



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:26 PM UTC

PDB ID : 8G2C / pdb_00008g2c
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with tylosin, mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.65Å 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 : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12

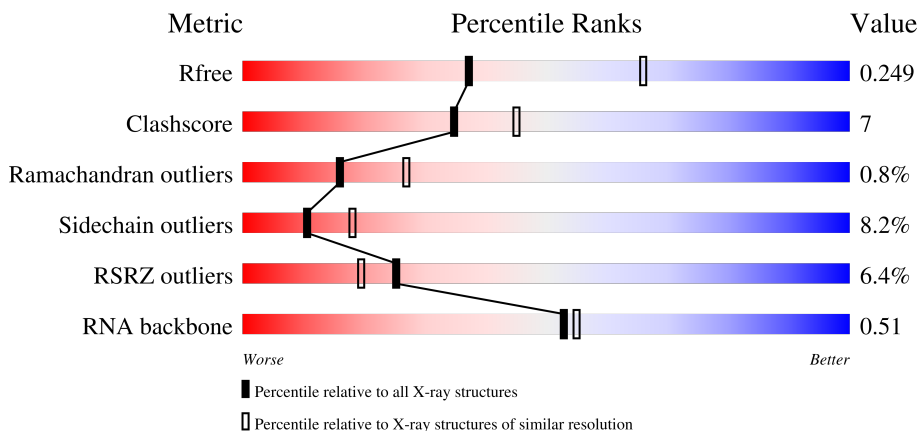
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

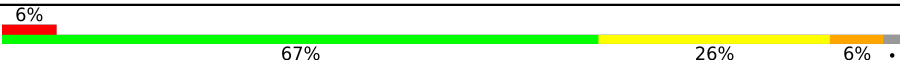
The reported resolution of this entry is 2.65 Å.

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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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	

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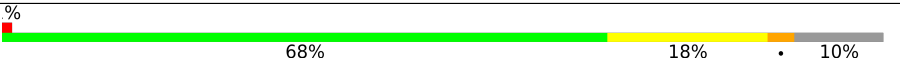
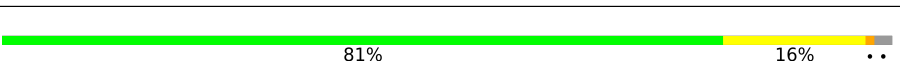
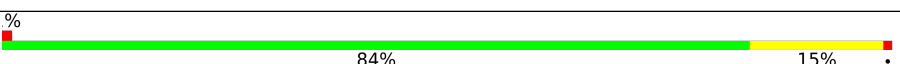
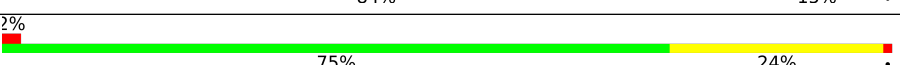
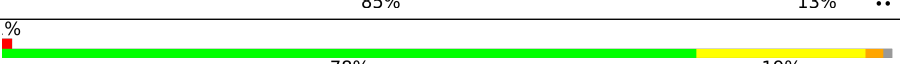
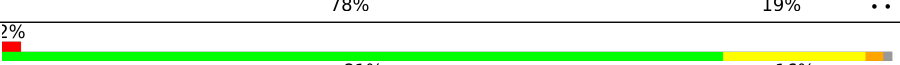
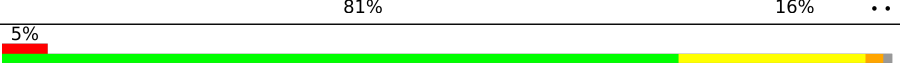
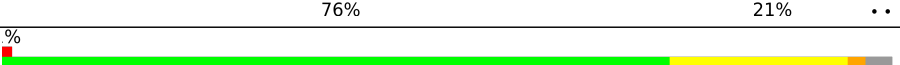
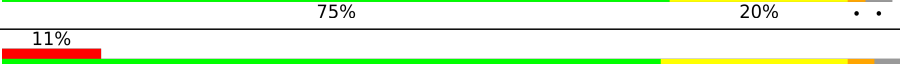
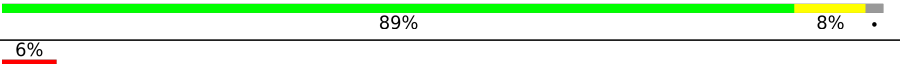
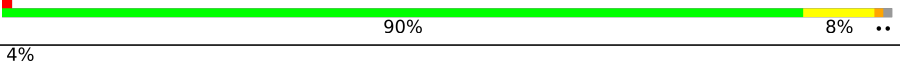
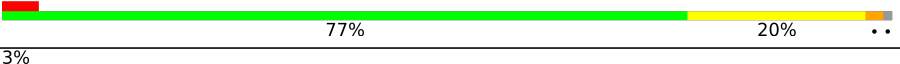
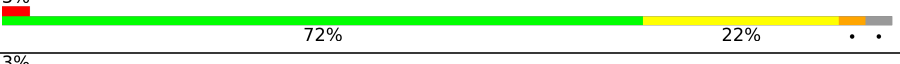
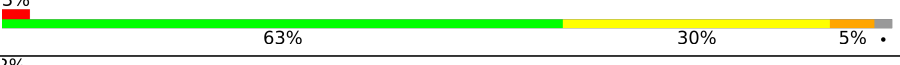
Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	2A	2915	
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	

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Mol	Chain	Length	Quality of chain
14	1S	112	
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	

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Mol	Chain	Length	Quality of chain
26	24	71	25% 49% 45% • •
27	15	60	83% 13% • •
27	25	60	2% 83% 15% •
28	16	54	63% 31% • •
28	26	54	59% 31% 7% •
29	17	49	2% 80% 14% • •
29	27	49	4% 78% 18% • •
30	18	65	77% 20% • •
30	28	65	2% 68% 31% •
31	19	37	86% 14%
31	29	37	5% 78% 19% •
32	1a	1521	4% 62% 32% 5% •
32	2a	1521	6% 56% 36% 8% •
33	1b	256	16% 55% 31% • 10%
33	2b	256	16% 52% 32% 5% 10%
34	1c	239	5% 64% 19% • 14%
34	2c	239	15% 56% 26% • 14%
35	1d	209	7% 68% 27% •
35	2d	209	5% 67% 30% •
36	1e	162	62% 23% 6% 9%
36	2e	162	6% 63% 28% • 9%
37	1f	101	2% 76% 20% • •
37	2f	101	3% 73% 25% • •
38	1g	156	6% 71% 22% 6% •
38	2g	156	14% 69% 29% • •

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Mol	Chain	Length	Quality of chain
39	1h	138	
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	

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Mol	Chain	Length	Quality of chain
51	2t	106	
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
56	PSU	2y	55	-	-	X	-
57	MG	2A	3177	-	-	-	X
57	MG	2A	3252	-	-	-	X
57	MG	2A	3775	-	-	-	X
57	MG	2a	1610	-	-	-	X
57	MG	2a	1629	-	-	-	X
57	MG	2v	102	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300115 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	1099	Total	Mg	0	0
			1099	1099		
57	1B	34	Total	Mg	0	0
			34	34		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	10	Total	Mg	0	0
			10	10		
57	1F	15	Total	Mg	0	0
			15	15		

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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	1I	1	Total 1	Mg 1	0	0
57	1N	5	Total 5	Mg 5	0	0
57	1O	6	Total 6	Mg 6	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	10	Total 10	Mg 10	0	0
57	1V	5	Total 5	Mg 5	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	6	Total 6	Mg 6	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	10	Total 10	Mg 10	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	3	Total 3	Mg 3	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	15	6	Total 6	Mg 6	0	0
57	16	1	Total 1	Mg 1	0	0
57	17	5	Total 5	Mg 5	0	0
57	18	7	Total 7	Mg 7	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	214	Total 214	Mg 214	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1h	1	Total 1	Mg 1	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	1r	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	5	Total 5	Mg 5	0	0
57	1x	13	Total 13	Mg 13	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	797	Total 797	Mg 797	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2B	19	Total 19	Mg 19	0	0
57	2D	8	Total 8	Mg 8	0	0
57	2E	9	Total 9	Mg 9	0	0
57	2F	8	Total 8	Mg 8	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2T	2	Total 2	Mg 2	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	2	Total 2	Mg 2	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	2	Total 2	Mg 2	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	4	Total 4	Mg 4	0	0
57	27	2	Total 2	Mg 2	0	0

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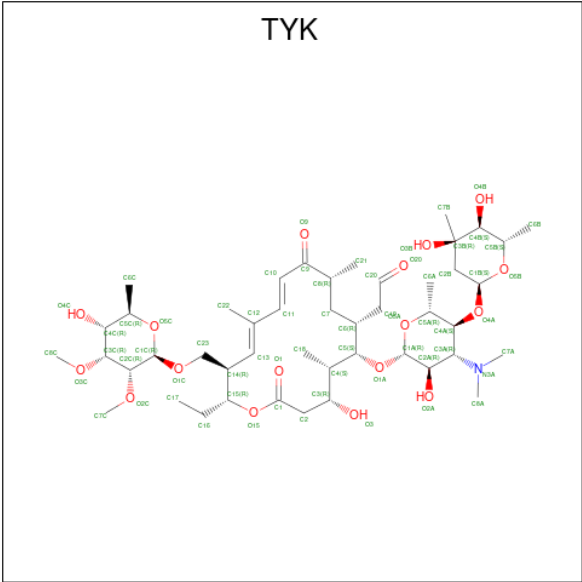
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	28	5	Total 5	Mg 5	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	221	Total 221	Mg 221	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	3	Total 3	Mg 3	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	1	Total 1	Mg 1	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	4	Total 4	Mg 4	0	0
57	2w	7	Total 7	Mg 7	0	0
57	2x	9	Total 9	Mg 9	0	0
57	2y	2	Total 2	Mg 2	0	0

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

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

- Molecule 59 is TYLOSIN (CCD ID: TYK) (formula: C₄₆H₇₇NO₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1A	1	Total	C	N	O	0	0
			64	46	1	17		
59	2A	1	Total	C	N	O	0	0
			64	46	1	17		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

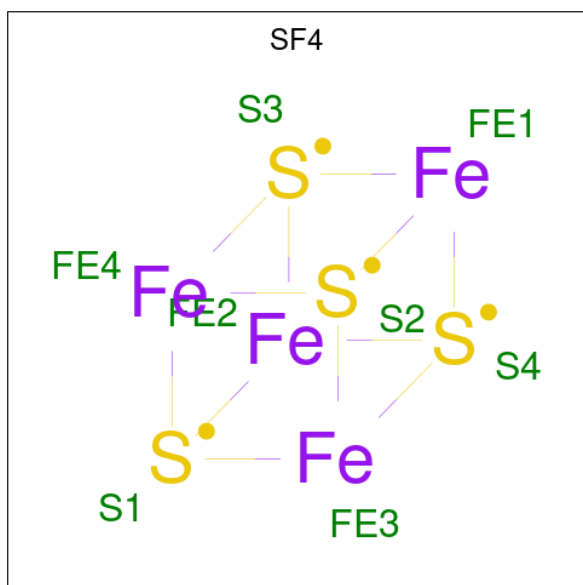
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1975	Total	O	0	0
			1975	1975		
62	1B	59	Total	O	0	0
			59	59		
62	1D	25	Total	O	0	0
			25	25		
62	1E	25	Total	O	0	0
			25	25		
62	1F	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1G	2	Total	O	0	0
			2	2		
62	1H	2	Total	O	0	0
			2	2		
62	1N	5	Total	O	0	0
			5	5		
62	1O	4	Total	O	0	0
			4	4		
62	1P	23	Total	O	0	0
			23	23		
62	1Q	6	Total	O	0	0
			6	6		
62	1R	9	Total	O	0	0
			9	9		
62	1S	2	Total	O	0	0
			2	2		
62	1T	7	Total	O	0	0
			7	7		
62	1U	11	Total	O	0	0
			11	11		
62	1V	8	Total	O	0	0
			8	8		
62	1W	7	Total	O	0	0
			7	7		
62	1X	6	Total	O	0	0
			6	6		
62	1Y	3	Total	O	0	0
			3	3		
62	1Z	1	Total	O	0	0
			1	1		
62	10	10	Total	O	0	0
			10	10		
62	11	6	Total	O	0	0
			6	6		
62	12	3	Total	O	0	0
			3	3		
62	13	3	Total	O	0	0
			3	3		
62	14	1	Total	O	0	0
			1	1		
62	15	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	16	2	Total 2	O 2	0	0
62	17	10	Total 10	O 10	0	0
62	18	12	Total 12	O 12	0	0
62	1a	377	Total 377	O 377	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	2	Total 2	O 2	0	0
62	1f	2	Total 2	O 2	0	0
62	1l	6	Total 6	O 6	0	0
62	1m	1	Total 1	O 1	0	0
62	1o	1	Total 1	O 1	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	12	Total 12	O 12	0	0
62	1x	15	Total 15	O 15	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1136	Total 1136	O 1136	0	0
62	2B	22	Total 22	O 22	0	0
62	2D	21	Total 21	O 21	0	0
62	2E	16	Total 16	O 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2F	13	Total 13	O 13	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	5	Total 5	O 5	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	2	Total 2	O 2	0	0
62	2T	7	Total 7	O 7	0	0
62	2U	4	Total 4	O 4	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	2	Total 2	O 2	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	4	Total 4	O 4	0	0
62	21	7	Total 7	O 7	0	0
62	23	2	Total 2	O 2	0	0
62	25	1	Total 1	O 1	0	0
62	26	2	Total 2	O 2	0	0
62	27	4	Total 4	O 4	0	0
62	28	4	Total 4	O 4	0	0
62	29	1	Total 1	O 1	0	0
62	2a	254	Total 254	O 254	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0

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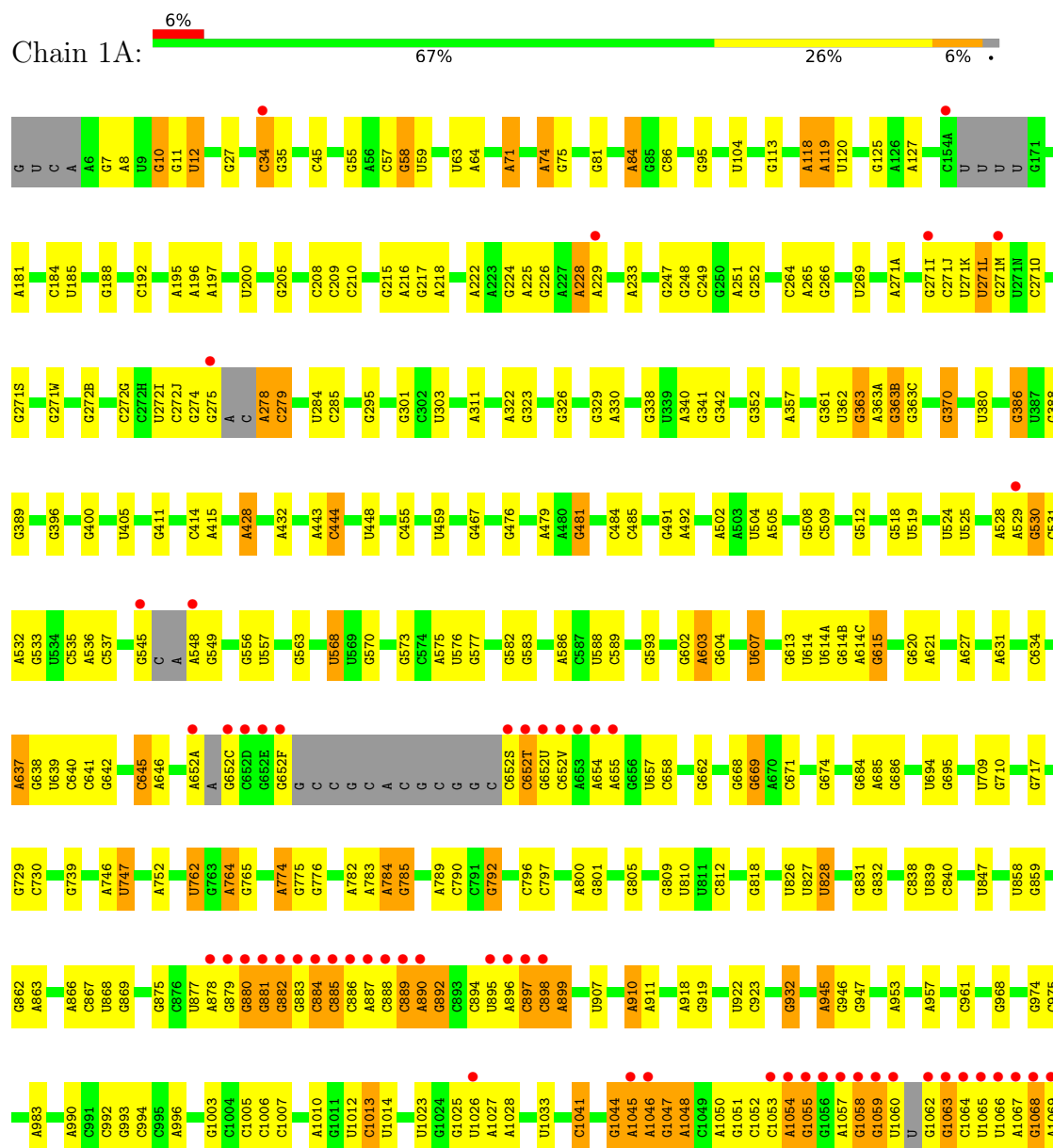
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2e	1	Total 1	O 1	0	0
62	2j	4	Total 4	O 4	0	0
62	2l	4	Total 4	O 4	0	0
62	2n	1	Total 1	O 1	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	1	Total 1	O 1	0	0
62	2q	2	Total 2	O 2	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	10	Total 10	O 10	0	0
62	2y	1	Total 1	O 1	0	0

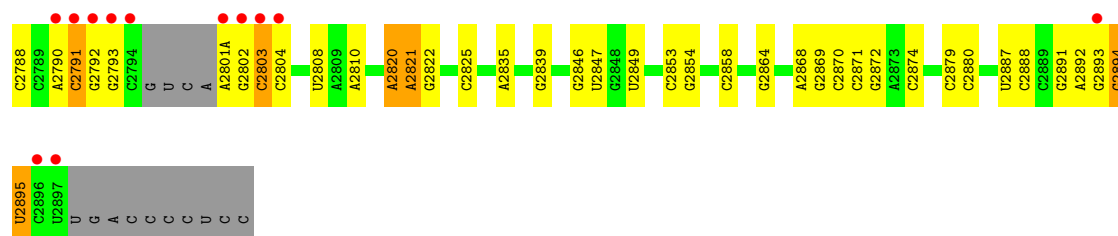
3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA

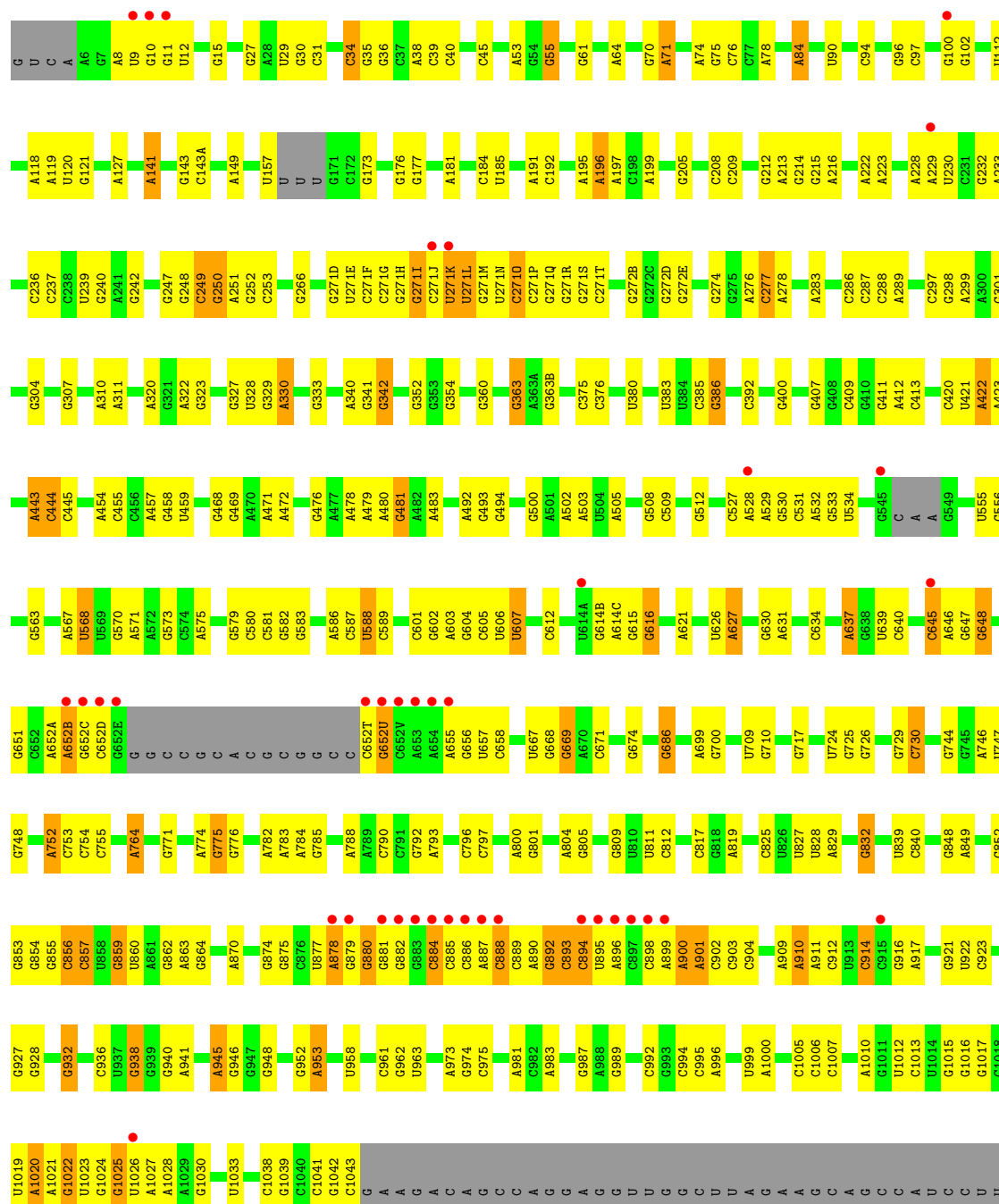


C2667	G2668	U2537	C2538	G2410	C2306	G2181	U2121	A2020	C1882	U1739	C1584	A1445	A1301	A1424A	A1070
G2668	U2537	C2538	G2307	A2422	G2307	G2182	U2122	C2021	G1883	G1740	A1586	G1445	A1302	A1143	G1071
C2683	U2549	C2540	G2308	A2423	G2308	G2183	G2123	C2022	A1587	G1741	C1587	G1448	G1303	A1144	C1072
G2685	G2500	A2424	U2312	A2425	U2312	G2184	G2124	G2023	C1588	U1742	C1588	G1449	U1313	C1163	G1073
U2689	U2552	A2426	C2316	A2426	C2316	G2185	A2126	G2029	C1589	G1745	C1589	G1450	U1314	C1164	G1074
C2690	U2553	C2427	C2317	A2427	C2317	G2186	G2127	A2030	G1593	G1756	U1453	U1453	C1315	C1165	G1075
C2691	U2554	G2428	G2319	A2428	G2319	U2189	C2129	A2031	G1594	A1762	U1455	G1456	C1316	A1165	G1076
U2693	U2563	A2430	A2320	A2430	A2320	G2190	G2130	A2032	G1595	G1763	U1456	G1456	A1317	A1166	A1077
A2693	U2564	U2431	G2325	A2431	G2325	G2191	G2131	A2033	U1602	G1764	U1602	G1461	G1324	U1165	C1078
G2694	U2565	C2326	C2326	A2435	C2326	G2192	G2132	G2038	A1603	A1773	A1603	C1467	G1332	U1166	C1080
C2699	U2566	A2327	A2327	A2435	A2327	G2193	G2133	C2039	C1607	A1773	C1607	C1467	G1332	G1171	U1081
C2700	U2567	G2329	A2329	A2439	G2329	U2198	A2135	C2039	A1608	U1779	A1608	G1467	G1338	G1172	U1082
C2701	A2572	G2330	G2330	A2440	G2330	U2189	A2136	C2040	A1609	A1780	A1609	G1467	G1338	G1173	U1083
U2702	C2573	G2331	G2331	C2441	G2331	G2190	G2137	U2041	A1610	U1781	A1610	G1467	G1338	G1174	A1085
C2703	G2574	G2332	G2332	C2441	G2332	G2191	G2138	A2042	A1610	C1782	A1610	G1467	G1338	U1175	A1086
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A2713	U2583	A2336	G2336	A2448	A2336	G2193	G2140	G2053	G1622	A1786	G1622	G1467	G1338	C1177	A1088
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U2721	G2588	U2344	G2344	A2458	U2344	A2225	C2145	A2060	G1628	A1791	G1628	G1467	G1338	C1179	A1090
U2726	U2590	G2345	G2345	A2464	G2345	U2203	C2146	C2061	U1629	A1791	U1629	G1467	G1338	U1188	G1091
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C2774	U2646	G2384	G2384	C2502	G2384	G2275	G2162	G2103	C1516	U1813	C1516	G1467	G1338	G1191	U1108
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U2776	U2648	C2520	U2390	U2504	U2390	A2277	G2164	G2105	C1518	U1815	C1518	G1467	G1338	G1191	G1110
A2778	U2649	G2529	G2405	U2505	G2405	G2278	G2165	G2106	C1519	U1816	C1519	G1467	G1338	G1191	A1111
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				U2518		G2292	G2179	G2120	C1533	U1830	C1533	G1467	G1338	G1191	C1293
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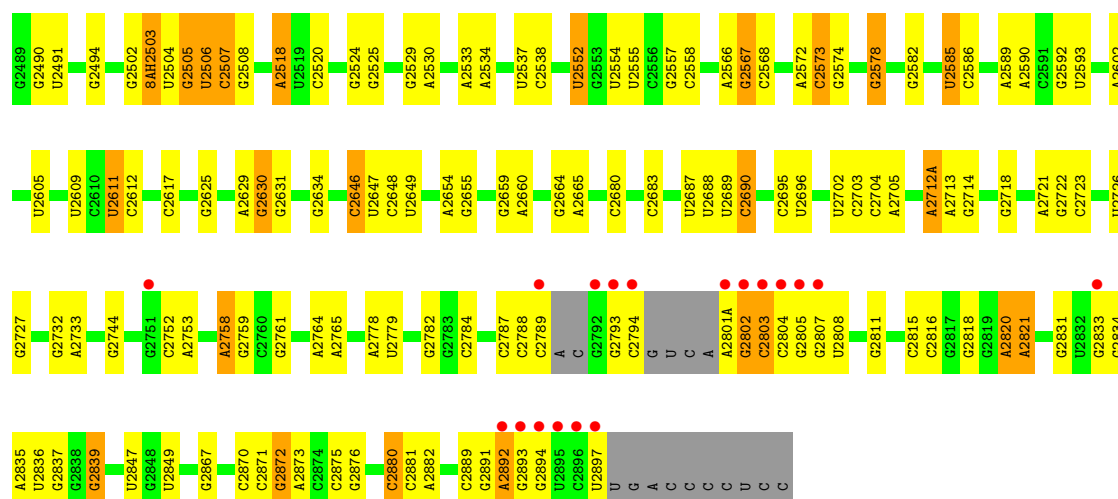


