1/1	0.98	0.13	53,53,53,53	0
57	MG	2A	3379	1/1	0.98	0.11	25,25,25,25	0
57	MG	2A	3734	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3227	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3614	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	4069	1/1	0.98	0.14	47,47,47,47	0
57	MG	1A	3924	1/1	0.98	0.04	54,54,54,54	0
57	MG	1A	3150	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3792	1/1	0.98	0.04	27,27,27,27	0
57	MG	2A	3741	1/1	0.98	0.09	47,47,47,47	0
57	MG	1a	1707	1/1	0.98	0.03	32,32,32,32	0
57	MG	1a	1708	1/1	0.98	0.08	34,34,34,34	0
57	MG	23	102	1/1	0.98	0.06	59,59,59,59	0
57	MG	1a	1709	1/1	0.98	0.07	36,36,36,36	0
57	MG	2A	3389	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3793	1/1	0.98	0.29	24,24,24,24	0
57	MG	1A	3670	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3616	1/1	0.98	0.04	28,28,28,28	0
57	MG	1a	1622	1/1	0.98	0.06	53,53,53,53	0
57	MG	1D	301	1/1	0.98	0.14	35,35,35,35	0
57	MG	2A	3629	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	4000	1/1	0.98	0.05	36,36,36,36	0
57	MG	1V	201	1/1	0.98	0.19	40,40,40,40	0
57	MG	1A	3733	1/1	0.98	0.07	58,58,58,58	0
57	MG	1D	304	1/1	0.98	0.04	21,21,21,21	0
57	MG	1a	1719	1/1	0.98	0.06	58,58,58,58	0
57	MG	2A	3759	1/1	0.98	0.13	63,63,63,63	0
57	MG	1A	3037	1/1	0.98	0.14	37,37,37,37	0
57	MG	2A	3075	1/1	0.98	0.23	40,40,40,40	0
57	MG	2A	3637	1/1	0.98	0.05	56,56,56,56	0
57	MG	1A	3326	1/1	0.98	0.17	40,40,40,40	0
57	MG	1A	3481	1/1	0.98	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1D	308	1/1	0.98	0.17	44,44,44,44	0
57	MG	1A	3401	1/1	0.98	0.17	39,39,39,39	0
57	MG	1D	310	1/1	0.98	0.23	27,27,27,27	0
57	MG	2A	3768	1/1	0.98	0.06	45,45,45,45	0
57	MG	1W	203	1/1	0.98	0.23	43,43,43,43	0
57	MG	1A	3571	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3363	1/1	0.98	0.31	44,44,44,44	0
57	MG	1A	4085	1/1	0.98	0.05	61,61,61,61	0
57	MG	1A	3623	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3134	1/1	0.98	0.27	41,41,41,41	0
57	MG	1A	3057	1/1	0.98	0.06	38,38,38,38	0
57	MG	2A	3088	1/1	0.98	0.06	47,47,47,47	0
57	MG	1A	3366	1/1	0.98	0.17	27,27,27,27	0
57	MG	1A	3807	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	3154	1/1	0.98	0.06	42,42,42,42	0
59	ZN	29	501	1/1	0.98	0.04	84,84,84,84	0
57	MG	1A	3178	1/1	0.98	0.10	41,41,41,41	0
60	SF4	2d	501	8/8	0.98	0.04	61,68,76,83	0
57	MG	1A	4078	1/1	0.99	0.06	34,34,34,34	0
57	MG	1a	1728	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	4016	1/1	0.99	0.02	23,23,23,23	0
57	MG	2A	3754	1/1	0.99	0.06	33,33,33,33	0
57	MG	15	101	1/1	0.99	0.21	44,44,44,44	0
57	MG	1A	3894	1/1	0.99	0.07	43,43,43,43	0
57	MG	1a	1759	1/1	0.99	0.07	70,70,70,70	0
57	MG	1a	1760	1/1	0.99	0.04	57,57,57,57	0
57	MG	2A	3643	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3034	1/1	0.99	0.27	29,29,29,29	0
57	MG	1A	3747	1/1	0.99	0.05	44,44,44,44	0
57	MG	2A	3646	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	3981	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3095	1/1	0.99	0.12	19,19,19,19	0
57	MG	1A	3024	1/1	0.99	0.16	29,29,29,29	0
57	MG	1a	1766	1/1	0.99	0.03	48,48,48,48	0
57	MG	2A	3038	1/1	0.99	0.15	31,31,31,31	0
57	MG	1A	3899	1/1	0.99	0.02	24,24,24,24	0
57	MG	1A	3828	1/1	0.99	0.11	33,33,33,33	0
57	MG	1A	3690	1/1	0.99	0.04	15,15,15,15	0
57	MG	1A	3987	1/1	0.99	0.04	40,40,40,40	0
57	MG	1R	203	1/1	0.99	0.28	39,39,39,39	0
57	MG	1A	3169	1/1	0.99	0.04	31,31,31,31	0
57	MG	2A	3512	1/1	0.99	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3202	1/1	0.99	0.13	33,33,33,33	0
57	MG	1a	1774	1/1	0.99	0.05	61,61,61,61	0
57	MG	1A	4049	1/1	0.99	0.06	28,28,28,28	0
57	MG	1a	1745	1/1	0.99	0.04	67,67,67,67	0
57	MG	1A	3672	1/1	0.99	0.08	32,32,32,32	0
57	MG	1A	3071	1/1	0.99	0.10	15,15,15,15	0
57	MG	1a	1779	1/1	0.99	0.04	62,62,62,62	0
57	MG	1A	3171	1/1	0.99	0.04	35,35,35,35	0
57	MG	1A	3039	1/1	0.99	0.15	31,31,31,31	0
59	ZN	1Y	203	1/1	0.99	0.03	72,72,72,72	0
57	MG	2A	3486	1/1	0.99	0.05	45,45,45,45	0
59	ZN	15	109	1/1	0.99	0.03	43,43,43,43	0
59	ZN	16	103	1/1	0.99	0.03	42,42,42,42	0
59	ZN	19	102	1/1	0.99	0.04	46,46,46,46	0
59	ZN	1n	102	1/1	0.99	0.03	68,68,68,68	0
57	MG	1A	3013	1/1	0.99	0.07	29,29,29,29	0
57	MG	2A	3419	1/1	0.99	0.06	64,64,64,64	0
59	ZN	25	104	1/1	0.99	0.05	60,60,60,60	0
57	MG	1A	3709	1/1	0.99	0.06	23,23,23,23	0
57	MG	13	101	1/1	0.99	0.05	32,32,32,32	0
60	SF4	1d	302	8/8	0.99	0.04	58,66,72,72	0
57	MG	1A	3926	1/1	0.99	0.04	51,51,51,51	0
57	MG	2A	3742	1/1	1.00	0.06	37,37,37,37	0
59	ZN	26	501	1/1	1.00	0.03	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.