• Molecule 1: 23S Ribosomal RNA

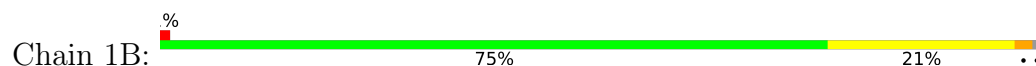
Chain 2A: 5% 60% 30% 6%



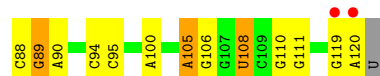




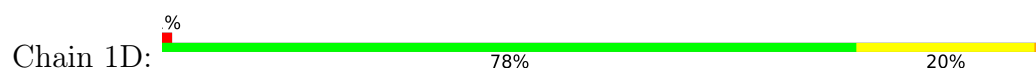
• Molecule 2: 5S Ribosomal RNA



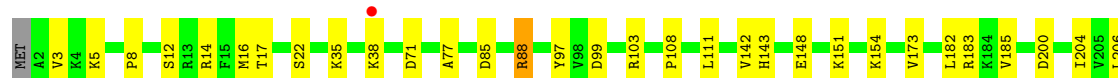
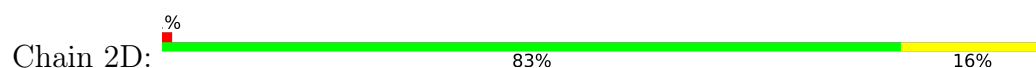
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2



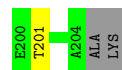
• Molecule 3: 50S ribosomal protein L2





- Molecule 4: 50S ribosomal protein L3

Chain 1E: 82% 16% ..



- Molecule 4: 50S ribosomal protein L3

Chain 2E: 75% 21% ..



- Molecule 5: 50S ribosomal protein L4

Chain 1F: 69% 23% ..



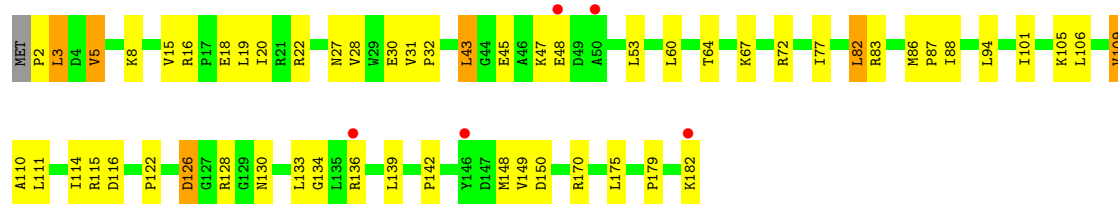
- Molecule 5: 50S ribosomal protein L4

Chain 2F: 68% 27% ..

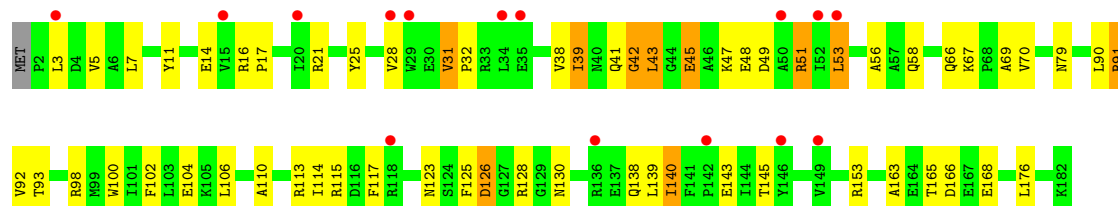


- Molecule 6: 50S ribosomal protein L5

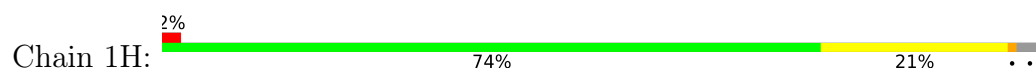
Chain 1G: 69% 27% ..



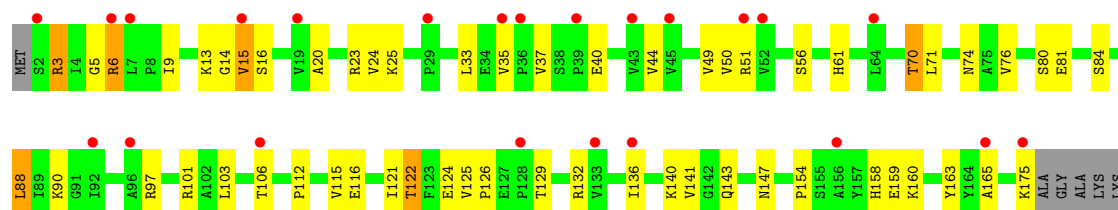
• Molecule 6: 50S ribosomal protein L5



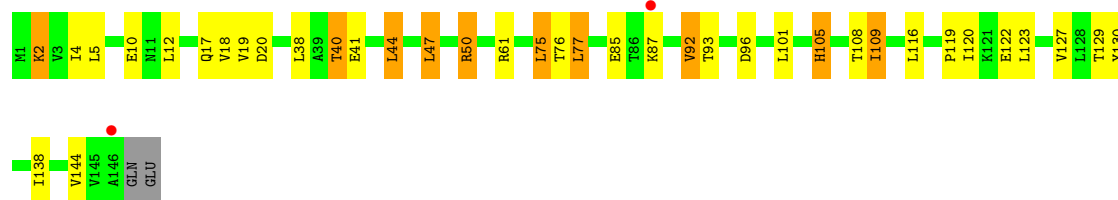
• Molecule 7: 50S ribosomal protein L6



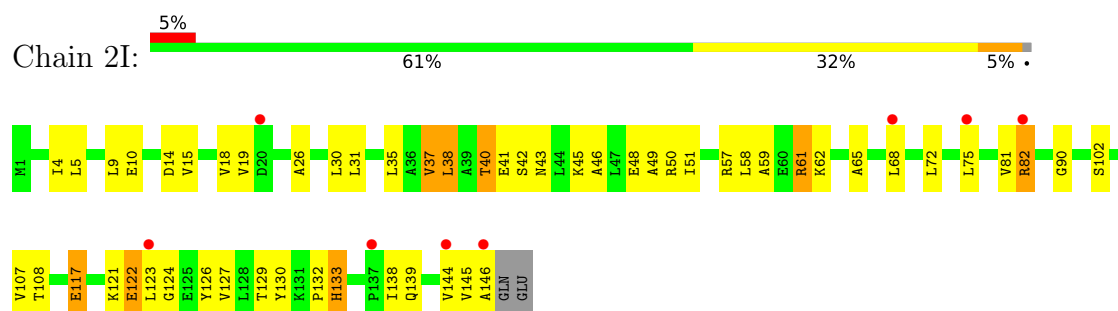
• Molecule 7: 50S ribosomal protein L6



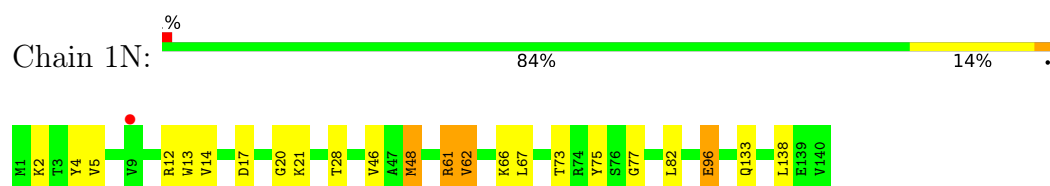
• Molecule 8: 50S ribosomal protein L9



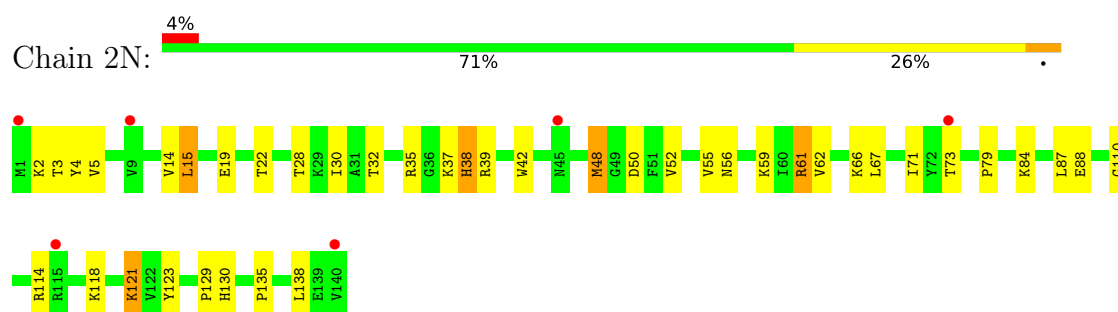
- Molecule 8: 50S ribosomal protein L9



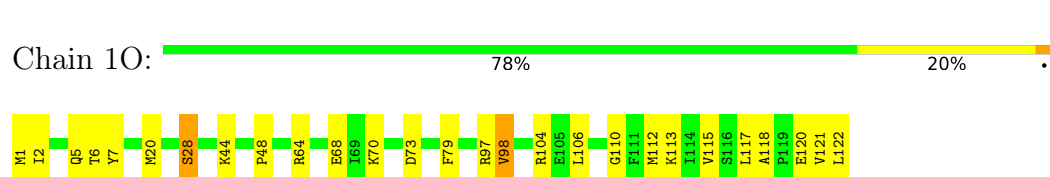
- Molecule 9: 50S ribosomal protein L13



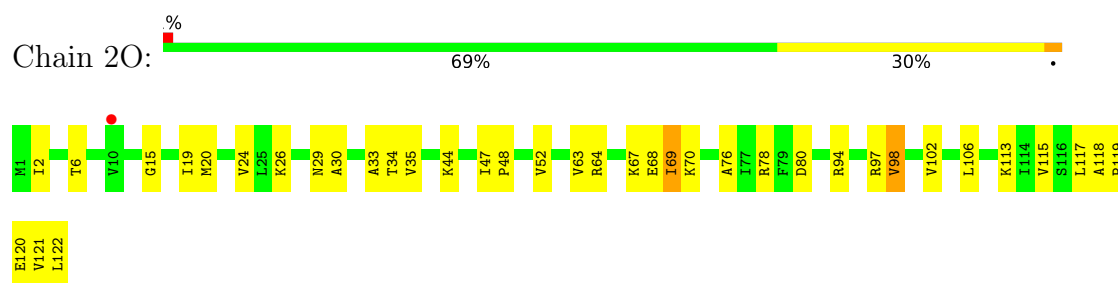
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

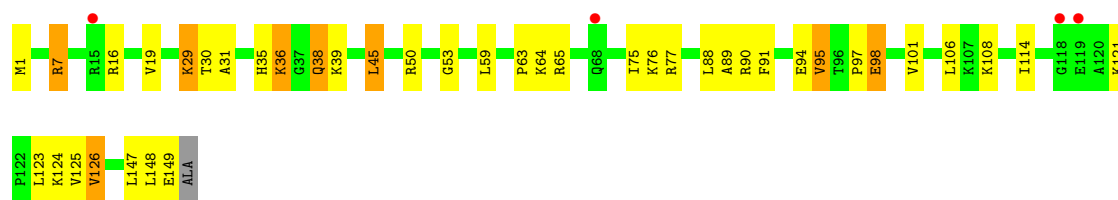


- Molecule 10: 50S ribosomal protein L14

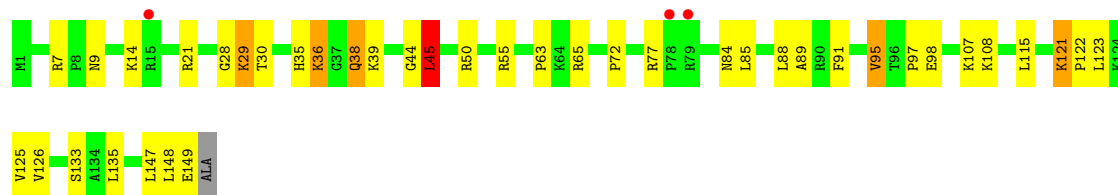
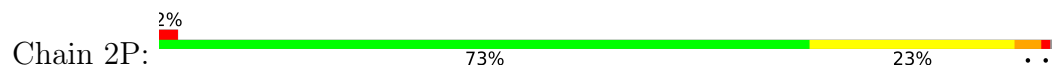


- Molecule 11: 50S ribosomal protein L15

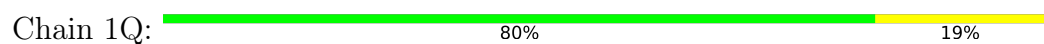




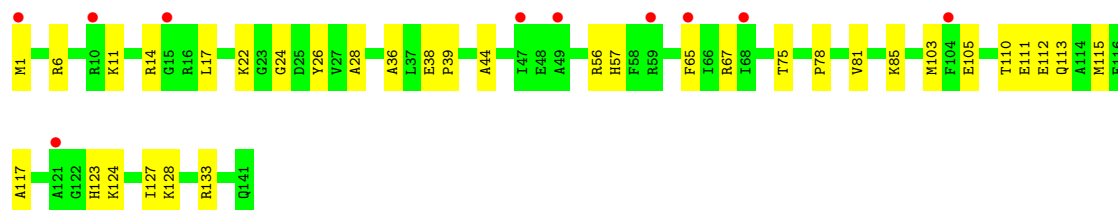
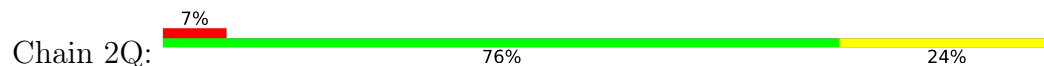
- Molecule 11: 50S ribosomal protein L15



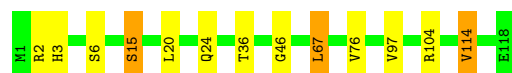
- Molecule 12: 50S ribosomal protein L16



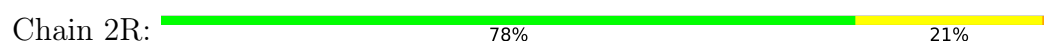
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

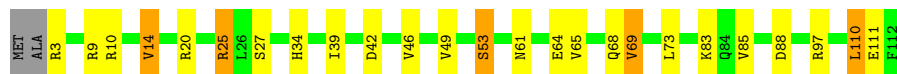


- Molecule 13: 50S ribosomal protein L17



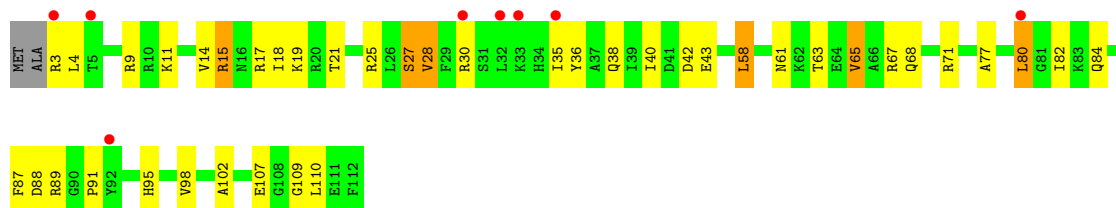
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  76% 18% . .



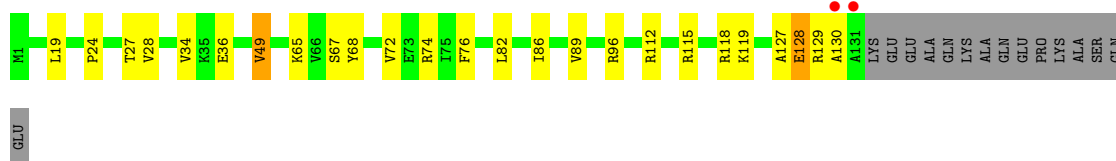
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  7% 62% 31% 5% .



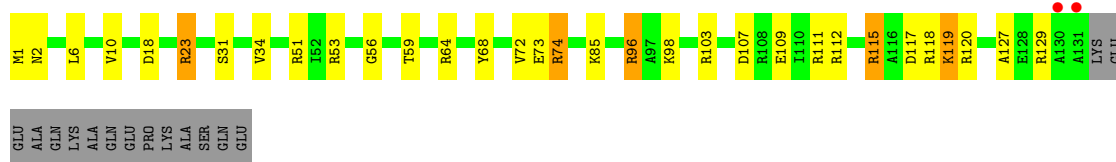
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  % 73% 16% . 10%



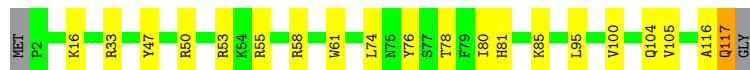
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  % 68% 18% . 10%



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  81% 16% . .

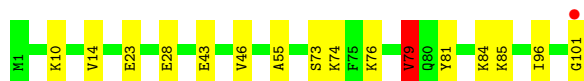
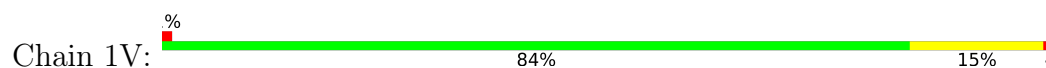


- Molecule 16: 50S ribosomal protein L20

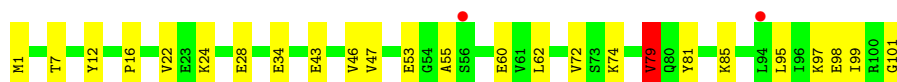
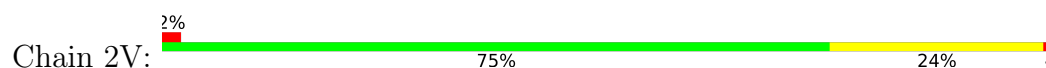
Chain 2U:  % 79% 18% . .



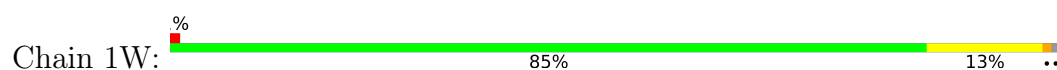
- Molecule 17: 50S ribosomal protein L21



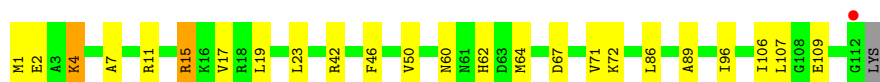
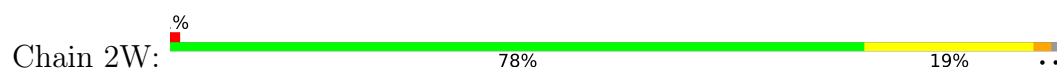
- Molecule 17: 50S ribosomal protein L21



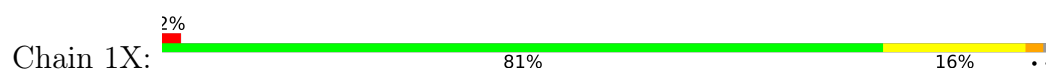
- Molecule 18: 50S ribosomal protein L22



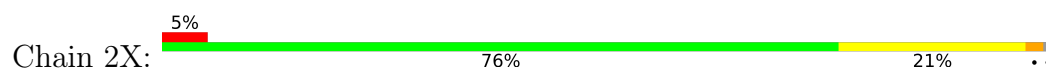
- Molecule 18: 50S ribosomal protein L22



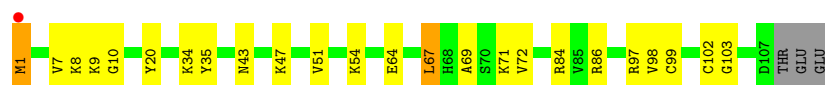
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



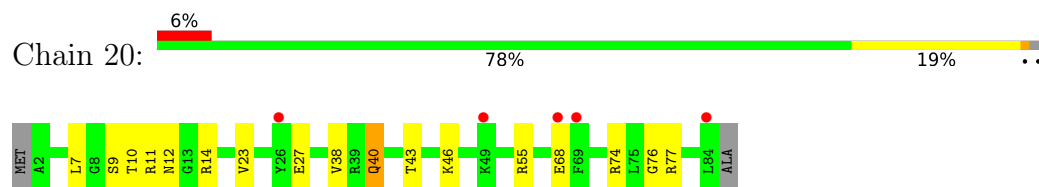
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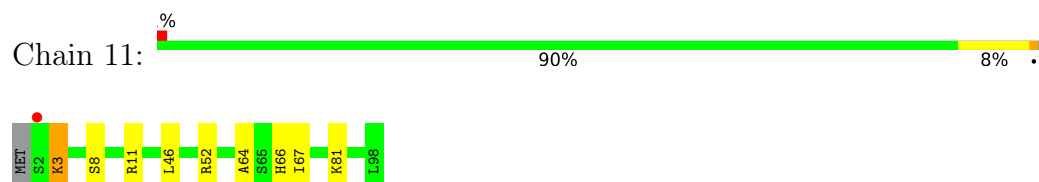
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|------|------|------|------|------|------|---|
| P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P130 | R131 | N132 | I133 | F136 | I137 | E138 | V139 | D140 | V141 | S142 | G143 | L144 | E145 | I146 | G147 | D148 | S149 | L150 | H151 | A152 | S153 | D154 | L155 | L156 | L157 | P158 | P159 | G160 | V161 | E162 | L163 | A164 | V165 | S166 | P167 | E168 | E169 | T170 | T171 | A172 | A173 | V174 | VAL | PRO | PRO | GLU | ASP | VAL | GLU | LYS | LEU | ALA | GLU | GLU | LYS | GLY | GLY | GLY | GLY | VAL | LEU | GLN | GLU | ILE | H121 | H124 | L125 | A126 | K127 | V128 | S129 | P |
|------|------|------|------|------|------|------|------|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|------|------|------|------|------|------|---|

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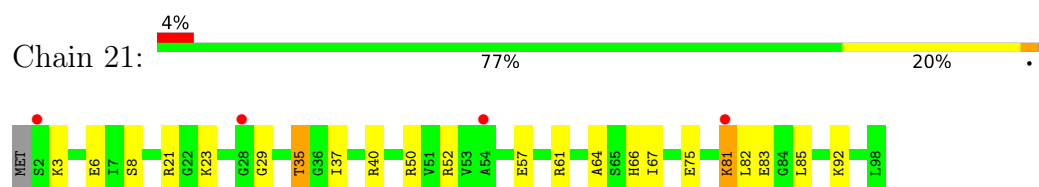
- Molecule 22: 50S ribosomal protein L27



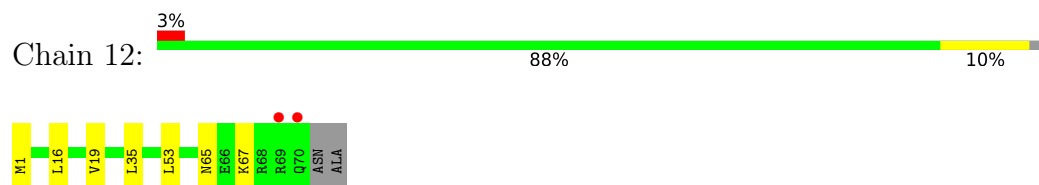
- Molecule 23: 50S ribosomal protein L28



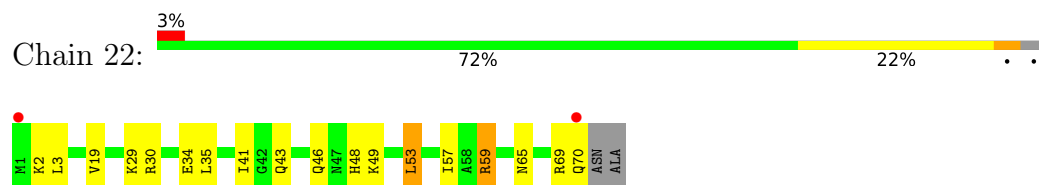
- Molecule 23: 50S ribosomal protein L28



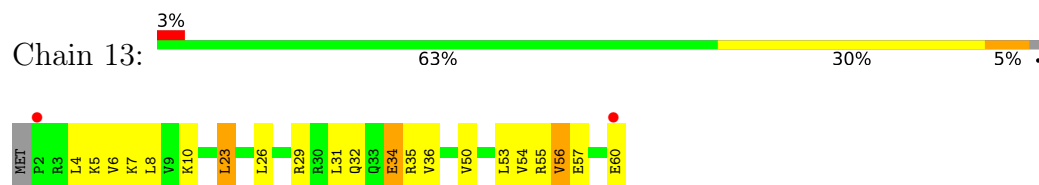
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

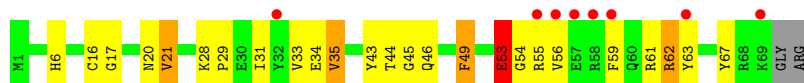


- Molecule 25: 50S ribosomal protein L30





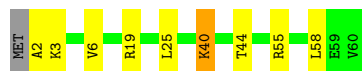
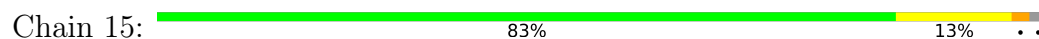
- Molecule 26: 50S ribosomal protein L31



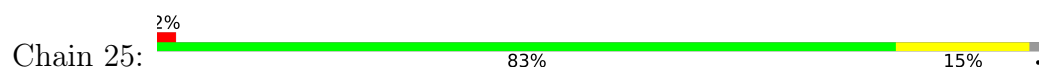
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



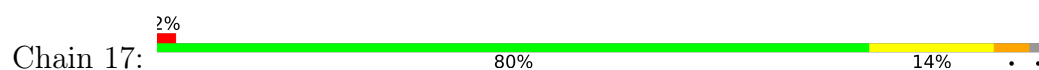
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

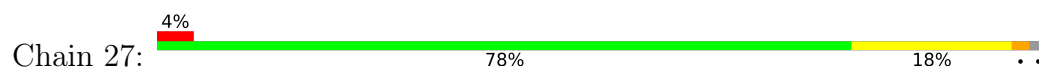


- Molecule 29: 50S ribosomal protein L34

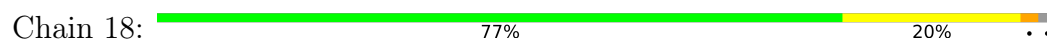




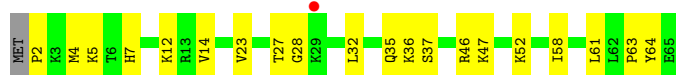
- Molecule 29: 50S ribosomal protein L34



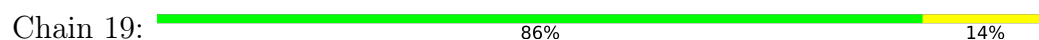
- Molecule 30: 50S ribosomal protein L35



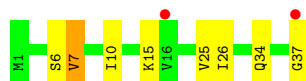
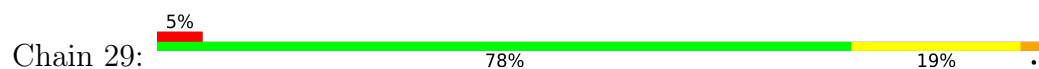
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

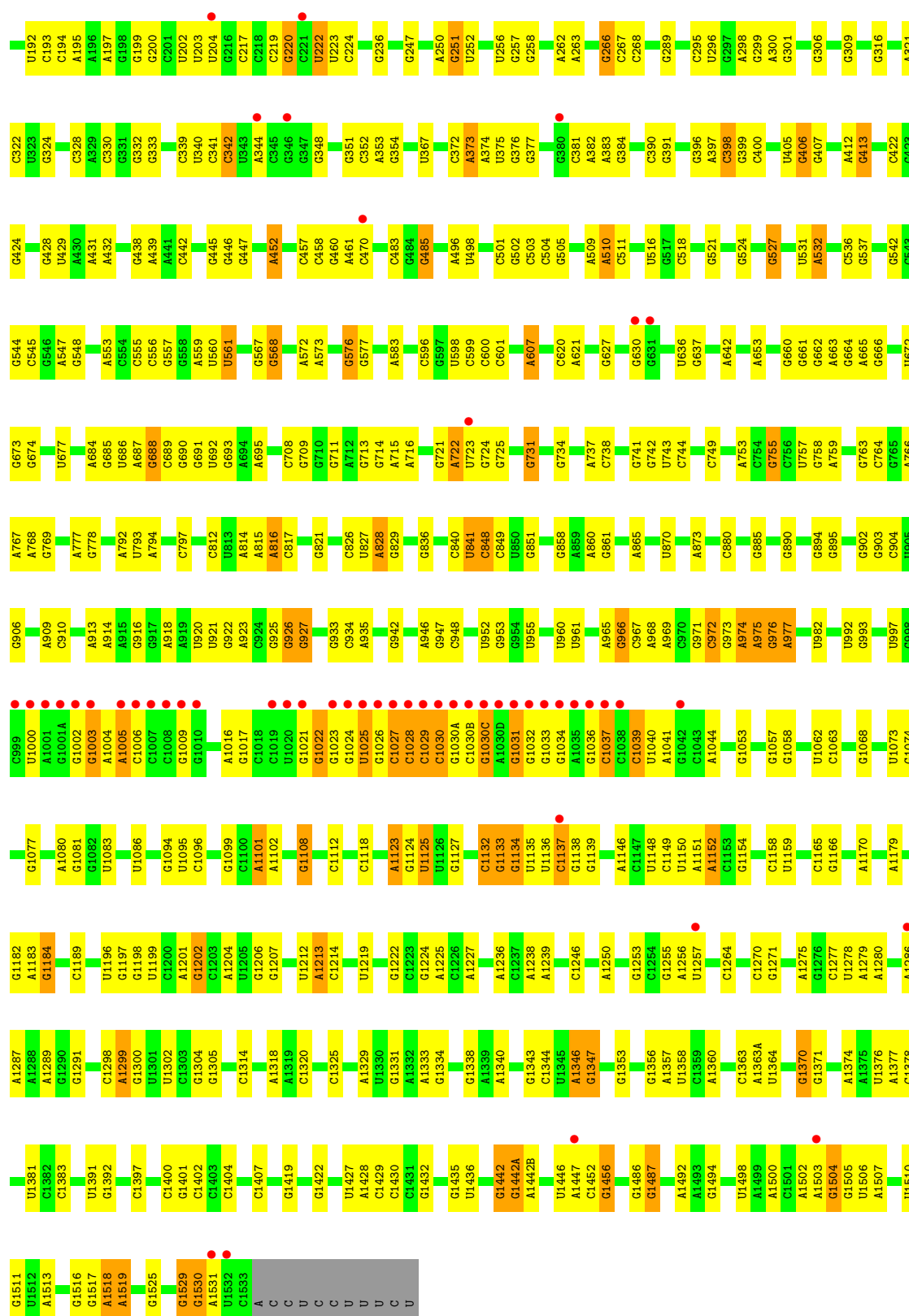


- Molecule 31: 50S ribosomal protein L36

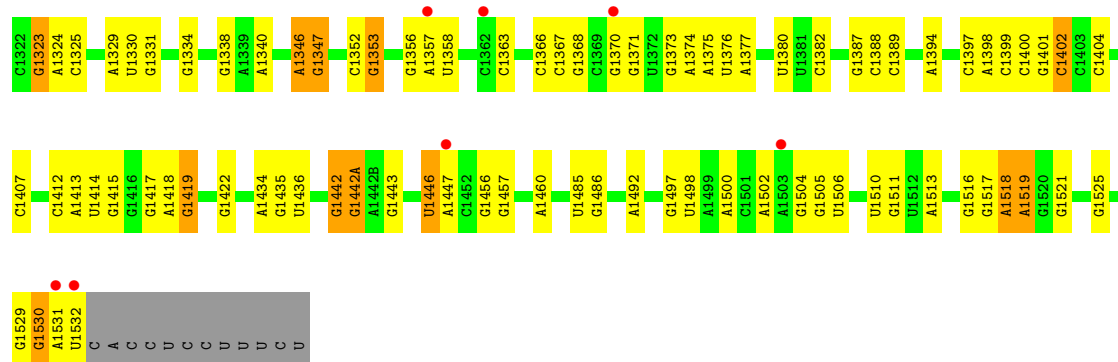


- Molecule 32: 16S Ribosomal RNA

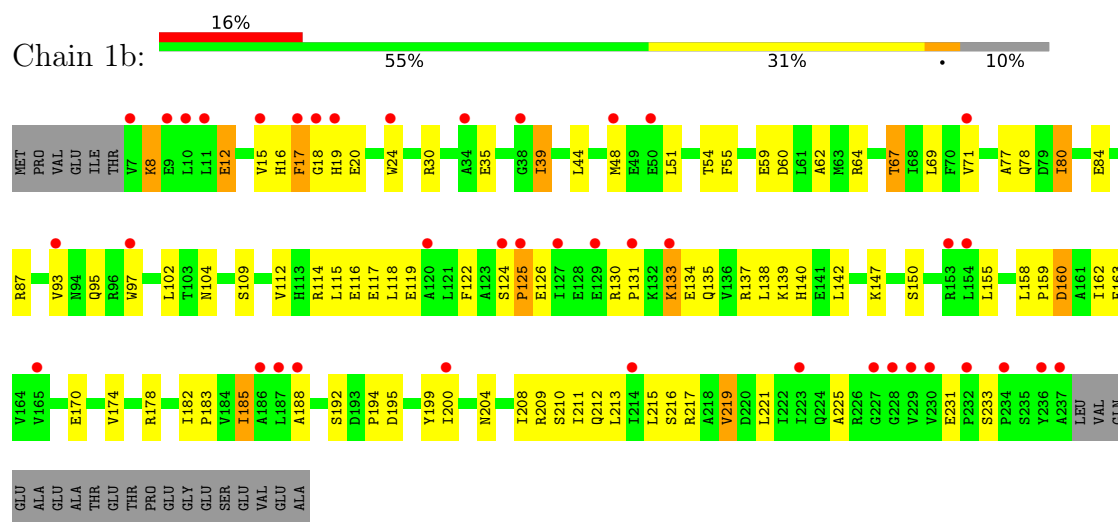




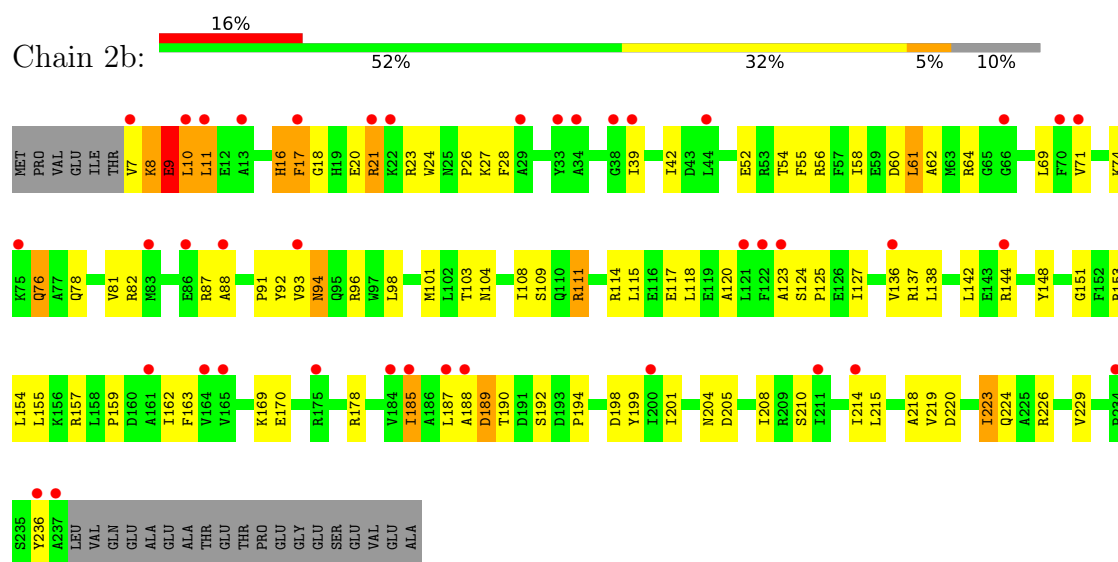




• Molecule 33: 30S ribosomal protein S2

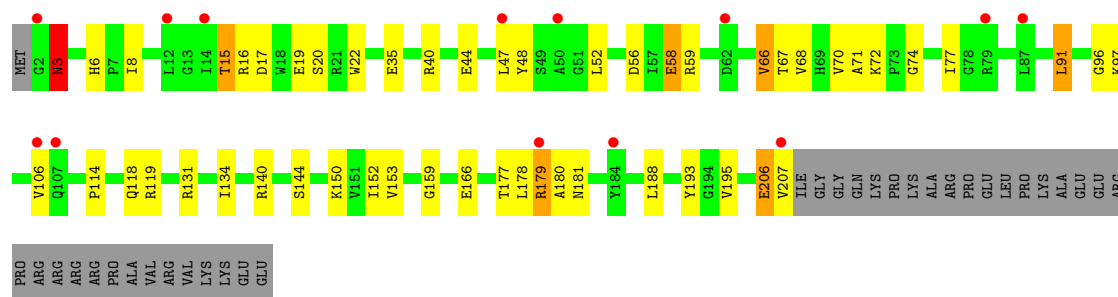


• Molecule 33: 30S ribosomal protein S2

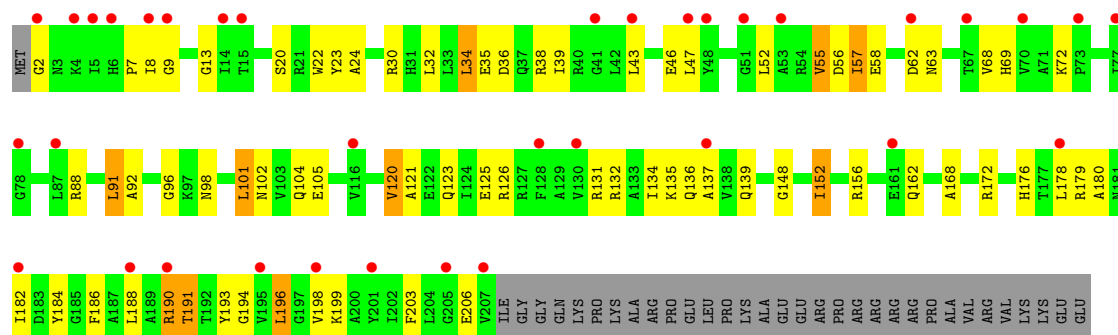


• Molecule 34: 30S ribosomal protein S3

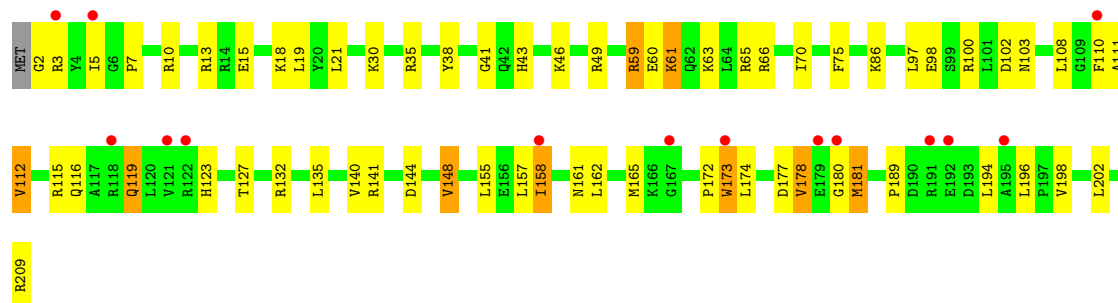




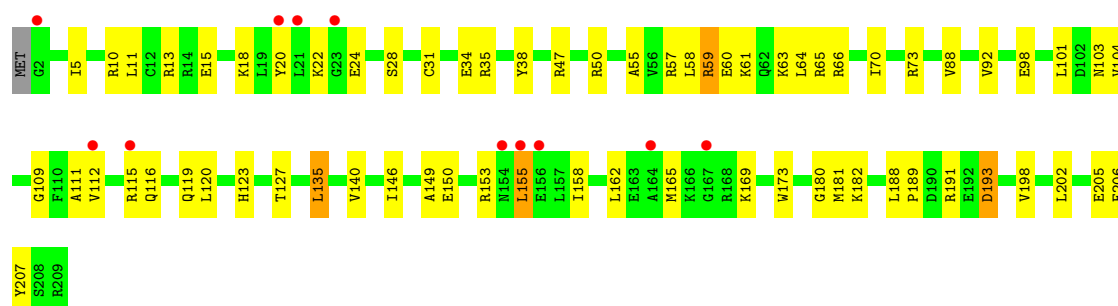
• Molecule 34: 30S ribosomal protein S3



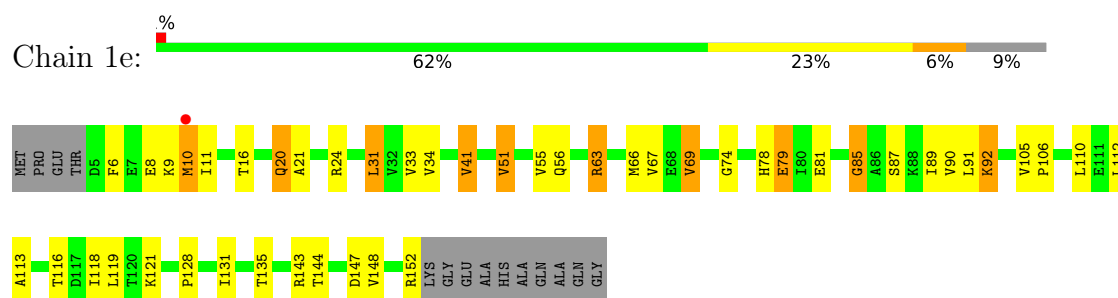
• Molecule 35: 30S ribosomal protein S4



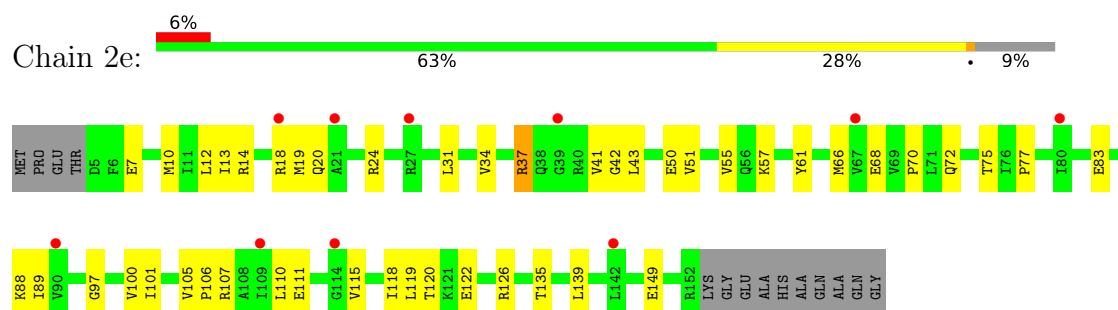
• Molecule 35: 30S ribosomal protein S4



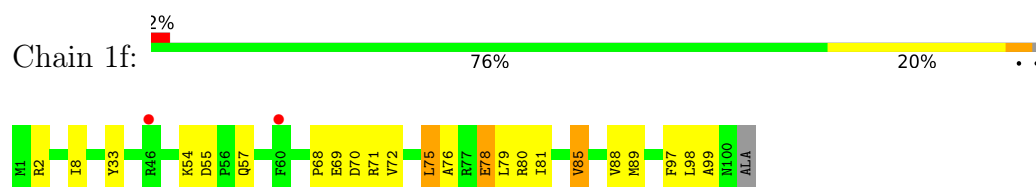
- Molecule 36: 30S ribosomal protein S5



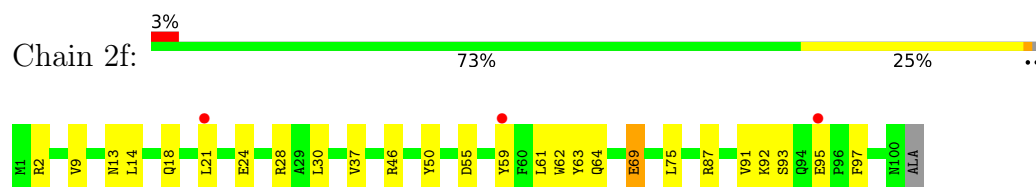
- Molecule 36: 30S ribosomal protein S5



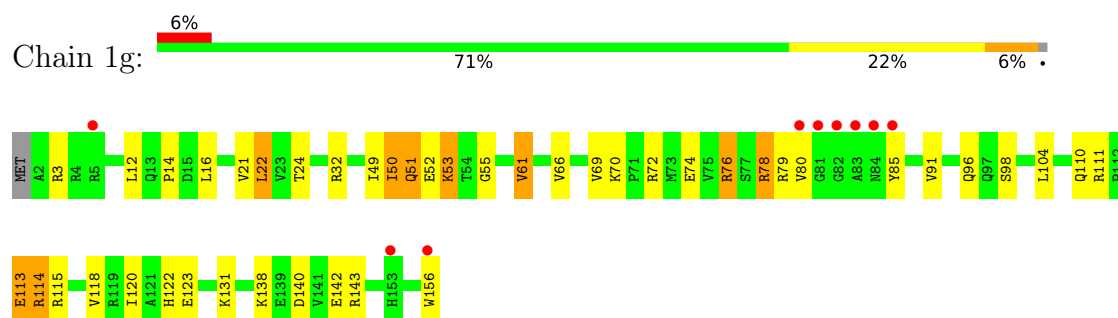
- Molecule 37: 30S ribosomal protein S6



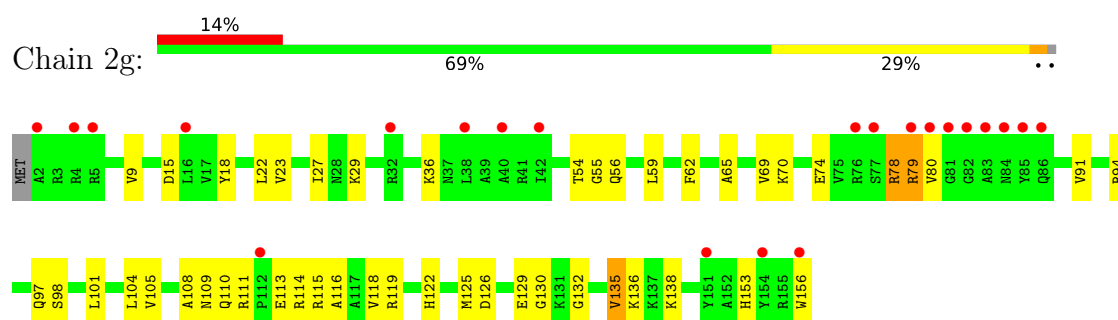
- Molecule 37: 30S ribosomal protein S6



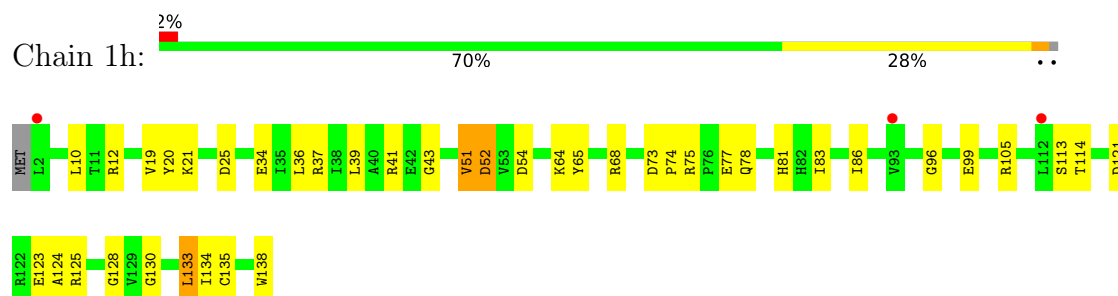
- Molecule 38: 30S ribosomal protein S7



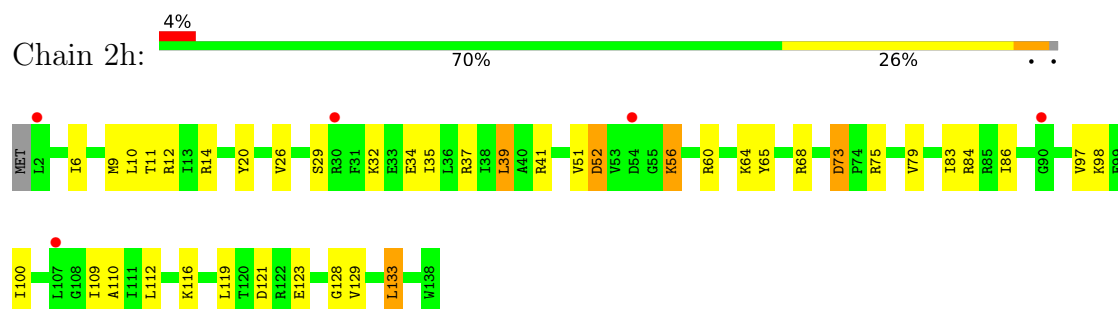
- Molecule 38: 30S ribosomal protein S7



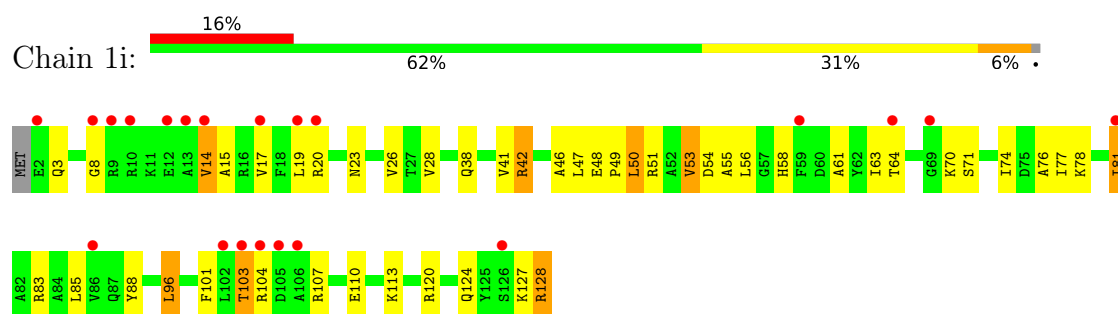
- Molecule 39: 30S ribosomal protein S8



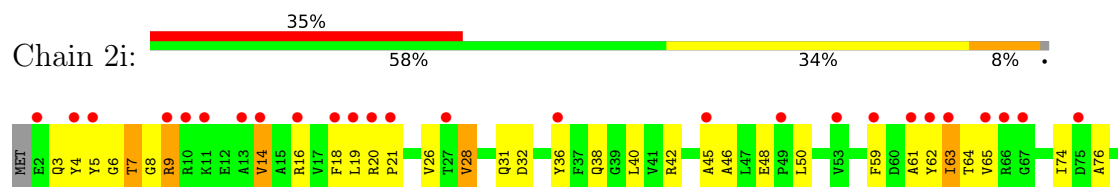
- Molecule 39: 30S ribosomal protein S8

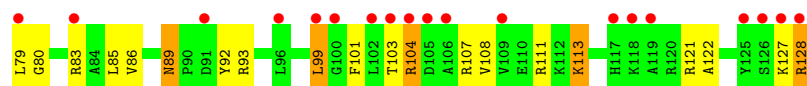


- Molecule 40: 30S ribosomal protein S9

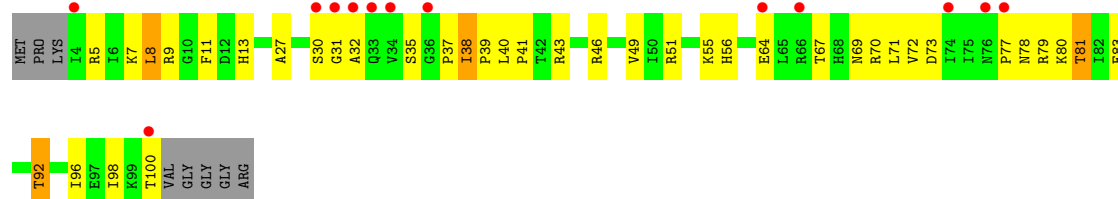


- Molecule 40: 30S ribosomal protein S9

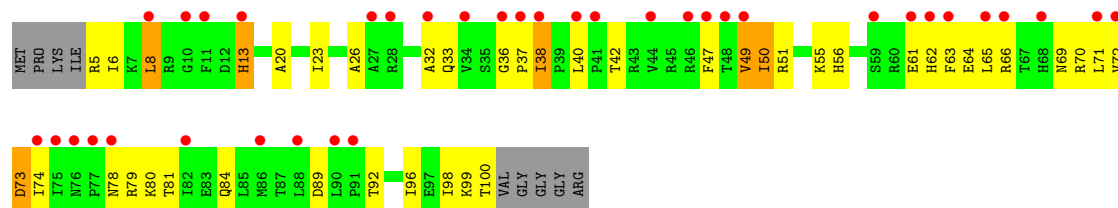




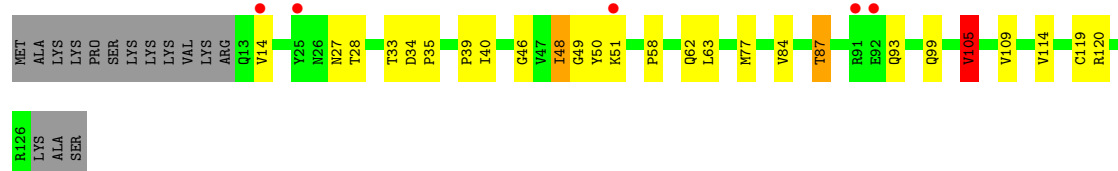
- Molecule 41: 30S ribosomal protein S10



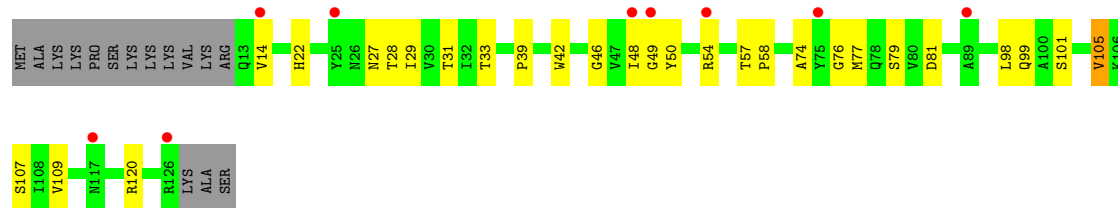
- Molecule 41: 30S ribosomal protein S10



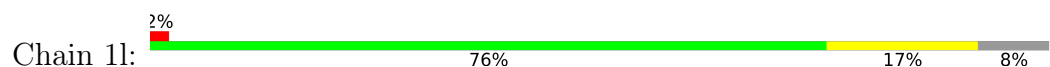
- Molecule 42: 30S ribosomal protein S11

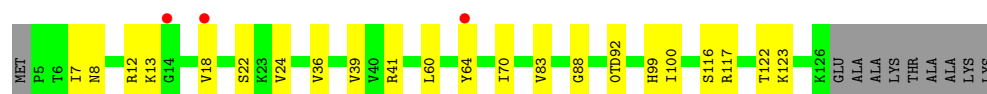


- Molecule 42: 30S ribosomal protein S11

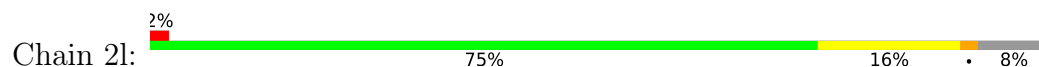


- Molecule 43: 30S ribosomal protein S12





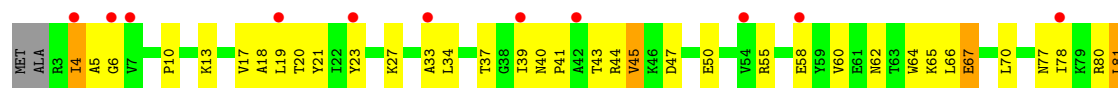
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



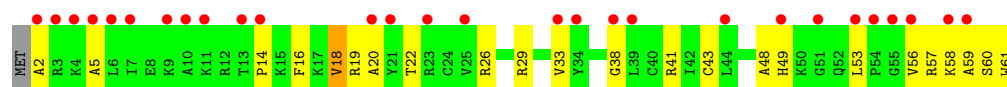
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

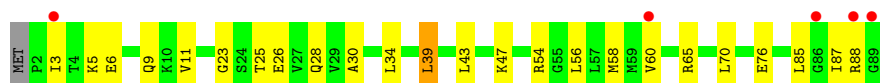
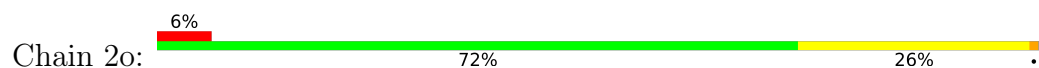


- Molecule 46: 30S ribosomal protein S15





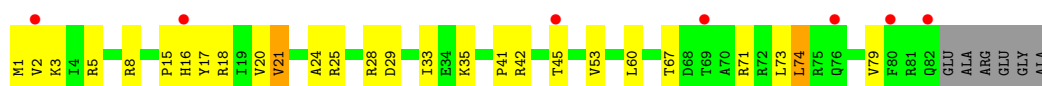
- Molecule 46: 30S ribosomal protein S15



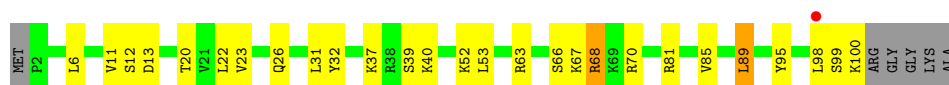
- Molecule 47: 30S ribosomal protein S16



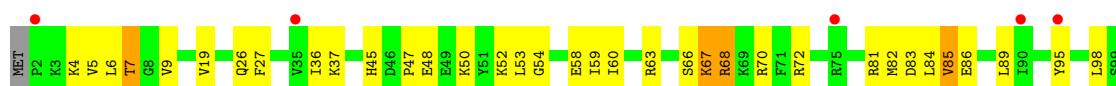
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

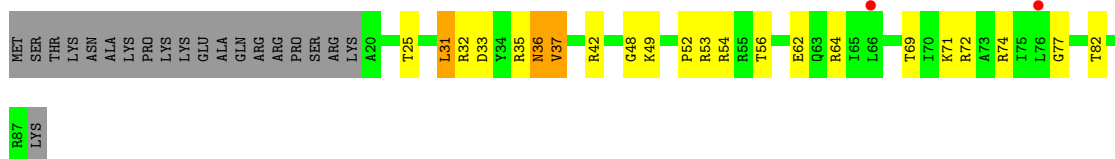


- Molecule 49: 30S ribosomal protein S18





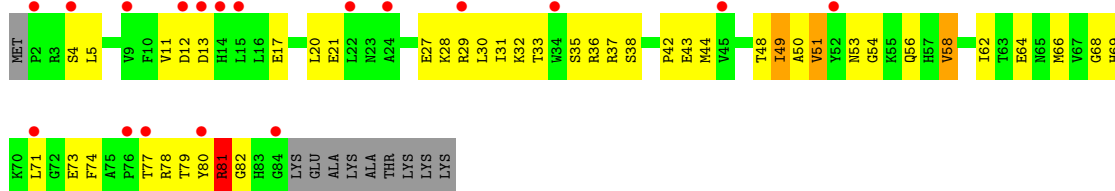
- Molecule 49: 30S ribosomal protein S18



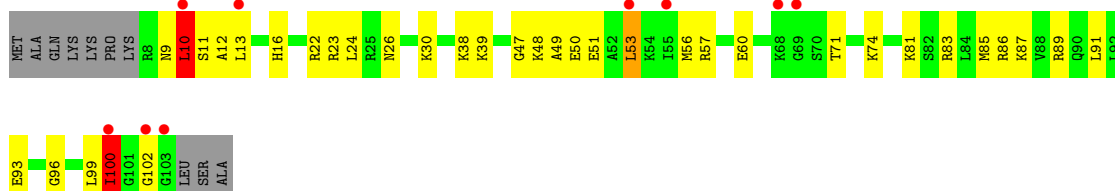
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

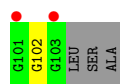


- Molecule 51: 30S ribosomal protein S20

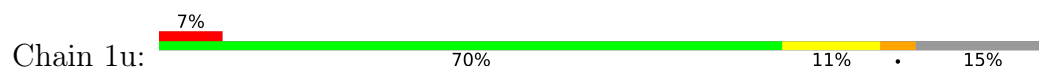


- Molecule 51: 30S ribosomal protein S20

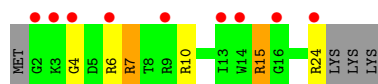




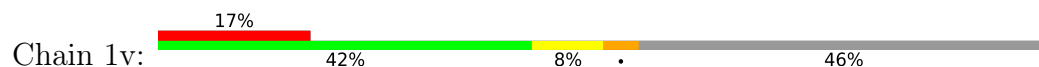
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



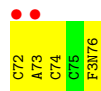
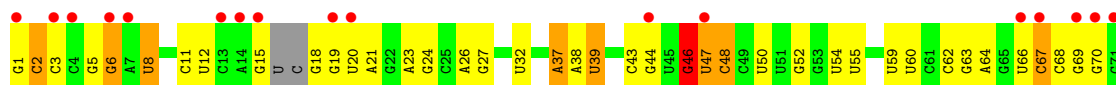
- Molecule 53: MF-mRNA



- Molecule 53: MF-mRNA

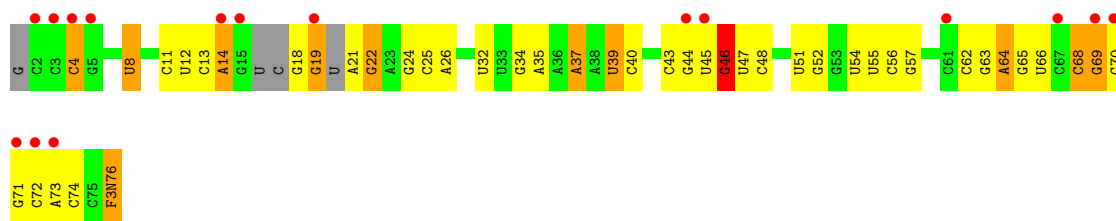


- Molecule 54: A-site Aminoacylated Phe-tRNAphe

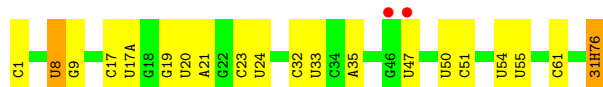
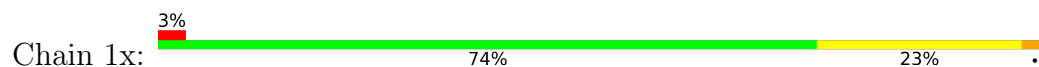


- Molecule 54: A-site Aminoacylated Phe-tRNAphe





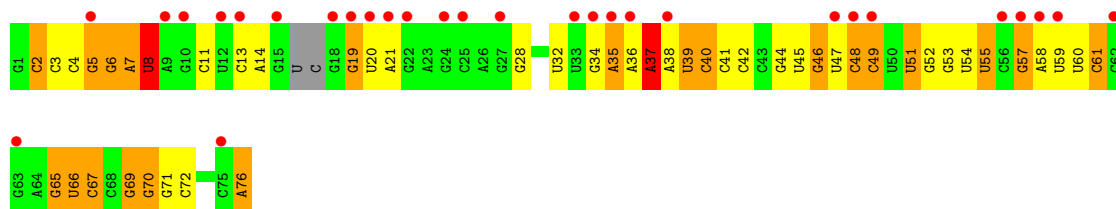
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



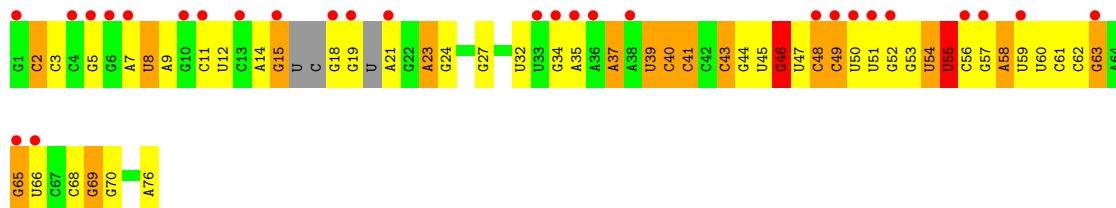
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



- Molecule 56: E-site Deacylated tRNA^{Phe}



- Molecule 56: E-site Deacylated tRNA^{Phe}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.65Å 448.12Å 621.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	162.05 – 2.65 162.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (162.05-2.65) 98.7 (162.05-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.249 0.209 , 0.249	Depositor DCC
R_{free} test set	82773 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	300115	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: 2MU, M2G, 5MC, TYK, 8AH, G7M, K, OMC, SF4, 2MG, F3N, OMG, 5MU, MA6, PSU, 4OC, UR3, MG, 0TD, MIA, 31H, 4SU, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	0/69010	0.46	3/107716 (0.0%)
1	2A	0.21	0/67294	0.39	1/105038 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.34	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.47	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.25	0/1618	0.47	0/2191
5	2F	0.21	0/1614	0.48	3/2186 (0.1%)
6	1G	0.24	0/1448	0.50	1/1957 (0.1%)
6	2G	0.19	0/1453	0.43	0/1963
7	1H	0.22	0/1356	0.42	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.21	0/1112	0.50	1/1514 (0.1%)
8	2I	0.21	0/1079	0.45	0/1475
9	1N	0.25	0/1144	0.49	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.21	0/943	0.45	0/1269
11	1P	0.25	0/1152	0.61	0/1533
11	2P	0.20	0/1152	0.49	0/1533
12	1Q	0.28	0/1143	0.47	0/1527
12	2Q	0.21	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.47	0/1312
13	2R	0.21	0/982	0.50	0/1312
14	1S	0.23	0/883	0.46	0/1176
14	2S	0.20	0/880	0.41	0/1172
15	1T	0.24	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.28	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.25	0/782	0.47	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.20	0/897	0.39	0/1205
19	1X	0.27	0/764	0.55	2/1025 (0.2%)
19	2X	0.20	0/764	0.48	2/1025 (0.2%)
20	1Y	0.22	0/819	0.48	0/1095
20	2Y	0.19	0/819	0.43	0/1095
21	1Z	0.21	0/1267	0.44	0/1717
21	2Z	0.20	0/1299	0.44	0/1763
22	10	0.28	0/662	0.51	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.44	0/1014
23	21	0.22	0/762	0.39	0/1014
24	12	0.24	0/590	0.41	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.24	0/474	0.44	0/635
25	23	0.20	0/469	0.45	0/630
26	14	0.24	0/565	0.61	0/761
26	24	0.26	0/545	0.44	0/737
27	15	0.27	0/469	0.50	0/635
27	25	0.22	0/469	0.44	0/635
28	16	0.27	0/460	0.48	0/613
28	26	0.23	0/456	0.44	0/608
29	17	0.29	0/426	0.53	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.28	0/525	0.47	0/691
30	28	0.21	0/525	0.40	0/691
31	19	0.26	0/310	0.51	0/407
31	29	0.20	0/310	0.55	1/407 (0.2%)
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.22	0/1881	0.47	0/2542
33	2b	0.23	0/1860	0.46	0/2518
34	1c	0.20	0/1572	0.40	1/2126 (0.0%)
34	2c	0.25	0/1566	0.44	0/2119
35	1d	0.19	0/1685	0.42	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.20	0/1145	0.44	0/1543
36	2e	0.22	0/1149	0.45	0/1548
37	1f	0.19	0/823	0.40	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	0.19	0/1250	0.39	0/1679
38	2g	0.22	0/1254	0.43	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.23	0/1108	0.42	0/1494
40	1i	0.22	0/1002	0.47	0/1346
40	2i	0.21	0/997	0.44	0/1343
41	1j	0.22	0/722	0.45	0/982
41	2j	0.22	0/727	0.50	0/988
42	1k	0.25	0/844	0.38	0/1145
42	2k	0.20	0/848	0.41	0/1149
43	1l	0.25	0/937	0.45	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.19	0/969	0.50	0/1302
44	2m	0.23	0/961	0.58	2/1291 (0.2%)
45	1n	0.21	0/501	0.45	0/664
45	2n	0.20	0/501	0.46	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.19	0/697	0.44	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.19	0/836	0.45	0/1117
48	2q	0.17	0/836	0.43	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.19	0/560	0.41	0/746
50	1s	0.22	0/667	0.45	0/900
50	2s	0.30	0/661	0.58	0/893
51	1t	0.21	0/730	0.48	0/965
51	2t	0.20	0/729	0.42	0/965
52	1u	0.18	0/203	0.42	0/266
52	2u	0.23	0/203	0.45	0/266
53	1v	0.23	0/310	0.37	0/480
53	2v	0.20	0/310	0.33	0/480
54	1w	0.30	1/1581 (0.1%)	0.40	0/2458
54	2w	0.29	1/1531 (0.1%)	0.40	0/2379
55	1x	0.27	0/1723	0.40	0/2684
55	2x	0.25	0/1723	0.37	0/2684
56	1y	0.31	2/1606 (0.1%)	0.40	0/2497
56	2y	0.30	2/1583 (0.1%)	0.40	0/2459
All	All	0.23	6/316632 (0.0%)	0.42	20/474029 (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
33	1b	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	5.75	1.61	1.56
54	2w	46	G7M	O3'-P	5.52	1.61	1.56
56	2y	46	G7M	O3'-P	5.44	1.61	1.56
56	1y	46	G7M	O3'-P	5.43	1.61	1.56
56	1y	8	4SU	O3'-P	5.30	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1G	150	ASP	N-CA-C	-9.76	103.50	114.62
8	1I	50	ARG	N-CA-C	-9.26	104.07	114.62
1	1A	1992	G	C2'-C3'-O3'	7.09	120.14	109.50
44	2m	107	ALA	N-CA-C	-7.07	104.59	112.57
19	1X	94	GLY	CA-C-N	5.73	132.02	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61853	0	31182	521	0
1	2A	60323	0	30412	600	0
2	1B	2577	0	1305	19	0
2	2B	2575	0	1303	34	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	19	0
4	2E	1559	0	1618	31	0
5	1F	1583	0	1625	33	0
5	2F	1579	0	1619	37	0
6	1G	1423	0	1436	35	0
6	2G	1428	0	1438	42	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	23	0
8	2I	1064	0	1082	36	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	21	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	32	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	18	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	7	0
13	2R	968	0	1033	18	0
14	1S	873	0	927	17	0
14	2S	870	0	923	31	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	17	0
17	1V	771	0	830	9	0
17	2V	771	0	830	13	0
18	1W	886	0	940	8	0
18	2W	886	0	940	12	0
19	1X	750	0	814	13	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	14	0
20	2Y	806	0	881	13	0
21	1Z	1240	0	1240	24	0
21	2Z	1271	0	1273	34	0
22	10	653	0	674	8	0
22	20	653	0	674	16	0
23	11	755	0	826	5	0
23	21	755	0	826	15	0
24	12	588	0	643	4	0
24	22	588	0	643	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	12	0
25	23	464	0	514	14	0
26	14	552	0	533	19	0
26	24	532	0	503	26	0
27	15	455	0	465	5	0
27	25	455	0	465	6	0
28	16	453	0	473	9	0
28	26	449	0	469	10	0
29	17	418	0	467	5	0
29	27	418	0	467	7	0
30	18	517	0	582	12	0
30	28	517	0	582	15	0
31	19	307	0	335	3	0
31	29	307	0	335	4	0
32	1a	32246	0	16295	315	0
32	2a	32327	0	16338	443	0
33	1b	1846	0	1867	58	0
33	2b	1825	0	1828	62	0
34	1c	1548	0	1535	33	0
34	2c	1542	0	1517	48	0
35	1d	1655	0	1672	48	0
35	2d	1674	0	1714	53	0
36	1e	1129	0	1185	26	0
36	2e	1133	0	1191	31	0
37	1f	810	0	804	12	0
37	2f	816	0	808	17	0
38	1g	1231	0	1238	24	0
38	2g	1235	0	1249	33	0
39	1h	1088	0	1126	26	0
39	2h	1088	0	1126	26	0
40	1i	983	0	986	31	0
40	2i	978	0	966	38	0
41	1j	709	0	650	28	0
41	2j	714	0	672	35	0
42	1k	829	0	825	15	0
42	2k	833	0	836	18	0
43	1l	932	0	981	10	0
43	2l	932	0	981	13	0
44	1m	958	0	1002	19	0
44	2m	950	0	988	38	0
45	1n	492	0	529	11	0
45	2n	492	0	529	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	16	0
46	2o	728	0	760	15	0
47	1p	681	0	697	15	0
47	2p	677	0	686	16	0
48	1q	823	0	891	15	0
48	2q	823	0	891	19	0
49	1r	555	0	618	10	0
49	2r	555	0	618	18	0
50	1s	652	0	662	17	0
50	2s	646	0	644	34	0
51	1t	728	0	798	22	0
51	2t	727	0	796	14	0
52	1u	199	0	208	4	0
52	2u	199	0	208	6	0
53	1v	277	0	140	2	0
53	2v	277	0	140	1	0
54	1w	1603	0	828	18	0
54	2w	1555	0	797	28	0
55	1x	1656	0	849	11	0
55	2x	1656	0	850	19	0
56	1y	1585	0	803	26	0
56	2y	1565	0	794	33	0
57	10	10	0	0	0	0
57	11	5	0	0	0	0
57	12	3	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	6	0	0	0	0
57	16	1	0	0	0	0
57	17	5	0	0	0	0
57	18	7	0	0	0	0
57	19	1	0	0	0	0
57	1A	1099	0	0	0	0
57	1B	34	0	0	0	0
57	1D	12	0	0	0	0
57	1E	10	0	0	0	0
57	1F	15	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	5	0	0	0	0
57	1O	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1P	5	0	0	0	0
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	10	0	0	0	0
57	1V	5	0	0	0	0
57	1W	6	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	214	0	0	0	0
57	1b	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	1	0	0	0	0
57	1h	1	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	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	5	0	0	0	0
57	1x	13	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	21	2	0	0	0	0
57	23	2	0	0	0	0
57	25	4	0	0	0	0
57	27	2	0	0	0	0
57	28	5	0	0	0	0
57	29	1	0	0	0	0
57	2A	797	0	0	0	0
57	2B	19	0	0	0	0
57	2D	8	0	0	0	0
57	2E	9	0	0	0	0
57	2F	8	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2Q	4	0	0	0	0
57	2R	2	0	0	0	0
57	2T	2	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	221	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	3	0	0	0	0
57	2j	1	0	0	0	0
57	2k	1	0	0	0	0
57	2l	1	0	0	0	0
57	2q	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	4	0	0	0	0
57	2w	7	0	0	0	0
57	2x	9	0	0	0	0
57	2y	2	0	0	0	0
58	1A	1	0	0	0	0
59	1A	64	0	76	1	0
59	2A	64	0	76	1	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	1	0
61	2d	8	0	0	1	0
62	10	10	0	0	0	0
62	11	6	0	0	0	0
62	12	3	0	0	0	0
62	13	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	14	1	0	0	0	0
62	15	6	0	0	0	0
62	16	2	0	0	0	0
62	17	10	0	0	0	0
62	18	12	0	0	1	0
62	1A	1975	0	0	69	0
62	1B	59	0	0	0	0
62	1D	25	0	0	1	0
62	1E	25	0	0	1	0
62	1F	13	0	0	0	0
62	1G	2	0	0	0	0
62	1H	2	0	0	0	0
62	1N	5	0	0	0	0
62	1O	4	0	0	0	0
62	1P	23	0	0	1	0
62	1Q	6	0	0	0	0
62	1R	9	0	0	0	0
62	1S	2	0	0	0	0
62	1T	7	0	0	0	0
62	1U	11	0	0	0	0
62	1V	8	0	0	0	0
62	1W	7	0	0	1	0
62	1X	6	0	0	0	0
62	1Y	3	0	0	1	0
62	1Z	1	0	0	0	0
62	1a	377	0	0	24	0
62	1b	1	0	0	0	0
62	1e	2	0	0	0	0
62	1f	2	0	0	0	0
62	1l	6	0	0	0	0
62	1m	1	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	12	0	0	1	0
62	1x	15	0	0	0	0
62	1y	1	0	0	0	0
62	20	4	0	0	0	0
62	21	7	0	0	0	0
62	23	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	25	1	0	0	0	0
62	26	2	0	0	1	0
62	27	4	0	0	0	0
62	28	4	0	0	0	0
62	29	1	0	0	0	0
62	2A	1136	0	0	67	0
62	2B	22	0	0	0	0
62	2D	21	0	0	1	0
62	2E	16	0	0	0	0
62	2F	13	0	0	0	0
62	2O	2	0	0	0	0
62	2P	5	0	0	2	0
62	2Q	1	0	0	0	0
62	2R	2	0	0	0	0
62	2T	7	0	0	0	0
62	2U	4	0	0	0	0
62	2W	3	0	0	0	0
62	2X	2	0	0	1	0
62	2Z	1	0	0	0	0
62	2a	254	0	0	29	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2e	1	0	0	0	0
62	2j	4	0	0	1	0
62	2l	4	0	0	1	0
62	2n	1	0	0	0	0
62	2o	1	0	0	0	0
62	2p	1	0	0	0	0
62	2q	2	0	0	0	0
62	2t	2	0	0	0	0
62	2v	2	0	0	0	0
62	2w	3	0	0	0	0
62	2x	10	0	0	1	0
62	2y	1	0	0	0	0
All	All	300115	0	196876	3588	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 3588 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	1.47	1.13
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.47	0.96
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.48	0.95
1:1A:1082:U:O4	1:1A:1086:A:N1	2.01	0.94
22:20:10:THR:HG22	22:20:12:ASN:H	1.33	0.94

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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	39
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	39
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	24	39
5	2F	200/210 (95%)	194 (97%)	4 (2%)	2 (1%)	12	20
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
6	2G	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	7	12
7	1H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	21	34
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	14
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	30
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	27
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	10
11	2P	147/150 (98%)	130 (88%)	11 (8%)	6 (4%)	2	3
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	4 (4%)	2 (2%)	6	10
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	20
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	20
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	14	24
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	20
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	135 (91%)	12 (8%)	1 (1%)	18	30
21	2Z	156/206 (76%)	130 (83%)	22 (14%)	4 (3%)	4	6
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	19
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	11
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	197 (86%)	27 (12%)	5 (2%)	5	9
33	2b	229/256 (90%)	194 (85%)	28 (12%)	7 (3%)	3	5
34	1c	204/239 (85%)	186 (91%)	17 (8%)	1 (0%)	24	39
34	2c	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	24	39
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	14
36	2e	146/162 (90%)	137 (94%)	7 (5%)	2 (1%)	9	14
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	18	30
38	2g	153/156 (98%)	133 (87%)	18 (12%)	2 (1%)	9	16
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	13 (10%)	1 (1%)	18	30
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	27
40	2i	125/128 (98%)	104 (83%)	21 (17%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5	9
41	2j	94/105 (90%)	82 (87%)	10 (11%)	2 (2%)	5	9
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	4	6
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16	27
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	7	12
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	7	12
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	12
46	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	20
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	5	9
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8	13
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	10	17
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	2
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	9
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10509 (92%)	769 (7%)	90 (1%)	16	27

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	29	LYS
11	1P	36	LYS
21	1Z	53	ILE
26	14	45	GLY

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	21	36
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	24
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26	44
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	38
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	8
5	2F	159/166 (96%)	151 (95%)	8 (5%)	22	37
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10	17
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	7
7	1H	144/148 (97%)	138 (96%)	6 (4%)	26	45
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	7
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	2
8	2I	105/124 (85%)	90 (86%)	15 (14%)	3	4
9	1N	118/119 (99%)	107 (91%)	11 (9%)	8	13
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	13
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	57
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	47
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9	16
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9	16
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	31	51
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	31	51
13	1R	101/101 (100%)	95 (94%)	6 (6%)	18	30
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	47
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	10
14	2S	85/88 (97%)	72 (85%)	13 (15%)	3	4
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	44
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	29
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	55
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	35
17	1V	80/82 (98%)	75 (94%)	5 (6%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	11
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	25
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	25
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	63
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	48
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	23
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	6
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	18
21	2Z	137/179 (76%)	123 (90%)	14 (10%)	7	10
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	29
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	64
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	15
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	56
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	14
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	11
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	11
26	14	59/63 (94%)	54 (92%)	5 (8%)	10	17
26	24	53/63 (84%)	49 (92%)	4 (8%)	12	21
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	19
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	47
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	7
28	26	50/52 (96%)	41 (82%)	9 (18%)	2	2
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	7
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	22
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	32
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	32
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	30
33	1b	192/220 (87%)	174 (91%)	18 (9%)	8	13
33	2b	187/220 (85%)	163 (87%)	24 (13%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	10
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	11
35	1d	169/181 (93%)	152 (90%)	17 (10%)	7	11
35	2d	173/181 (96%)	162 (94%)	11 (6%)	16	28
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5	8
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	12
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	9
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18	30
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	3
38	2g	120/127 (94%)	114 (95%)	6 (5%)	22	37
39	1h	114/119 (96%)	108 (95%)	6 (5%)	20	35
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	30
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2	3
40	2i	89/99 (90%)	72 (81%)	17 (19%)	1	2
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	7
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	4
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	11
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	39
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	29
43	2l	96/108 (89%)	91 (95%)	5 (5%)	21	36
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	12
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	6
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	18
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	10
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	49
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	28
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	11
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	7
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	44
48	2q	94/97 (97%)	85 (90%)	9 (10%)	8	12
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	36
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	58
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	5
51	1t	70/82 (85%)	63 (90%)	7 (10%)	7	11
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	16
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	32
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	9
All	All	9303/10064 (92%)	8544 (92%)	759 (8%)	10	18

5 of 759 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	2P	147	LEU
28	26	23	THR
14	2S	27	SER
11	2P	135	LEU
20	2Y	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	98	ASN
49	2r	63	GLN
35	2d	77	ASN
40	2i	58	HIS
36	1e	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	435 (15%)	30 (1%)
1	2A	2791/2915 (95%)	463 (16%)	26 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1497/1521 (98%)	242 (16%)	0
32	2a	1501/1521 (98%)	272 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	1 (8%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	72/76 (94%)	35 (48%)	0
56	2y	70/76 (92%)	25 (35%)	0
All	All	9345/9620 (97%)	1569 (16%)	56 (0%)

5 of 1569 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	58	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2689	U
1	2A	2689	U
1	2A	271(M)	G
1	2A	2439	A
1	2A	1913	A

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

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	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.07	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.46	6 (31%)	27,32,35	2.18	6 (22%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
54	PSU	1w	39	54	18,21,22	1.40	3 (16%)	21,30,33	1.82	3 (14%)
56	PSU	2y	39	56	18,21,22	1.41	2 (11%)	21,30,33	1.76	3 (14%)
32	G7M	1a	527	32,57	23,26,27	1.51	3 (13%)	34,39,42	1.73	5 (14%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	1.07	3 (12%)
54	5MU	1w	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.94	6 (22%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	1.96	3 (14%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	2.06	9 (27%)
32	MA6	1a	1519	32	23,26,27	0.46	0	33,38,41	2.13	8 (24%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	21,30,33	1.98	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.49	3 (15%)	26,32,35	1.11	2 (7%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	27,32,35	2.15	6 (22%)
1	5MU	2A	1939	57,1	19,22,23	1.40	5 (26%)	27,32,35	2.29	6 (22%)
54	F3N	1w	76	1,54	33,36,37	1.56	5 (15%)	41,51,54	1.82	10 (24%)
1	5MU	1A	1939	57,1	19,22,23	1.35	5 (26%)	27,32,35	2.19	6 (22%)
56	PSU	2y	55	56	18,21,22	1.32	3 (16%)	21,30,33	1.99	4 (19%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.18	3 (11%)
56	G7M	2y	46	56	23,26,27	1.66	4 (17%)	34,39,42	1.96	4 (11%)
1	8AH	1A	2503	57,1	22,26,27	1.61	5 (22%)	29,39,42	2.24	5 (17%)
56	MIA	1y	37	56	21,24,32	1.65	4 (19%)	30,35,47	1.98	6 (20%)
54	4SU	1w	8	54	18,21,22	1.75	4 (22%)	25,30,33	1.89	4 (16%)
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.06	3 (14%)
32	2MG	1a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.27	8 (24%)
32	5MC	1a	1404	32	19,22,23	1.76	3 (15%)	26,32,35	1.19	4 (15%)
54	4SU	2w	8	54	18,21,22	1.72	4 (22%)	25,30,33	2.81	5 (20%)
43	0TD	2l	92	43	8,9,10	4.52	1 (12%)	6,11,13	1.91	2 (33%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.86	0
32	5MC	1a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	2A	1962	57,1	19,22,23	1.67	3 (15%)	26,32,35	1.17	2 (7%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.70	4 (19%)
55	4SU	1x	8	55	18,21,22	2.32	5 (27%)	25,30,33	1.74	6 (24%)
32	G7M	2a	527	32,57	23,26,27	1.53	3 (13%)	34,39,42	1.67	5 (14%)
1	5MC	1A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.19	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	4SU	2y	8	56	18,21,22	1.72	4 (22%)	25,30,33	2.41	6 (24%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
55	31H	1x	76	55,57	31,34,35	1.23	3 (9%)	35,47,50	2.08	11 (31%)
1	PSU	1A	2605	57,1	18,21,22	1.32	3 (16%)	21,30,33	2.03	4 (19%)
43	0TD	1l	92	43	8,9,10	4.54	2 (25%)	6,11,13	7.49	2 (33%)
54	G7M	2w	46	54	23,26,27	1.51	3 (13%)	34,39,42	1.74	4 (11%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.03	4 (19%)
54	MIA	1w	37	54	28,31,32	2.35	6 (21%)	38,44,47	2.59	12 (31%)
55	31H	2x	76	55,57	31,34,35	1.20	3 (9%)	35,47,50	2.16	13 (37%)
56	PSU	1y	55	56	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.06	2 (10%)	26,32,35	1.78	4 (15%)
56	PSU	1y	39	56	18,21,22	1.44	2 (11%)	21,30,33	1.81	4 (19%)
54	G7M	1w	46	54	23,26,27	1.56	3 (13%)	34,39,42	1.68	4 (11%)
1	OMG	1A	2251	55,57,1	23,26,27	1.27	3 (13%)	32,38,41	1.94	6 (18%)
56	PSU	1y	32	56	18,21,22	1.35	2 (11%)	21,30,33	1.95	3 (14%)
56	5MU	1y	54	56	19,22,23	1.40	5 (26%)	27,32,35	2.16	7 (25%)
32	2MG	2a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.15	7 (21%)
55	5MC	2x	32	55	19,22,23	1.77	3 (15%)	26,32,35	1.23	3 (11%)
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.92	6 (22%)
54	PSU	1w	32	57,54	18,21,22	1.31	2 (11%)	21,30,33	1.95	3 (14%)
1	5MC	1A	1962	1	19,22,23	1.69	3 (15%)	26,32,35	1.17	2 (7%)
55	5MU	1x	54	55,57	19,22,23	1.39	5 (26%)	27,32,35	2.02	6 (22%)
1	5MC	2A	1942	1	19,22,23	1.70	3 (15%)	26,32,35	1.11	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.46	0	33,38,41	2.16	8 (24%)
1	2MU	1A	2552	57,1	19,22,24	1.19	2 (10%)	25,31,36	1.99	6 (24%)
56	PSU	2y	32	56	18,21,22	1.32	2 (11%)	21,30,33	1.95	3 (14%)
56	MIA	2y	37	56	21,24,32	1.66	4 (19%)	30,35,47	1.99	7 (23%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.81	6 (18%)
32	UR3	2a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.75	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.93	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)
54	F3N	2w	76	1,54	33,36,37	1.49	4 (12%)	41,51,54	1.76	8 (19%)
54	MIA	2w	37	54	24,27,32	2.15	5 (20%)	32,39,47	2.62	11 (34%)
32	5MC	2a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.23	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	4SU	1y	8	56	18,21,22	1.77	4 (22%)	25,30,33	2.10	5 (20%)
32	M2G	2a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.84	6 (18%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.96	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	5 (23%)
1	2MU	2A	2552	1	19,22,24	1.31	3 (15%)	25,31,36	1.86	6 (24%)
1	8AH	2A	2503	57,1	22,26,27	1.66	5 (22%)	29,39,42	2.09	5 (17%)
1	OMG	2A	2251	55,1	23,26,27	1.23	3 (13%)	32,38,41	1.96	6 (18%)
32	4OC	1a	1402	32	20,23,24	0.72	0	25,32,35	0.97	1 (4%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.04	3 (14%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.96	6 (28%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.07	9 (27%)
56	G7M	1y	46	56	23,26,27	1.63	3 (13%)	34,39,42	1.87	4 (11%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.16	3 (11%)
55	5MC	1x	32	55	19,22,23	1.68	3 (15%)	26,32,35	1.25	3 (11%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.21	7 (25%)
56	5MU	2y	54	56	19,22,23	1.48	4 (21%)	27,32,35	2.00	6 (22%)
55	4SU	2x	8	55	18,21,22	2.15	5 (27%)	25,30,33	1.44	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	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	39	56	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	3/7/25/26	0/3/3/3
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	2/19/37/38	0/4/4/4
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	6/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
1	8AH	1A	2503	57,1	-	1/7/25/26	0/3/3/3
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,57	-	3/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,57	-	3/22/40/41	0/3/3/3
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
55	31H	2x	76	55,57	-	3/22/40/41	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	OMG	1A	2251	55,57,1	-	0/9/27/28	0/3/3/3
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	2MU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	1,54	-	1/19/37/38	0/4/4/4
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
1	8AH	2A	2503	57,1	-	0/7/25/26	0/3/3/3
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
56	G7M	1y	46	56	-	2/7/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.45	1.69	1.82
43	1l	92	0TD	CB-SB	-12.32	1.69	1.82
54	1w	37	MIA	C13-C14	7.03	1.53	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	MIA	C2-S10	-6.98	1.70	1.75
54	1w	37	MIA	C2-S10	-6.77	1.70	1.75

The worst 5 of 429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.81	70.35	102.36
54	2w	37	MIA	C5-C4-N3	-9.04	117.66	127.18
54	2w	8	4SU	C4-N3-C2	-8.98	118.71	127.31
1	1A	2503	8AH	C5-C4-N3	-8.24	118.50	127.18
1	2A	2503	8AH	C5-C4-N3	-8.22	118.52	127.18

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C15
55	1x	76	31H	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

36 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1915	5MU	1	0
54	1w	39	PSU	1	0
56	2y	39	PSU	1	0
32	2a	1402	4OC	1	0
32	1a	1518	MA6	3	0
32	1a	1519	MA6	2	0
1	2A	1939	5MU	1	0
1	1A	1939	5MU	2	0
56	2y	55	PSU	7	0
56	2y	46	G7M	1	0
56	1y	37	MIA	2	0
54	2w	8	4SU	2	0
54	2w	39	PSU	2	0
55	1x	8	4SU	2	0
56	2y	8	4SU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	55	PSU	1	0
55	1x	76	31H	1	0
54	2w	46	G7M	1	0
54	1w	37	MIA	1	0
55	2x	76	31H	2	0
56	1y	55	PSU	1	0
56	1y	39	PSU	1	0
54	1w	46	G7M	1	0
1	1A	2251	OMG	1	0
32	2a	1207	2MG	3	0
32	2a	1519	MA6	3	0
1	1A	2552	2MU	1	0
32	1a	966	M2G	1	0
54	2w	76	F3N	3	0
54	2w	37	MIA	1	0
56	1y	8	4SU	1	0
1	2A	2552	2MU	1	0
1	2A	2503	8AH	2	0
1	1A	1917	PSU	1	0
32	2a	1518	MA6	3	0
55	2x	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2685 ligands modelled in this entry, 2681 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	SF4	1d	501	35	0,12,12	-	-	-		
59	TYK	2A	3798	1	67,67,67	1.82	8 (11%)	87,97,97	1.52	16 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TYK	1A	4101	1	67,67,67	1.77	7 (10%)	87,97,97	1.35	15 (17%)
61	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	501	35	-	-	0/6/5/5
59	TYK	2A	3798	1	-	4/67/126/126	1/3/4/4
59	TYK	1A	4101	1	-	3/67/126/126	1/3/4/4
61	SF4	2d	303	35	-	-	0/6/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4101	TYK	C8-C9	-8.59	1.38	1.51
59	2A	3798	TYK	C8-C9	-8.57	1.38	1.51
59	2A	3798	TYK	C14-C13	-7.21	1.37	1.50
59	1A	4101	TYK	C14-C13	-6.61	1.39	1.50
59	2A	3798	TYK	C2-C1	-4.91	1.41	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3798	TYK	C10-C11-C12	-4.40	119.72	126.23
59	1A	4101	TYK	C3B-C2B-C1B	-4.35	106.69	114.77
59	2A	3798	TYK	C1B-O4A-C4A	3.84	122.36	114.72
59	2A	3798	TYK	O4B-C4B-C5B	-3.73	103.04	109.46
59	2A	3798	TYK	C3B-C2B-C1B	-3.72	107.85	114.77

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4101	TYK	C15-C14-C23-O1C
59	2A	3798	TYK	C15-C14-C23-O1C
59	1A	4101	TYK	C18-C4-C5-C6
59	2A	3798	TYK	C18-C4-C5-C6
59	2A	3798	TYK	C3-C4-C5-O1A

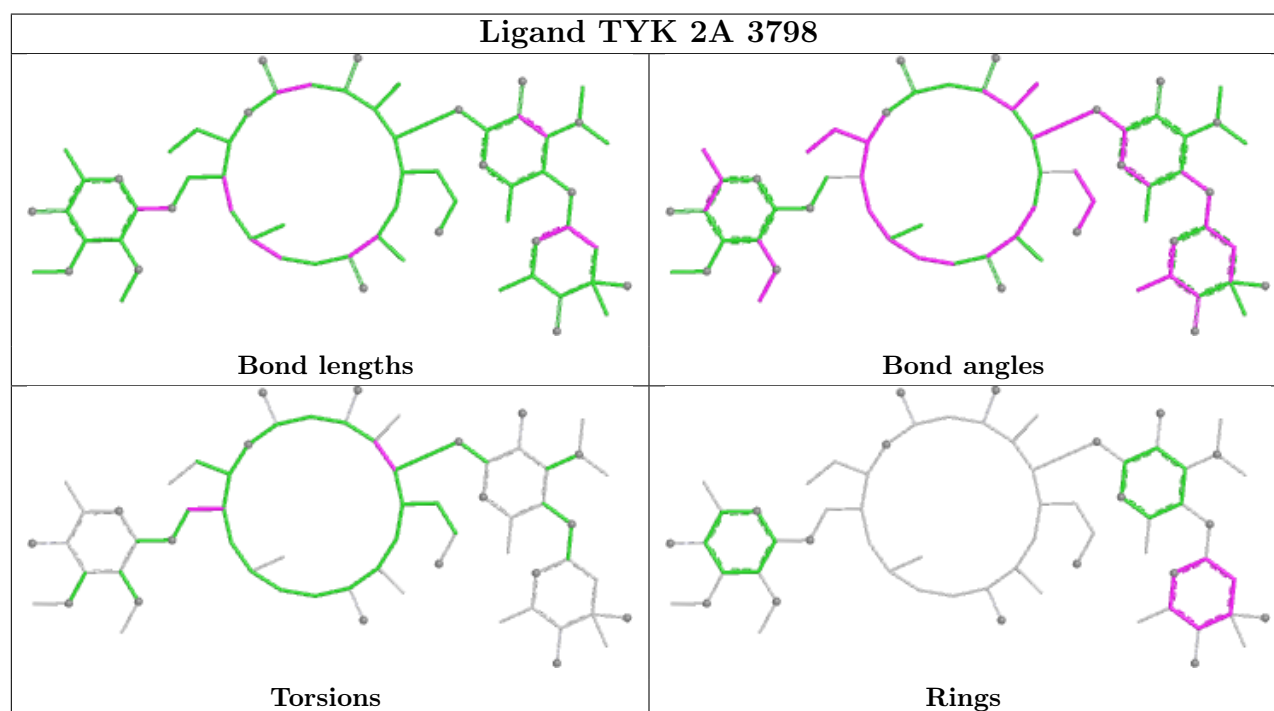
All (2) ring outliers are listed below:

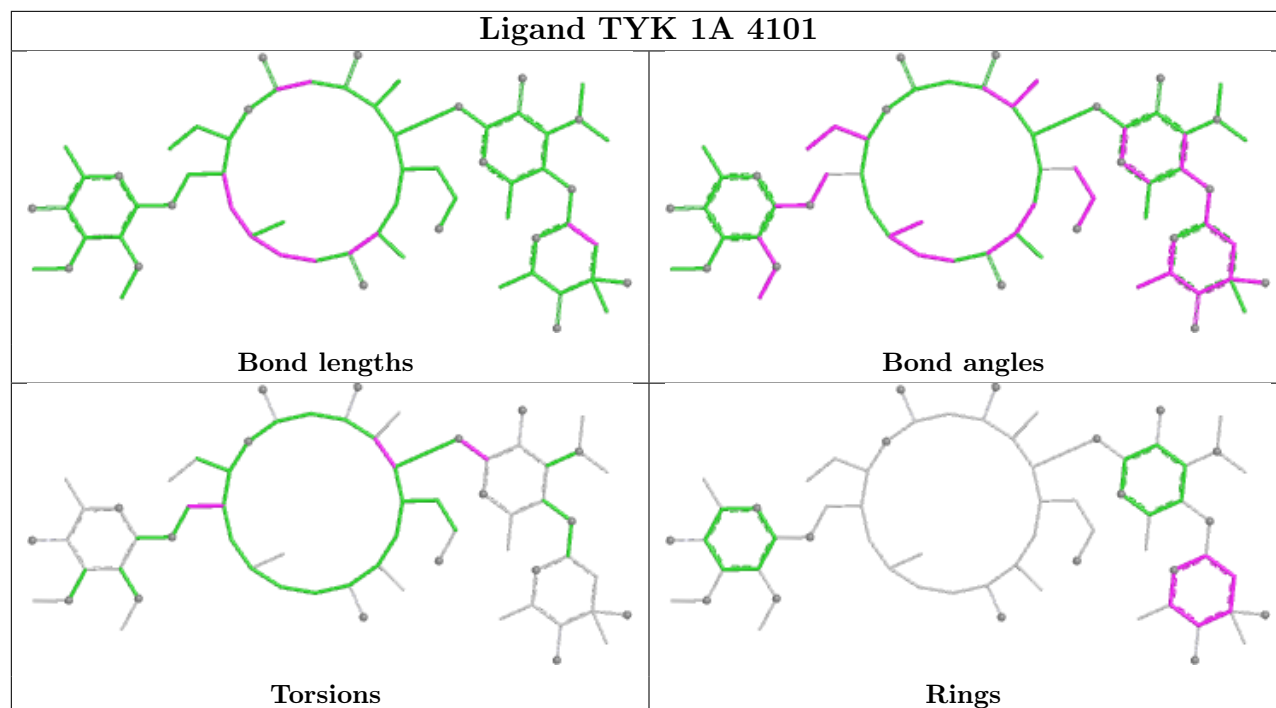
Mol	Chain	Res	Type	Atoms
59	2A	3798	TYK	C1B-C2B-C3B-C4B-C5B-O5B
59	1A	4101	TYK	C1B-C2B-C3B-C4B-C5B-O5B

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	1d	501	SF4	1	0
59	2A	3798	TYK	1	0
59	1A	4101	TYK	1	0
61	2d	303	SF4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	1A	2860/2915 (98%)	-0.42	186 (6%) 25 19	20, 36, 98, 108	0
1	2A	2789/2915 (95%)	0.07	147 (5%) 32 25	33, 57, 95, 107	0
2	1B	120/121 (99%)	-0.34	1 (0%) 82 79	29, 48, 63, 89	0
2	2B	120/121 (99%)	0.78	2 (1%) 69 64	61, 75, 84, 91	0
3	1D	275/276 (99%)	-0.26	3 (1%) 78 75	21, 37, 52, 77	0
3	2D	275/276 (99%)	0.13	2 (0%) 84 82	33, 50, 62, 82	0
4	1E	204/206 (99%)	-0.20	1 (0%) 87 85	20, 39, 59, 76	0
4	2E	204/206 (99%)	0.41	4 (1%) 65 59	38, 59, 72, 81	0
5	1F	202/210 (96%)	-0.15	1 (0%) 87 85	19, 41, 66, 84	0
5	2F	202/210 (96%)	0.45	1 (0%) 87 85	37, 66, 79, 87	0
6	1G	181/182 (99%)	0.39	5 (2%) 55 48	39, 56, 71, 81	0
6	2G	181/182 (99%)	1.03	15 (8%) 17 12	67, 77, 85, 94	0
7	1H	174/180 (96%)	0.27	4 (2%) 61 54	36, 53, 67, 73	0
7	2H	174/180 (96%)	1.25	23 (13%) 7 6	69, 83, 90, 95	0
8	1I	146/148 (98%)	0.71	2 (1%) 73 69	46, 72, 80, 83	0
8	2I	146/148 (98%)	0.87	8 (5%) 30 24	53, 73, 80, 85	0
9	1N	140/140 (100%)	-0.21	1 (0%) 84 82	25, 38, 61, 67	0
9	2N	140/140 (100%)	0.62	6 (4%) 40 32	48, 66, 79, 85	0
10	1O	122/122 (100%)	-0.28	0 100 100	28, 39, 57, 61	0
10	2O	122/122 (100%)	0.28	1 (0%) 82 79	47, 58, 70, 76	0
11	1P	149/150 (99%)	0.03	4 (2%) 56 49	23, 45, 68, 73	0
11	2P	149/150 (99%)	0.53	3 (2%) 65 59	40, 65, 80, 89	0
12	1Q	141/141 (100%)	-0.11	0 100 100	25, 39, 55, 72	0
12	2Q	141/141 (100%)	0.99	10 (7%) 22 16	48, 66, 77, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.40	0 100 100	25, 34, 46, 56	0
13	2R	118/118 (100%)	0.23	0 100 100	44, 53, 63, 70	0
14	1S	110/112 (98%)	0.17	0 100 100	38, 49, 60, 66	0
14	2S	110/112 (98%)	1.02	8 (7%) 21 15	61, 70, 78, 84	0
15	1T	131/146 (89%)	0.01	2 (1%) 72 67	33, 44, 68, 78	0
15	2T	131/146 (89%)	0.53	2 (1%) 72 67	52, 62, 75, 82	0
16	1U	116/118 (98%)	-0.43	0 100 100	22, 30, 44, 64	0
16	2U	116/118 (98%)	0.49	1 (0%) 81 78	44, 62, 72, 77	0
17	1V	101/101 (100%)	-0.43	1 (0%) 79 76	23, 38, 55, 65	0
17	2V	101/101 (100%)	0.79	2 (1%) 65 59	43, 71, 77, 83	0
18	1W	112/113 (99%)	-0.35	1 (0%) 81 78	25, 32, 49, 85	0
18	2W	112/113 (99%)	0.29	1 (0%) 81 78	40, 51, 69, 86	0
19	1X	95/96 (98%)	-0.17	2 (2%) 63 57	26, 38, 62, 77	0
19	2X	95/96 (98%)	0.51	5 (5%) 32 25	45, 58, 75, 82	0
20	1Y	107/110 (97%)	0.22	1 (0%) 81 78	36, 50, 67, 80	0
20	2Y	107/110 (97%)	1.07	12 (11%) 10 8	58, 71, 80, 86	0
21	1Z	154/206 (74%)	0.84	21 (13%) 7 5	38, 64, 83, 91	0
21	2Z	160/206 (77%)	1.65	47 (29%) 1 1	64, 81, 88, 92	0
22	10	83/85 (97%)	-0.14	0 100 100	29, 37, 50, 67	0
22	20	83/85 (97%)	0.88	5 (6%) 27 21	47, 61, 73, 78	0
23	11	97/98 (98%)	0.12	1 (1%) 79 76	29, 47, 71, 75	0
23	21	97/98 (98%)	0.35	4 (4%) 41 33	39, 55, 75, 84	0
24	12	70/72 (97%)	0.25	2 (2%) 53 46	35, 48, 59, 76	0
24	22	70/72 (97%)	0.78	2 (2%) 53 46	58, 69, 76, 80	0
25	13	59/60 (98%)	-0.22	2 (3%) 48 40	26, 36, 62, 79	0
25	23	59/60 (98%)	0.50	1 (1%) 69 64	57, 66, 79, 87	0
26	14	69/71 (97%)	0.92	8 (11%) 9 8	52, 73, 88, 89	0
26	24	69/71 (97%)	1.47	18 (26%) 1 1	75, 84, 92, 94	0
27	15	59/60 (98%)	-0.45	0 100 100	20, 32, 51, 54	0
27	25	59/60 (98%)	0.33	1 (1%) 69 64	39, 54, 66, 78	0
28	16	53/54 (98%)	-0.16	0 100 100	33, 43, 57, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.57	0 100 100	51, 60, 68, 72	0
29	17	48/49 (97%)	-0.27	1 (2%) 63 57	24, 29, 54, 63	0
29	27	48/49 (97%)	0.14	2 (4%) 40 32	35, 42, 64, 74	0
30	18	64/65 (98%)	-0.28	0 100 100	29, 34, 42, 56	0
30	28	64/65 (98%)	0.38	1 (1%) 70 66	44, 55, 62, 65	0
31	19	37/37 (100%)	-0.25	0 100 100	30, 38, 54, 61	0
31	29	37/37 (100%)	1.01	2 (5%) 31 25	60, 68, 77, 83	0
32	1a	1488/1521 (97%)	0.26	62 (4%) 40 32	34, 64, 92, 105	0
32	2a	1491/1521 (98%)	0.62	96 (6%) 25 19	49, 75, 95, 106	0
33	1b	231/256 (90%)	1.22	40 (17%) 4 3	62, 77, 87, 92	0
33	2b	231/256 (90%)	1.34	40 (17%) 4 3	73, 83, 89, 92	0
34	1c	206/239 (86%)	0.75	13 (6%) 26 19	56, 68, 79, 86	0
34	2c	206/239 (86%)	1.27	35 (16%) 4 3	73, 82, 88, 92	0
35	1d	208/209 (99%)	0.74	14 (6%) 24 18	52, 67, 76, 82	0
35	2d	208/209 (99%)	0.84	11 (5%) 32 25	59, 71, 79, 82	0
36	1e	148/162 (91%)	0.34	1 (0%) 84 82	48, 62, 72, 80	0
36	2e	148/162 (91%)	1.04	10 (6%) 23 17	65, 75, 81, 86	0
37	1f	100/101 (99%)	0.46	2 (2%) 65 59	52, 65, 72, 77	0
37	2f	100/101 (99%)	0.52	3 (3%) 52 45	49, 67, 75, 82	0
38	1g	155/156 (99%)	0.73	9 (5%) 29 22	59, 70, 84, 88	0
38	2g	155/156 (99%)	1.17	22 (14%) 6 5	68, 78, 87, 92	0
39	1h	137/138 (99%)	0.50	3 (2%) 62 56	52, 65, 72, 76	0
39	2h	137/138 (99%)	0.85	5 (3%) 46 38	65, 74, 80, 83	0
40	1i	127/128 (99%)	1.20	21 (16%) 4 3	50, 74, 83, 87	0
40	2i	127/128 (99%)	1.78	45 (35%) 1 0	71, 83, 88, 92	0
41	1j	97/105 (92%)	1.16	13 (13%) 7 6	53, 76, 84, 91	0
41	2j	96/105 (91%)	1.82	37 (38%) 1 0	74, 84, 90, 92	0
42	1k	114/129 (88%)	0.61	5 (4%) 39 31	41, 66, 76, 80	0
42	2k	114/129 (88%)	0.88	9 (7%) 18 14	52, 72, 79, 82	0
43	1l	121/132 (91%)	0.26	3 (2%) 58 52	41, 50, 63, 71	0
43	2l	121/132 (91%)	0.63	3 (2%) 58 52	50, 66, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.83	10 (8%) 18 13	53, 67, 76, 88	0
44	2m	122/126 (96%)	1.52	24 (19%) 3 2	67, 80, 85, 88	0
45	1n	60/61 (98%)	0.96	5 (8%) 17 12	54, 64, 71, 76	0
45	2n	60/61 (98%)	2.21	28 (46%) 0 0	73, 82, 87, 90	0
46	1o	88/89 (98%)	0.60	4 (4%) 38 31	47, 63, 72, 79	0
46	2o	88/89 (98%)	0.69	5 (5%) 29 23	59, 70, 80, 85	0
47	1p	82/88 (93%)	1.27	10 (12%) 8 7	58, 69, 77, 86	0
47	2p	82/88 (93%)	0.98	7 (8%) 16 12	59, 69, 77, 81	0
48	1q	99/105 (94%)	0.64	1 (1%) 79 76	48, 66, 75, 76	0
48	2q	99/105 (94%)	0.68	5 (5%) 33 26	62, 72, 80, 81	0
49	1r	68/88 (77%)	0.47	1 (1%) 72 67	53, 64, 76, 77	0
49	2r	68/88 (77%)	0.66	2 (2%) 53 46	59, 69, 78, 83	0
50	1s	83/93 (89%)	0.78	4 (4%) 35 28	59, 69, 79, 84	0
50	2s	83/93 (89%)	1.56	18 (21%) 2 1	78, 83, 89, 95	0
51	1t	96/106 (90%)	0.97	9 (9%) 14 11	61, 68, 78, 82	0
51	2t	96/106 (90%)	0.84	8 (8%) 17 12	60, 70, 81, 87	0
52	1u	23/27 (85%)	0.88	2 (8%) 16 12	59, 64, 70, 74	0
52	2u	23/27 (85%)	1.74	9 (39%) 1 0	74, 78, 83, 89	0
53	1v	13/24 (54%)	0.92	4 (30%) 1 0	47, 51, 92, 98	0
53	2v	13/24 (54%)	1.30	4 (30%) 1 0	63, 73, 96, 102	0
54	1w	66/76 (86%)	1.32	19 (28%) 1 1	29, 86, 98, 103	0
54	2w	64/76 (84%)	1.53	16 (25%) 2 1	48, 91, 100, 102	0
55	1x	72/77 (93%)	0.12	2 (2%) 55 48	25, 58, 78, 91	0
55	2x	72/77 (93%)	0.53	1 (1%) 73 69	42, 73, 87, 97	0
56	1y	67/76 (88%)	2.02	29 (43%) 0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	2.00	28 (42%) 0 0	69, 101, 103, 105	0
All	All	20871/21748 (95%)	0.37	1343 (6%) 25 19	19, 63, 89, 108	0

The worst 5 of 1343 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	10.0
1	2A	652(U)	G	8.7

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Mol	Chain	Res	Type	RSRZ
1	2A	653	A	8.2
1	2A	652(V)	C	8.1
1	1A	653	A	7.7

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	0.43	0.19	95,104,112,126	0
56	G7M	2y	46	24/25	0.46	0.16	86,99,105,120	0
56	MIA	2y	37	22/30	0.52	0.16	83,97,109,123	0
56	PSU	1y	55	20/21	0.52	0.17	96,101,106,114	0
56	5MU	2y	54	21/22	0.54	0.18	91,96,106,126	0
56	G7M	1y	46	24/25	0.55	0.18	91,99,104,117	0
56	5MU	1y	54	21/22	0.59	0.15	89,99,104,118	0
56	PSU	2y	55	20/21	0.59	0.15	89,97,106,108	0
56	PSU	2y	39	20/21	0.61	0.16	90,95,104,111	0
56	MIA	1y	37	22/30	0.61	0.16	86,93,100,113	0
56	4SU	1y	8	20/21	0.63	0.14	93,97,105,116	0
56	PSU	2y	32	20/21	0.64	0.16	86,98,107,115	0
54	G7M	2w	46	24/25	0.66	0.17	84,94,109,123	0
56	PSU	1y	39	20/21	0.70	0.16	83,94,107,109	0
56	PSU	1y	32	20/21	0.70	0.14	88,96,106,112	0
54	G7M	1w	46	24/25	0.71	0.18	78,88,100,121	0
54	PSU	2w	55	20/21	0.82	0.12	77,83,94,96	0
54	4SU	2w	8	20/21	0.85	0.13	90,94,105,108	0
54	4SU	1w	8	20/21	0.85	0.14	71,85,92,94	0
54	5MU	2w	54	21/22	0.87	0.12	74,80,84,89	0
55	PSU	2x	55	20/21	0.88	0.10	69,75,84,86	0
55	5MU	2x	54	21/22	0.89	0.12	72,79,84,96	0
54	PSU	1w	55	20/21	0.89	0.10	61,73,81,81	0
32	2MG	2a	1207	24/25	0.89	0.12	76,83,86,90	0
54	PSU	2w	32	20/21	0.90	0.13	76,84,91,92	0
54	MIA	2w	37	25/30	0.90	0.12	68,76,85,103	0
55	4SU	2x	8	20/21	0.90	0.11	64,75,83,83	0
32	G7M	2a	527	24/25	0.90	0.13	61,67,71,76	0
32	M2G	2a	966	25/26	0.91	0.15	55,65,76,81	0
43	0TD	1l	92	10/11	0.91	0.11	41,49,50,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	967	21/22	0.92	0.12	62,66,76,82	0
54	PSU	1w	32	20/21	0.92	0.12	60,65,74,77	0
1	5MU	2A	1915	21/22	0.92	0.10	57,64,73,75	0
32	5MC	2a	1400	21/22	0.93	0.17	63,71,76,80	0
32	4OC	2a	1402	22/23	0.93	0.11	55,60,66,71	0
54	MIA	1w	37	29/30	0.93	0.14	43,53,70,87	0
55	5MC	2x	32	21/22	0.93	0.12	63,69,78,80	0
55	PSU	1x	55	20/21	0.93	0.10	49,56,67,70	0
32	2MG	1a	1207	24/25	0.93	0.11	61,67,71,71	0
32	PSU	2a	516	20/21	0.93	0.11	61,71,78,79	0
54	PSU	2w	39	20/21	0.94	0.10	62,78,85,85	0
55	4SU	1x	8	20/21	0.94	0.10	52,60,67,77	0
32	5MC	2a	1407	21/22	0.94	0.10	50,57,61,65	0
43	0TD	2l	92	10/11	0.94	0.09	61,65,67,78	0
1	PSU	2A	1917	20/21	0.94	0.09	54,61,69,72	0
1	OMC	2A	1920	21/22	0.94	0.09	53,61,63,65	0
55	5MU	1x	54	21/22	0.95	0.08	55,61,65,70	0
1	PSU	2A	1911	20/21	0.95	0.09	52,62,67,71	0
32	UR3	2a	1498	21/22	0.95	0.11	52,58,61,65	0
55	5MC	1x	32	21/22	0.95	0.11	51,53,59,70	0
32	5MC	2a	1404	21/22	0.95	0.09	53,57,62,66	0
1	5MC	2A	1962	21/22	0.95	0.10	39,51,58,67	0
55	31H	2x	76	32/33	0.96	0.10	36,46,54,63	0
32	PSU	1a	516	20/21	0.96	0.08	51,55,58,59	0
32	5MC	1a	1400	21/22	0.96	0.09	39,47,49,50	0
54	5MU	1w	54	21/22	0.96	0.07	46,62,67,69	0
32	5MC	1a	1404	21/22	0.96	0.08	33,39,42,45	0
32	5MC	1a	1407	21/22	0.96	0.10	30,39,42,43	0
32	G7M	1a	527	24/25	0.96	0.09	36,42,50,50	0
32	M2G	1a	966	25/26	0.96	0.10	46,50,57,61	0
54	F3N	2w	76	33/34	0.96	0.10	38,43,48,51	0
1	5MU	1A	1915	21/22	0.96	0.09	42,51,55,55	0
32	5MC	1a	967	21/22	0.96	0.09	45,51,59,61	0
32	MA6	2a	1518	24/25	0.96	0.10	49,60,69,69	0
32	MA6	2a	1519	24/25	0.96	0.11	55,61,67,71	0
1	5MC	1A	1942	21/22	0.96	0.08	34,39,43,51	0
55	31H	1x	76	32/33	0.96	0.09	22,26,37,41	10
54	F3N	1w	76	33/34	0.97	0.07	22,25,30,32	0
1	PSU	1A	1917	20/21	0.97	0.07	39,45,50,52	0
32	4OC	1a	1402	22/23	0.97	0.08	38,45,48,49	0
1	OMC	1A	1920	21/22	0.97	0.08	35,43,45,52	0
1	PSU	1A	1911	20/21	0.97	0.07	42,46,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1939	21/22	0.97	0.08	32,38,42,45	0
32	MA6	1a	1519	24/25	0.97	0.09	35,42,45,47	0
1	5MC	2A	1942	21/22	0.97	0.08	43,53,57,62	0
1	5MC	1A	1962	21/22	0.97	0.06	24,32,37,42	0
54	PSU	1w	39	20/21	0.97	0.08	53,61,67,76	0
1	OMG	2A	2251	24/25	0.97	0.08	35,43,45,51	0
1	8AH	2A	2503	24/25	0.97	0.09	32,38,44,45	0
1	2MU	2A	2552	21/23	0.97	0.08	35,41,45,55	0
1	PSU	2A	2605	20/21	0.97	0.07	30,38,42,44	0
1	5MU	1A	1939	21/22	0.98	0.06	21,28,30,32	0
1	8AH	1A	2503	24/25	0.98	0.06	15,21,26,27	0
32	MA6	1a	1518	24/25	0.98	0.08	31,39,45,46	0
1	2MU	1A	2552	21/23	0.98	0.07	23,27,34,36	0
32	UR3	1a	1498	21/22	0.98	0.07	36,41,45,46	0
1	PSU	1A	2605	20/21	0.98	0.07	23,26,31,32	0
1	OMG	1A	2251	24/25	0.98	0.06	22,25,28,30	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	2a	1808	1/1	0.33	0.20	91,91,91,91	0
57	MG	1a	1792	1/1	0.42	0.40	74,74,74,74	0
57	MG	2v	102	1/1	0.53	0.42	80,80,80,80	0
57	MG	1A	4078	1/1	0.57	0.25	62,62,62,62	0
57	MG	2A	3557	1/1	0.64	0.20	83,83,83,83	0
57	MG	1A	4042	1/1	0.65	0.26	70,70,70,70	0
57	MG	2A	3762	1/1	0.66	0.14	53,53,53,53	0
57	MG	1A	3909	1/1	0.67	0.24	85,85,85,85	0
57	MG	2A	3547	1/1	0.67	0.20	72,72,72,72	0
57	MG	2l	201	1/1	0.67	0.20	78,78,78,78	0
57	MG	1A	3979	1/1	0.67	0.14	70,70,70,70	0
57	MG	1B	213	1/1	0.68	0.26	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	228	1/1	0.68	0.27	77,77,77,77	0
57	MG	1A	3178	1/1	0.68	0.18	74,74,74,74	0
57	MG	1a	1673	1/1	0.69	0.26	77,77,77,77	0
57	MG	1w	104	1/1	0.69	0.28	81,81,81,81	0
57	MG	2A	3482	1/1	0.69	0.19	69,69,69,69	0
57	MG	1a	1743	1/1	0.70	0.36	81,81,81,81	0
57	MG	2A	3603	1/1	0.70	0.18	76,76,76,76	0
57	MG	2A	3690	1/1	0.70	0.19	58,58,58,58	0
57	MG	2A	3074	1/1	0.70	0.19	63,63,63,63	0
57	MG	2a	1781	1/1	0.70	0.23	81,81,81,81	0
57	MG	2A	3215	1/1	0.70	0.32	77,77,77,77	0
57	MG	1A	3841	1/1	0.70	0.18	24,24,24,24	0
57	MG	1a	1796	1/1	0.70	0.31	67,67,67,67	0
57	MG	2a	1643	1/1	0.71	0.25	73,73,73,73	0
57	MG	2a	1700	1/1	0.71	0.33	82,82,82,82	0
57	MG	2a	1770	1/1	0.71	0.21	70,70,70,70	0
57	MG	1a	1801	1/1	0.71	0.19	56,56,56,56	0
57	MG	2A	3645	1/1	0.71	0.23	48,48,48,48	0
57	MG	2a	1628	1/1	0.71	0.32	79,79,79,79	0
57	MG	2a	1632	1/1	0.71	0.37	74,74,74,74	0
57	MG	2A	3483	1/1	0.72	0.35	84,84,84,84	0
57	MG	2A	3573	1/1	0.72	0.30	68,68,68,68	0
57	MG	1A	4064	1/1	0.72	0.18	64,64,64,64	0
57	MG	1V	205	1/1	0.73	0.15	63,63,63,63	0
57	MG	2A	3516	1/1	0.73	0.14	40,40,40,40	0
57	MG	2A	3019	1/1	0.73	0.34	79,79,79,79	0
57	MG	1A	4023	1/1	0.73	0.18	50,50,50,50	0
57	MG	1A	3375	1/1	0.73	0.33	74,74,74,74	0
57	MG	1a	1812	1/1	0.73	0.19	67,67,67,67	0
57	MG	2Q	204	1/1	0.74	0.17	77,77,77,77	0
57	MG	1A	3766	1/1	0.74	0.30	51,51,51,51	0
57	MG	2A	3590	1/1	0.74	0.23	50,50,50,50	0
57	MG	1A	3394	1/1	0.74	0.34	69,69,69,69	0
57	MG	2A	3604	1/1	0.74	0.22	76,76,76,76	0
57	MG	1A	3747	1/1	0.74	0.25	82,82,82,82	0
57	MG	2A	3293	1/1	0.74	0.26	67,67,67,67	0
57	MG	2A	3436	1/1	0.74	0.20	66,66,66,66	0
57	MG	2A	3784	1/1	0.74	0.21	70,70,70,70	0
57	MG	2v	101	1/1	0.74	0.24	78,78,78,78	0
57	MG	2B	211	1/1	0.74	0.34	76,76,76,76	0
57	MG	2y	101	1/1	0.74	0.20	81,81,81,81	0
57	MG	2A	3580	1/1	0.75	0.17	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	2a	1756	1/1	0.75	0.29	59,59,59,59	0
57	MG	1B	227	1/1	0.75	0.12	81,81,81,81	0
57	MG	2A	3057	1/1	0.75	0.15	65,65,65,65	0
57	MG	2a	1790	1/1	0.75	0.26	75,75,75,75	0
57	MG	11	104	1/1	0.75	0.24	78,78,78,78	0
57	MG	20	102	1/1	0.75	0.31	73,73,73,73	0
57	MG	2A	3606	1/1	0.75	0.19	66,66,66,66	0
57	MG	2A	3564	1/1	0.75	0.15	75,75,75,75	0
57	MG	1A	3898	1/1	0.75	0.16	35,35,35,35	0
57	MG	1a	1738	1/1	0.76	0.36	76,76,76,76	0
57	MG	2A	3775	1/1	0.76	0.48	73,73,73,73	0
57	MG	2A	3779	1/1	0.76	0.29	82,82,82,82	0
57	MG	1v	101	1/1	0.76	0.35	82,82,82,82	0
57	MG	2a	1698	1/1	0.76	0.35	74,74,74,74	0
57	MG	2A	3662	1/1	0.76	0.29	60,60,60,60	0
57	MG	2a	1730	1/1	0.76	0.18	87,87,87,87	0
57	MG	2A	3419	1/1	0.76	0.32	61,61,61,61	0
57	MG	2y	102	1/1	0.76	0.33	75,75,75,75	0
57	MG	2A	3584	1/1	0.77	0.18	69,69,69,69	0
57	MG	2W	201	1/1	0.77	0.13	67,67,67,67	0
57	MG	1A	3863	1/1	0.77	0.13	44,44,44,44	0
57	MG	2A	3415	1/1	0.77	0.27	71,71,71,71	0
57	MG	2a	1629	1/1	0.77	0.44	73,73,73,73	0
57	MG	1A	3732	1/1	0.77	0.13	70,70,70,70	0
57	MG	1a	1662	1/1	0.77	0.32	71,71,71,71	0
57	MG	2a	1665	1/1	0.77	0.28	64,64,64,64	0
57	MG	2a	1670	1/1	0.77	0.33	74,74,74,74	0
57	MG	1A	3785	1/1	0.77	0.20	55,55,55,55	0
57	MG	2A	3658	1/1	0.77	0.22	67,67,67,67	0
57	MG	1A	3804	1/1	0.77	0.17	69,69,69,69	0
57	MG	2A	3675	1/1	0.77	0.29	69,69,69,69	0
57	MG	2a	1759	1/1	0.77	0.25	81,81,81,81	0
57	MG	1B	217	1/1	0.77	0.17	52,52,52,52	0
57	MG	2a	1777	1/1	0.77	0.17	75,75,75,75	0
57	MG	2A	3711	1/1	0.77	0.14	47,47,47,47	0
57	MG	1A	3491	1/1	0.77	0.23	64,64,64,64	0
57	MG	2A	3213	1/1	0.77	0.33	72,72,72,72	0
57	MG	1A	4039	1/1	0.77	0.14	48,48,48,48	0
57	MG	2A	3274	1/1	0.77	0.15	74,74,74,74	0
57	MG	2A	3289	1/1	0.77	0.17	62,62,62,62	0
57	MG	2B	214	1/1	0.77	0.29	66,66,66,66	0
57	MG	2N	201	1/1	0.77	0.25	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3176	1/1	0.78	0.14	63,63,63,63	0
57	MG	1a	1719	1/1	0.78	0.20	82,82,82,82	0
57	MG	2A	3749	1/1	0.78	0.14	58,58,58,58	0
57	MG	2a	1686	1/1	0.78	0.30	72,72,72,72	0
57	MG	1O	204	1/1	0.78	0.18	71,71,71,71	0
57	MG	2A	3227	1/1	0.78	0.28	71,71,71,71	0
57	MG	2A	3248	1/1	0.78	0.13	57,57,57,57	0
57	MG	2a	1732	1/1	0.78	0.35	83,83,83,83	0
57	MG	1A	3970	1/1	0.78	0.17	47,47,47,47	0
57	MG	1A	3600	1/1	0.78	0.18	66,66,66,66	0
57	MG	2A	3023	1/1	0.78	0.22	71,71,71,71	0
57	MG	1A	3810	1/1	0.78	0.20	69,69,69,69	0
57	MG	1A	4029	1/1	0.78	0.16	27,27,27,27	0
57	MG	2a	1783	1/1	0.78	0.34	66,66,66,66	0
57	MG	2V	202	1/1	0.78	0.24	67,67,67,67	0
57	MG	2A	3080	1/1	0.78	0.21	66,66,66,66	0
57	MG	2A	3450	1/1	0.78	0.18	49,49,49,49	0
57	MG	2q	202	1/1	0.78	0.18	82,82,82,82	0
57	MG	2A	3460	1/1	0.78	0.19	51,51,51,51	0
57	MG	2A	3102	1/1	0.78	0.24	66,66,66,66	0
57	MG	2A	3112	1/1	0.78	0.27	75,75,75,75	0
57	MG	2a	1633	1/1	0.78	0.36	73,73,73,73	0
57	MG	1a	1684	1/1	0.79	0.15	68,68,68,68	0
57	MG	1A	3690	1/1	0.79	0.19	62,62,62,62	0
57	MG	2A	3225	1/1	0.79	0.34	75,75,75,75	0
57	MG	2a	1696	1/1	0.79	0.39	74,74,74,74	0
57	MG	2a	1697	1/1	0.79	0.27	81,81,81,81	0
57	MG	1A	4040	1/1	0.79	0.19	67,67,67,67	0
57	MG	2A	3233	1/1	0.79	0.14	69,69,69,69	0
57	MG	2a	1711	1/1	0.79	0.26	83,83,83,83	0
57	MG	2A	3236	1/1	0.79	0.19	63,63,63,63	0
57	MG	2A	3055	1/1	0.79	0.18	57,57,57,57	0
57	MG	2A	3252	1/1	0.79	0.50	62,62,62,62	0
57	MG	2D	306	1/1	0.79	0.39	54,54,54,54	0
57	MG	2F	302	1/1	0.79	0.30	74,74,74,74	0
57	MG	1A	3446	1/1	0.79	0.16	65,65,65,65	0
57	MG	1A	3528	1/1	0.79	0.17	57,57,57,57	0
57	MG	1A	3989	1/1	0.79	0.14	58,58,58,58	0
57	MG	2A	3399	1/1	0.79	0.24	83,83,83,83	0
57	MG	1a	1657	1/1	0.79	0.16	65,65,65,65	0
57	MG	1A	3467	1/1	0.79	0.21	60,60,60,60	0
57	MG	2A	3156	1/1	0.79	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3643	1/1	0.79	0.23	72,72,72,72	0
57	MG	2A	3177	1/1	0.79	0.51	80,80,80,80	0
57	MG	2a	1642	1/1	0.79	0.33	73,73,73,73	0
57	MG	2A	3474	1/1	0.79	0.30	78,78,78,78	0
57	MG	2A	3001	1/1	0.80	0.26	59,59,59,59	0
57	MG	14	101	1/1	0.80	0.20	80,80,80,80	0
57	MG	1A	3488	1/1	0.80	0.36	60,60,60,60	0
57	MG	2A	3044	1/1	0.80	0.22	58,58,58,58	0
57	MG	1A	3704	1/1	0.80	0.20	61,61,61,61	0
57	MG	2A	3294	1/1	0.80	0.26	69,69,69,69	0
57	MG	2A	3639	1/1	0.80	0.15	72,72,72,72	0
57	MG	2a	1666	1/1	0.80	0.35	68,68,68,68	0
57	MG	2A	3320	1/1	0.80	0.10	69,69,69,69	0
57	MG	2A	3354	1/1	0.80	0.29	65,65,65,65	0
57	MG	1A	3854	1/1	0.80	0.16	58,58,58,58	0
57	MG	1A	3727	1/1	0.80	0.12	26,26,26,26	0
57	MG	1A	3039	1/1	0.80	0.29	63,63,63,63	0
57	MG	2A	3427	1/1	0.80	0.23	74,74,74,74	0
57	MG	2a	1710	1/1	0.80	0.29	79,79,79,79	0
57	MG	1a	1728	1/1	0.80	0.25	67,67,67,67	0
57	MG	2A	3760	1/1	0.80	0.17	73,73,73,73	0
57	MG	2A	3448	1/1	0.80	0.14	47,47,47,47	0
57	MG	1A	3314	1/1	0.80	0.18	54,54,54,54	0
57	MG	1A	3954	1/1	0.80	0.16	31,31,31,31	0
57	MG	2a	1768	1/1	0.80	0.14	69,69,69,69	0
57	MG	1A	3356	1/1	0.80	0.33	34,34,34,34	0
57	MG	1A	3607	1/1	0.80	0.18	68,68,68,68	0
57	MG	1O	201	1/1	0.80	0.13	72,72,72,72	0
57	MG	1a	1802	1/1	0.80	0.15	84,84,84,84	0
57	MG	2E	301	1/1	0.80	0.19	68,68,68,68	0
57	MG	2a	1793	1/1	0.80	0.23	64,64,64,64	0
57	MG	1a	1809	1/1	0.80	0.27	69,69,69,69	0
57	MG	2A	3548	1/1	0.80	0.20	65,65,65,65	0
57	MG	1A	3795	1/1	0.80	0.19	60,60,60,60	0
57	MG	2A	3560	1/1	0.80	0.16	74,74,74,74	0
57	MG	1A	3796	1/1	0.80	0.17	49,49,49,49	0
57	MG	1A	3374	1/1	0.80	0.22	61,61,61,61	0
57	MG	2a	1610	1/1	0.80	0.48	78,78,78,78	0
57	MG	2B	206	1/1	0.81	0.33	73,73,73,73	0
57	MG	2A	3582	1/1	0.81	0.15	70,70,70,70	0
57	MG	1A	3907	1/1	0.81	0.11	70,70,70,70	0
57	MG	2A	3223	1/1	0.81	0.19	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	1708	1/1	0.81	0.15	62,62,62,62	0
57	MG	1A	3514	1/1	0.81	0.26	48,48,48,48	0
57	MG	1A	3915	1/1	0.81	0.15	62,62,62,62	0
57	MG	2a	1714	1/1	0.81	0.23	74,74,74,74	0
57	MG	2a	1723	1/1	0.81	0.33	80,80,80,80	0
57	MG	2G	201	1/1	0.81	0.14	77,77,77,77	0
57	MG	1A	3620	1/1	0.81	0.14	65,65,65,65	0
57	MG	1l	103	1/1	0.81	0.10	42,42,42,42	0
57	MG	1A	4060	1/1	0.81	0.15	53,53,53,53	0
57	MG	1A	3962	1/1	0.81	0.15	58,58,58,58	0
57	MG	1A	3526	1/1	0.81	0.39	56,56,56,56	0
57	MG	2A	3281	1/1	0.81	0.26	67,67,67,67	0
57	MG	2a	1626	1/1	0.81	0.40	77,77,77,77	0
57	MG	1A	3395	1/1	0.81	0.23	69,69,69,69	0
57	MG	2a	1788	1/1	0.81	0.42	83,83,83,83	0
57	MG	1a	1670	1/1	0.81	0.32	75,75,75,75	0
57	MG	1A	3533	1/1	0.81	0.12	38,38,38,38	0
57	MG	2a	1798	1/1	0.81	0.26	73,73,73,73	0
57	MG	2A	3754	1/1	0.81	0.24	77,77,77,77	0
57	MG	2A	3559	1/1	0.81	0.17	67,67,67,67	0
57	MG	2A	3171	1/1	0.81	0.32	70,70,70,70	0
57	MG	1A	3432	1/1	0.81	0.16	64,64,64,64	0
57	MG	2A	3776	1/1	0.81	0.25	67,67,67,67	0
57	MG	1x	107	1/1	0.81	0.23	72,72,72,72	0
57	MG	1x	111	1/1	0.81	0.23	70,70,70,70	0
57	MG	2A	3441	1/1	0.82	0.23	59,59,59,59	0
57	MG	2a	1638	1/1	0.82	0.22	82,82,82,82	0
57	MG	2A	3680	1/1	0.82	0.11	63,63,63,63	0
57	MG	1A	3680	1/1	0.82	0.21	56,56,56,56	0
57	MG	2A	3695	1/1	0.82	0.13	70,70,70,70	0
57	MG	1A	3222	1/1	0.82	0.16	63,63,63,63	0
57	MG	1A	3802	1/1	0.82	0.17	50,50,50,50	0
57	MG	2a	1671	1/1	0.82	0.24	65,65,65,65	0
57	MG	1a	1704	1/1	0.82	0.36	72,72,72,72	0
57	MG	2A	3235	1/1	0.82	0.27	68,68,68,68	0
57	MG	2A	3035	1/1	0.82	0.34	69,69,69,69	0
57	MG	2A	3774	1/1	0.82	0.18	68,68,68,68	0
57	MG	1A	3558	1/1	0.82	0.15	55,55,55,55	0
57	MG	1A	3500	1/1	0.82	0.18	59,59,59,59	0
57	MG	2A	3255	1/1	0.82	0.14	65,65,65,65	0
57	MG	1A	3239	1/1	0.82	0.12	64,64,64,64	0
57	MG	2B	202	1/1	0.82	0.11	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	2A	3277	1/1	0.82	0.12	72,72,72,72	0
57	MG	2B	210	1/1	0.82	0.16	78,78,78,78	0
57	MG	1A	3844	1/1	0.82	0.15	30,30,30,30	0
57	MG	1A	3485	1/1	0.82	0.18	65,65,65,65	0
57	MG	10	108	1/1	0.82	0.23	70,70,70,70	0
57	MG	1A	3855	1/1	0.82	0.15	34,34,34,34	0
57	MG	2A	3305	1/1	0.82	0.26	58,58,58,58	0
57	MG	2F	308	1/1	0.82	0.16	69,69,69,69	0
57	MG	2A	3309	1/1	0.82	0.19	66,66,66,66	0
57	MG	1A	3057	1/1	0.82	0.15	63,63,63,63	0
57	MG	2A	3353	1/1	0.82	0.17	81,81,81,81	0
57	MG	2A	3158	1/1	0.82	0.14	70,70,70,70	0
57	MG	2a	1792	1/1	0.82	0.28	76,76,76,76	0
57	MG	1A	3783	1/1	0.82	0.14	49,49,49,49	0
57	MG	2A	3615	1/1	0.82	0.37	68,68,68,68	0
57	MG	2I	101	1/1	0.82	0.17	54,54,54,54	0
57	MG	2a	1811	1/1	0.82	0.17	70,70,70,70	0
57	MG	2A	3633	1/1	0.82	0.12	64,64,64,64	0
57	MG	1a	1622	1/1	0.82	0.27	65,65,65,65	0
57	MG	1a	1639	1/1	0.82	0.35	67,67,67,67	0
57	MG	1A	3670	1/1	0.82	0.24	62,62,62,62	0
57	MG	2a	1631	1/1	0.82	0.25	66,66,66,66	0
57	MG	1A	3794	1/1	0.82	0.16	59,59,59,59	0
57	MG	2a	1608	1/1	0.83	0.22	67,67,67,67	0
57	MG	2A	3613	1/1	0.83	0.28	56,56,56,56	0
57	MG	1A	3765	1/1	0.83	0.19	54,54,54,54	0
57	MG	2A	3617	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3631	1/1	0.83	0.22	86,86,86,86	0
57	MG	2A	3181	1/1	0.83	0.28	65,65,65,65	0
57	MG	2A	3634	1/1	0.83	0.15	45,45,45,45	0
57	MG	2A	3636	1/1	0.83	0.17	67,67,67,67	0
57	MG	2A	3367	1/1	0.83	0.28	74,74,74,74	0
57	MG	2A	3199	1/1	0.83	0.18	55,55,55,55	0
57	MG	2A	3405	1/1	0.83	0.26	61,61,61,61	0
57	MG	1B	220	1/1	0.83	0.18	57,57,57,57	0
57	MG	1a	1661	1/1	0.83	0.27	65,65,65,65	0
57	MG	2A	3678	1/1	0.83	0.17	68,68,68,68	0
57	MG	1B	221	1/1	0.83	0.24	56,56,56,56	0
57	MG	1A	3536	1/1	0.83	0.21	63,63,63,63	0
57	MG	1A	4028	1/1	0.83	0.11	62,62,62,62	0
57	MG	2A	3230	1/1	0.83	0.12	81,81,81,81	0
57	MG	1A	3372	1/1	0.83	0.33	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3822	1/1	0.83	0.18	61,61,61,61	0
57	MG	1R	206	1/1	0.83	0.14	71,71,71,71	0
57	MG	1A	3583	1/1	0.83	0.18	58,58,58,58	0
57	MG	10	102	1/1	0.83	0.23	66,66,66,66	0
57	MG	2A	3509	1/1	0.83	0.17	68,68,68,68	0
57	MG	1A	3949	1/1	0.83	0.12	57,57,57,57	0
57	MG	2A	3777	1/1	0.83	0.20	70,70,70,70	0
57	MG	2A	3523	1/1	0.83	0.15	59,59,59,59	0
57	MG	2A	3256	1/1	0.83	0.16	73,73,73,73	0
57	MG	10	109	1/1	0.83	0.21	69,69,69,69	0
57	MG	2a	1763	1/1	0.83	0.27	67,67,67,67	0
57	MG	2A	3275	1/1	0.83	0.45	78,78,78,78	0
57	MG	2A	3083	1/1	0.83	0.21	75,75,75,75	0
57	MG	1A	3445	1/1	0.83	0.17	58,58,58,58	0
57	MG	2B	213	1/1	0.83	0.11	65,65,65,65	0
57	MG	2A	3562	1/1	0.83	0.19	68,68,68,68	0
57	MG	1a	1800	1/1	0.83	0.30	76,76,76,76	0
57	MG	1A	3674	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3574	1/1	0.83	0.15	71,71,71,71	0
57	MG	1A	3677	1/1	0.83	0.13	42,42,42,42	0
57	MG	2A	3159	1/1	0.83	0.26	82,82,82,82	0
57	MG	1A	3858	1/1	0.83	0.12	56,56,56,56	0
57	MG	2a	1810	1/1	0.83	0.09	77,77,77,77	0
57	MG	1a	1637	1/1	0.83	0.34	57,57,57,57	0
57	MG	2a	1816	1/1	0.83	0.19	81,81,81,81	0
57	MG	2A	3325	1/1	0.83	0.19	67,67,67,67	0
57	MG	2A	3333	1/1	0.83	0.22	61,61,61,61	0
57	MG	2A	3350	1/1	0.83	0.22	59,59,59,59	0
57	MG	2A	3612	1/1	0.83	0.27	68,68,68,68	0
57	MG	28	102	1/1	0.83	0.34	69,69,69,69	0
57	MG	2a	1602	1/1	0.83	0.21	81,81,81,81	0
57	MG	1A	3936	1/1	0.84	0.10	68,68,68,68	0
57	MG	2A	3278	1/1	0.84	0.22	59,59,59,59	0
57	MG	1A	3701	1/1	0.84	0.09	19,19,19,19	0
57	MG	2A	3283	1/1	0.84	0.34	83,83,83,83	0
57	MG	1A	3636	1/1	0.84	0.16	56,56,56,56	0
57	MG	1A	3722	1/1	0.84	0.14	30,30,30,30	0
57	MG	2A	3586	1/1	0.84	0.15	67,67,67,67	0
57	MG	1F	304	1/1	0.84	0.26	69,69,69,69	0
57	MG	2A	3298	1/1	0.84	0.38	76,76,76,76	0
57	MG	1A	3641	1/1	0.84	0.12	43,43,43,43	0
57	MG	1A	3821	1/1	0.84	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	3119	1/1	0.84	0.18	69,69,69,69	0
57	MG	2a	1619	1/1	0.84	0.13	71,71,71,71	0
57	MG	1A	3556	1/1	0.84	0.31	72,72,72,72	0
57	MG	1a	1755	1/1	0.84	0.14	64,64,64,64	0
57	MG	1a	1779	1/1	0.84	0.13	75,75,75,75	0
57	MG	2A	3628	1/1	0.84	0.19	76,76,76,76	0
57	MG	2A	3165	1/1	0.84	0.13	67,67,67,67	0
57	MG	1A	3477	1/1	0.84	0.14	74,74,74,74	0
57	MG	2A	3359	1/1	0.84	0.41	73,73,73,73	0
57	MG	2A	3360	1/1	0.84	0.33	67,67,67,67	0
57	MG	2A	3363	1/1	0.84	0.26	65,65,65,65	0
57	MG	2a	1652	1/1	0.84	0.24	73,73,73,73	0
57	MG	1a	1795	1/1	0.84	0.14	68,68,68,68	0
57	MG	2A	3655	1/1	0.84	0.23	70,70,70,70	0
57	MG	1A	3757	1/1	0.84	0.13	61,61,61,61	0
57	MG	2A	3400	1/1	0.84	0.14	73,73,73,73	0
57	MG	2a	1673	1/1	0.84	0.15	64,64,64,64	0
57	MG	1A	3307	1/1	0.84	0.35	60,60,60,60	0
57	MG	2a	1688	1/1	0.84	0.22	71,71,71,71	0
57	MG	2A	3185	1/1	0.84	0.14	63,63,63,63	0
57	MG	1A	3139	1/1	0.84	0.13	47,47,47,47	0
57	MG	2A	3425	1/1	0.84	0.25	73,73,73,73	0
57	MG	2A	3692	1/1	0.84	0.13	71,71,71,71	0
57	MG	2a	1707	1/1	0.84	0.19	76,76,76,76	0
57	MG	1A	3773	1/1	0.84	0.15	58,58,58,58	0
57	MG	1a	1806	1/1	0.84	0.13	60,60,60,60	0
57	MG	2A	3733	1/1	0.84	0.13	68,68,68,68	0
57	MG	2A	3738	1/1	0.84	0.15	58,58,58,58	0
57	MG	2a	1722	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3216	1/1	0.84	0.22	73,73,73,73	0
57	MG	1A	3237	1/1	0.84	0.14	56,56,56,56	0
57	MG	1A	4044	1/1	0.84	0.16	59,59,59,59	0
57	MG	1a	1814	1/1	0.84	0.28	65,65,65,65	0
57	MG	2A	3767	1/1	0.84	0.32	66,66,66,66	0
57	MG	1t	201	1/1	0.84	0.22	57,57,57,57	0
57	MG	2A	3478	1/1	0.84	0.15	50,50,50,50	0
57	MG	18	107	1/1	0.84	0.25	70,70,70,70	0
57	MG	2a	1776	1/1	0.84	0.33	75,75,75,75	0
57	MG	1A	3683	1/1	0.84	0.13	62,62,62,62	0
57	MG	2A	3485	1/1	0.84	0.11	67,67,67,67	0
57	MG	1A	3793	1/1	0.84	0.14	57,57,57,57	0
57	MG	2A	3795	1/1	0.84	0.15	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3796	1/1	0.84	0.35	77,77,77,77	0
57	MG	2A	3797	1/1	0.84	0.15	69,69,69,69	0
57	MG	2A	3244	1/1	0.84	0.09	63,63,63,63	0
57	MG	2A	3246	1/1	0.84	0.09	68,68,68,68	0
57	MG	2B	209	1/1	0.84	0.32	69,69,69,69	0
57	MG	1A	3185	1/1	0.84	0.15	57,57,57,57	0
57	MG	1A	4085	1/1	0.84	0.14	62,62,62,62	0
57	MG	1a	1659	1/1	0.84	0.18	61,61,61,61	0
57	MG	1A	3694	1/1	0.84	0.10	57,57,57,57	0
57	MG	2B	216	1/1	0.84	0.14	68,68,68,68	0
57	MG	1A	3930	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3561	1/1	0.84	0.26	67,67,67,67	0
57	MG	2x	105	1/1	0.84	0.18	65,65,65,65	0
57	MG	2x	108	1/1	0.84	0.10	56,56,56,56	0
57	MG	2E	309	1/1	0.84	0.21	67,67,67,67	0
57	MG	1a	1666	1/1	0.84	0.27	72,72,72,72	0
57	MG	2A	3498	1/1	0.85	0.12	79,79,79,79	0
57	MG	2A	3702	1/1	0.85	0.13	69,69,69,69	0
57	MG	1A	3696	1/1	0.85	0.11	66,66,66,66	0
57	MG	1A	3997	1/1	0.85	0.11	53,53,53,53	0
57	MG	1A	4018	1/1	0.85	0.19	72,72,72,72	0
57	MG	2A	3741	1/1	0.85	0.12	48,48,48,48	0
57	MG	2A	3529	1/1	0.85	0.21	62,62,62,62	0
57	MG	2A	3196	1/1	0.85	0.38	74,74,74,74	0
57	MG	2A	3757	1/1	0.85	0.11	64,64,64,64	0
57	MG	2A	3310	1/1	0.85	0.16	64,64,64,64	0
57	MG	2a	1669	1/1	0.85	0.27	72,72,72,72	0
57	MG	2A	3552	1/1	0.85	0.11	39,39,39,39	0
57	MG	1A	3789	1/1	0.85	0.14	60,60,60,60	0
57	MG	1A	3623	1/1	0.85	0.15	30,30,30,30	0
57	MG	1a	1711	1/1	0.85	0.13	55,55,55,55	0
57	MG	2A	3347	1/1	0.85	0.23	70,70,70,70	0
57	MG	2a	1695	1/1	0.85	0.09	67,67,67,67	0
57	MG	1A	3144	1/1	0.85	0.23	32,32,32,32	0
57	MG	1A	3034	1/1	0.85	0.12	46,46,46,46	0
57	MG	1A	3541	1/1	0.85	0.17	65,65,65,65	0
57	MG	2A	3356	1/1	0.85	0.25	53,53,53,53	0
57	MG	2a	1704	1/1	0.85	0.20	69,69,69,69	0
57	MG	2A	3576	1/1	0.85	0.20	42,42,42,42	0
57	MG	1a	1740	1/1	0.85	0.17	43,43,43,43	0
57	MG	2A	3047	1/1	0.85	0.20	69,69,69,69	0
57	MG	1A	3546	1/1	0.85	0.15	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	2B	208	1/1	0.85	0.17	56,56,56,56	0
57	MG	2a	1720	1/1	0.85	0.23	68,68,68,68	0
57	MG	1A	3419	1/1	0.85	0.20	66,66,66,66	0
57	MG	2A	3390	1/1	0.85	0.22	64,64,64,64	0
57	MG	1A	3807	1/1	0.85	0.23	43,43,43,43	0
57	MG	2A	3078	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3428	1/1	0.85	0.16	57,57,57,57	0
57	MG	2A	3407	1/1	0.85	0.17	66,66,66,66	0
57	MG	2a	1762	1/1	0.85	0.15	63,63,63,63	0
57	MG	2D	303	1/1	0.85	0.12	61,61,61,61	0
57	MG	1A	4067	1/1	0.85	0.17	59,59,59,59	0
57	MG	1a	1615	1/1	0.85	0.11	56,56,56,56	0
57	MG	2a	1771	1/1	0.85	0.20	76,76,76,76	0
57	MG	2A	3423	1/1	0.85	0.14	64,64,64,64	0
57	MG	2A	3254	1/1	0.85	0.15	67,67,67,67	0
57	MG	1A	3939	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3258	1/1	0.85	0.20	55,55,55,55	0
57	MG	2A	3260	1/1	0.85	0.26	67,67,67,67	0
57	MG	2P	202	1/1	0.85	0.22	66,66,66,66	0
57	MG	2A	3143	1/1	0.85	0.34	72,72,72,72	0
57	MG	2R	202	1/1	0.85	0.14	50,50,50,50	0
57	MG	2U	201	1/1	0.85	0.19	54,54,54,54	0
57	MG	2A	3151	1/1	0.85	0.13	45,45,45,45	0
57	MG	1A	3262	1/1	0.85	0.14	51,51,51,51	0
57	MG	1A	3837	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3477	1/1	0.85	0.17	50,50,50,50	0
57	MG	2f	202	1/1	0.85	0.23	76,76,76,76	0
57	MG	1A	3287	1/1	0.85	0.09	30,30,30,30	0
57	MG	1A	3299	1/1	0.85	0.24	37,37,37,37	0
57	MG	1A	3981	1/1	0.85	0.11	69,69,69,69	0
57	MG	1b	301	1/1	0.85	0.17	68,68,68,68	0
57	MG	2a	1614	1/1	0.85	0.26	63,63,63,63	0
57	MG	2A	3687	1/1	0.85	0.25	70,70,70,70	0
57	MG	2A	3491	1/1	0.85	0.17	73,73,73,73	0
57	MG	2A	3494	1/1	0.85	0.17	76,76,76,76	0
57	MG	1A	3320	1/1	0.86	0.22	56,56,56,56	0
57	MG	2A	3382	1/1	0.86	0.10	72,72,72,72	0
57	MG	1A	3993	1/1	0.86	0.14	50,50,50,50	0
57	MG	2A	3392	1/1	0.86	0.17	47,47,47,47	0
57	MG	1A	3709	1/1	0.86	0.09	44,44,44,44	0
57	MG	2a	1611	1/1	0.86	0.39	75,75,75,75	0
57	MG	2A	3229	1/1	0.86	0.34	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3538	1/1	0.86	0.28	68,68,68,68	0
57	MG	2a	1620	1/1	0.86	0.25	76,76,76,76	0
57	MG	2A	3644	1/1	0.86	0.31	68,68,68,68	0
57	MG	1a	1717	1/1	0.86	0.18	67,67,67,67	0
57	MG	2A	3046	1/1	0.86	0.21	70,70,70,70	0
57	MG	1A	3881	1/1	0.86	0.10	26,26,26,26	0
57	MG	1A	3887	1/1	0.86	0.10	39,39,39,39	0
57	MG	1A	3479	1/1	0.86	0.26	67,67,67,67	0
57	MG	2A	3247	1/1	0.86	0.28	65,65,65,65	0
57	MG	2a	1640	1/1	0.86	0.13	67,67,67,67	0
57	MG	1A	3800	1/1	0.86	0.12	69,69,69,69	0
57	MG	2A	3077	1/1	0.86	0.15	60,60,60,60	0
57	MG	1a	1742	1/1	0.86	0.15	65,65,65,65	0
57	MG	1A	3328	1/1	0.86	0.10	57,57,57,57	0
57	MG	2A	3457	1/1	0.86	0.12	71,71,71,71	0
57	MG	1A	3335	1/1	0.86	0.16	56,56,56,56	0
57	MG	2A	3085	1/1	0.86	0.16	47,47,47,47	0
57	MG	2A	3723	1/1	0.86	0.18	43,43,43,43	0
57	MG	2A	3730	1/1	0.86	0.12	63,63,63,63	0
57	MG	2a	1677	1/1	0.86	0.20	68,68,68,68	0
57	MG	2A	3262	1/1	0.86	0.19	71,71,71,71	0
57	MG	2A	3263	1/1	0.86	0.14	73,73,73,73	0
57	MG	2A	3270	1/1	0.86	0.12	51,51,51,51	0
57	MG	2A	3271	1/1	0.86	0.18	73,73,73,73	0
57	MG	2A	3753	1/1	0.86	0.15	66,66,66,66	0
57	MG	2A	3095	1/1	0.86	0.21	75,75,75,75	0
57	MG	1A	3928	1/1	0.86	0.14	59,59,59,59	0
57	MG	1A	3755	1/1	0.86	0.12	42,42,42,42	0
57	MG	1A	3423	1/1	0.86	0.28	65,65,65,65	0
57	MG	2A	3279	1/1	0.86	0.18	60,60,60,60	0
57	MG	2A	3768	1/1	0.86	0.17	72,72,72,72	0
57	MG	2A	3123	1/1	0.86	0.14	57,57,57,57	0
57	MG	2A	3518	1/1	0.86	0.10	51,51,51,51	0
57	MG	2a	1718	1/1	0.86	0.11	82,82,82,82	0
57	MG	1a	1610	1/1	0.86	0.24	65,65,65,65	0
57	MG	2a	1721	1/1	0.86	0.23	76,76,76,76	0
57	MG	2A	3149	1/1	0.86	0.38	72,72,72,72	0
57	MG	2A	3542	1/1	0.86	0.19	72,72,72,72	0
57	MG	2a	1724	1/1	0.86	0.14	69,69,69,69	0
57	MG	2A	3783	1/1	0.86	0.29	75,75,75,75	0
57	MG	2A	3543	1/1	0.86	0.14	35,35,35,35	0
57	MG	2a	1751	1/1	0.86	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1754	1/1	0.86	0.13	49,49,49,49	0
57	MG	2A	3291	1/1	0.86	0.13	67,67,67,67	0
57	MG	1a	1798	1/1	0.86	0.17	70,70,70,70	0
57	MG	2a	1761	1/1	0.86	0.20	73,73,73,73	0
57	MG	1A	3068	1/1	0.86	0.25	58,58,58,58	0
57	MG	1A	3597	1/1	0.86	0.23	63,63,63,63	0
57	MG	2B	204	1/1	0.86	0.20	75,75,75,75	0
57	MG	2A	3299	1/1	0.86	0.28	75,75,75,75	0
57	MG	2A	3301	1/1	0.86	0.17	67,67,67,67	0
57	MG	2A	3303	1/1	0.86	0.13	72,72,72,72	0
57	MG	1a	1629	1/1	0.86	0.40	69,69,69,69	0
57	MG	1A	3823	1/1	0.86	0.12	29,29,29,29	0
57	MG	2A	3568	1/1	0.86	0.14	60,60,60,60	0
57	MG	1a	1638	1/1	0.86	0.20	60,60,60,60	0
57	MG	2B	215	1/1	0.86	0.17	66,66,66,66	0
57	MG	2A	3315	1/1	0.86	0.09	65,65,65,65	0
57	MG	1A	4095	1/1	0.86	0.15	47,47,47,47	0
57	MG	1A	3961	1/1	0.86	0.18	64,64,64,64	0
57	MG	2A	3330	1/1	0.86	0.31	56,56,56,56	0
57	MG	1B	214	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3096	1/1	0.86	0.24	65,65,65,65	0
57	MG	2a	1812	1/1	0.86	0.10	65,65,65,65	0
57	MG	2A	3195	1/1	0.86	0.14	56,56,56,56	0
57	MG	2A	3593	1/1	0.86	0.17	63,63,63,63	0
57	MG	2k	201	1/1	0.86	0.24	66,66,66,66	0
57	MG	2A	3597	1/1	0.86	0.21	74,74,74,74	0
57	MG	1A	3099	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	3277	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3605	1/1	0.86	0.34	67,67,67,67	0
57	MG	2w	106	1/1	0.86	0.17	75,75,75,75	0
57	MG	2x	104	1/1	0.86	0.36	72,72,72,72	0
57	MG	1x	101	1/1	0.86	0.17	60,60,60,60	0
57	MG	1A	3378	1/1	0.86	0.26	62,62,62,62	0
57	MG	1a	1671	1/1	0.86	0.34	65,65,65,65	0
57	MG	2A	3217	1/1	0.86	0.15	70,70,70,70	0
57	MG	25	101	1/1	0.87	0.31	67,67,67,67	0
57	MG	1a	1761	1/1	0.87	0.13	58,58,58,58	0
57	MG	2a	1601	1/1	0.87	0.10	81,81,81,81	0
57	MG	1a	1764	1/1	0.87	0.15	48,48,48,48	0
57	MG	1a	1765	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3339	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3341	1/1	0.87	0.40	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3343	1/1	0.87	0.36	64,64,64,64	0
57	MG	2a	1617	1/1	0.87	0.18	57,57,57,57	0
57	MG	2A	3346	1/1	0.87	0.34	68,68,68,68	0
57	MG	1A	3559	1/1	0.87	0.20	44,44,44,44	0
57	MG	2A	3164	1/1	0.87	0.21	66,66,66,66	0
57	MG	1a	1791	1/1	0.87	0.12	69,69,69,69	0
57	MG	2A	3166	1/1	0.87	0.16	65,65,65,65	0
57	MG	2A	3167	1/1	0.87	0.21	57,57,57,57	0
57	MG	1A	3427	1/1	0.87	0.20	55,55,55,55	0
57	MG	1A	3045	1/1	0.87	0.12	39,39,39,39	0
57	MG	2A	3653	1/1	0.87	0.12	64,64,64,64	0
57	MG	2a	1639	1/1	0.87	0.27	71,71,71,71	0
57	MG	1A	3308	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	4030	1/1	0.87	0.13	43,43,43,43	0
57	MG	2A	3182	1/1	0.87	0.18	64,64,64,64	0
57	MG	2A	3664	1/1	0.87	0.13	71,71,71,71	0
57	MG	2a	1659	1/1	0.87	0.13	64,64,64,64	0
57	MG	12	101	1/1	0.87	0.13	38,38,38,38	0
57	MG	12	102	1/1	0.87	0.11	50,50,50,50	0
57	MG	13	104	1/1	0.87	0.10	55,55,55,55	0
57	MG	1A	3434	1/1	0.87	0.22	60,60,60,60	0
57	MG	1a	1807	1/1	0.87	0.23	70,70,70,70	0
57	MG	1A	3618	1/1	0.87	0.09	21,21,21,21	0
57	MG	2A	3412	1/1	0.87	0.14	57,57,57,57	0
57	MG	2a	1684	1/1	0.87	0.21	67,67,67,67	0
57	MG	2a	1685	1/1	0.87	0.18	65,65,65,65	0
57	MG	1a	1810	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	3922	1/1	0.87	0.13	49,49,49,49	0
57	MG	2a	1689	1/1	0.87	0.23	67,67,67,67	0
57	MG	2A	3221	1/1	0.87	0.22	65,65,65,65	0
57	MG	2A	3729	1/1	0.87	0.19	74,74,74,74	0
57	MG	1A	3924	1/1	0.87	0.20	55,55,55,55	0
57	MG	1A	3927	1/1	0.87	0.18	65,65,65,65	0
57	MG	1A	3803	1/1	0.87	0.10	57,57,57,57	0
57	MG	1A	3313	1/1	0.87	0.19	53,53,53,53	0
57	MG	1w	103	1/1	0.87	0.21	73,73,73,73	0
57	MG	1A	3214	1/1	0.87	0.20	49,49,49,49	0
57	MG	2a	1709	1/1	0.87	0.31	72,72,72,72	0
57	MG	1w	105	1/1	0.87	0.10	68,68,68,68	0
57	MG	1A	3449	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3467	1/1	0.87	0.13	63,63,63,63	0
57	MG	2A	3238	1/1	0.87	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	104	1/1	0.87	0.18	66,66,66,66	0
57	MG	1a	1647	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3769	1/1	0.87	0.20	71,71,71,71	0
57	MG	1a	1648	1/1	0.87	0.33	66,66,66,66	0
57	MG	1A	3944	1/1	0.87	0.11	27,27,27,27	0
57	MG	1A	3456	1/1	0.87	0.12	58,58,58,58	0
57	MG	1A	3466	1/1	0.87	0.19	56,56,56,56	0
57	MG	2a	1749	1/1	0.87	0.14	78,78,78,78	0
57	MG	2A	3030	1/1	0.87	0.19	63,63,63,63	0
57	MG	1A	3758	1/1	0.87	0.08	49,49,49,49	0
57	MG	1A	3540	1/1	0.87	0.29	59,59,59,59	0
57	MG	2A	3785	1/1	0.87	0.13	57,57,57,57	0
57	MG	2A	3794	1/1	0.87	0.10	47,47,47,47	0
57	MG	1a	1668	1/1	0.87	0.16	56,56,56,56	0
57	MG	1A	3281	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3519	1/1	0.87	0.22	50,50,50,50	0
57	MG	2A	3264	1/1	0.87	0.30	69,69,69,69	0
57	MG	2B	203	1/1	0.87	0.23	73,73,73,73	0
57	MG	1B	224	1/1	0.87	0.19	57,57,57,57	0
57	MG	1A	3975	1/1	0.87	0.08	61,61,61,61	0
57	MG	2a	1779	1/1	0.87	0.40	71,71,71,71	0
57	MG	2A	3069	1/1	0.87	0.09	52,52,52,52	0
57	MG	1A	3252	1/1	0.87	0.09	46,46,46,46	0
57	MG	1a	1696	1/1	0.87	0.16	57,57,57,57	0
57	MG	1D	311	1/1	0.87	0.13	55,55,55,55	0
57	MG	2a	1791	1/1	0.87	0.26	79,79,79,79	0
57	MG	1E	310	1/1	0.87	0.08	39,39,39,39	0
57	MG	1A	3033	1/1	0.87	0.39	39,39,39,39	0
57	MG	2A	3282	1/1	0.87	0.25	76,76,76,76	0
57	MG	2a	1805	1/1	0.87	0.22	58,58,58,58	0
57	MG	1A	3784	1/1	0.87	0.18	54,54,54,54	0
57	MG	2A	3088	1/1	0.87	0.12	75,75,75,75	0
57	MG	2A	3092	1/1	0.87	0.27	65,65,65,65	0
57	MG	2A	3094	1/1	0.87	0.12	67,67,67,67	0
57	MG	1a	1727	1/1	0.87	0.11	64,64,64,64	0
57	MG	2a	1820	1/1	0.87	0.16	69,69,69,69	0
57	MG	2A	3099	1/1	0.87	0.23	77,77,77,77	0
57	MG	2f	203	1/1	0.87	0.18	75,75,75,75	0
57	MG	1A	3557	1/1	0.87	0.38	66,66,66,66	0
57	MG	2A	3106	1/1	0.87	0.24	59,59,59,59	0
57	MG	1O	206	1/1	0.87	0.24	65,65,65,65	0
57	MG	1R	205	1/1	0.87	0.13	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	3307	1/1	0.87	0.34	71,71,71,71	0
57	MG	2A	3121	1/1	0.87	0.25	42,42,42,42	0
57	MG	2x	102	1/1	0.87	0.39	82,82,82,82	0
57	MG	1A	3305	1/1	0.87	0.19	63,63,63,63	0
57	MG	1U	209	1/1	0.87	0.39	37,37,37,37	0
57	MG	2A	3599	1/1	0.87	0.22	67,67,67,67	0
57	MG	1A	4012	1/1	0.87	0.16	67,67,67,67	0
57	MG	2A	3321	1/1	0.87	0.16	64,64,64,64	0
57	MG	1a	1804	1/1	0.88	0.22	64,64,64,64	0
57	MG	1A	3770	1/1	0.88	0.20	68,68,68,68	0
57	MG	1A	3654	1/1	0.88	0.09	27,27,27,27	0
57	MG	1A	3906	1/1	0.88	0.18	48,48,48,48	0
57	MG	1A	3657	1/1	0.88	0.20	55,55,55,55	0
57	MG	15	106	1/1	0.88	0.13	61,61,61,61	0
57	MG	1A	3410	1/1	0.88	0.14	31,31,31,31	0
57	MG	1a	1605	1/1	0.88	0.12	62,62,62,62	0
57	MG	2a	1637	1/1	0.88	0.12	64,64,64,64	0
57	MG	2A	3205	1/1	0.88	0.38	47,47,47,47	0
57	MG	1l	3200	1/1	0.88	0.10	71,71,71,71	0
57	MG	2A	3214	1/1	0.88	0.17	77,77,77,77	0
57	MG	1A	3412	1/1	0.88	0.12	48,48,48,48	0
57	MG	1A	3413	1/1	0.88	0.13	67,67,67,67	0
57	MG	2a	1647	1/1	0.88	0.23	78,78,78,78	0
57	MG	2a	1650	1/1	0.88	0.28	66,66,66,66	0
57	MG	1A	3923	1/1	0.88	0.12	50,50,50,50	0
57	MG	2a	1654	1/1	0.88	0.19	64,64,64,64	0
57	MG	1A	4075	1/1	0.88	0.15	62,62,62,62	0
57	MG	2a	1661	1/1	0.88	0.19	59,59,59,59	0
57	MG	1A	4076	1/1	0.88	0.11	70,70,70,70	0
57	MG	1A	3547	1/1	0.88	0.09	42,42,42,42	0
57	MG	2A	3699	1/1	0.88	0.11	59,59,59,59	0
57	MG	1A	3475	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	4086	1/1	0.88	0.09	40,40,40,40	0
57	MG	2A	3720	1/1	0.88	0.10	58,58,58,58	0
57	MG	1x	108	1/1	0.88	0.21	67,67,67,67	0
57	MG	2a	1679	1/1	0.88	0.34	69,69,69,69	0
57	MG	2A	3231	1/1	0.88	0.13	71,71,71,71	0
57	MG	1A	4093	1/1	0.88	0.25	49,49,49,49	0
57	MG	1A	3414	1/1	0.88	0.10	51,51,51,51	0
57	MG	2A	3735	1/1	0.88	0.10	79,79,79,79	0
57	MG	1B	208	1/1	0.88	0.10	65,65,65,65	0
57	MG	2a	1691	1/1	0.88	0.38	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3418	1/1	0.88	0.22	54,54,54,54	0
57	MG	2A	3025	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3245	1/1	0.88	0.29	73,73,73,73	0
57	MG	1A	3363	1/1	0.88	0.29	41,41,41,41	0
57	MG	1a	1665	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3043	1/1	0.88	0.28	70,70,70,70	0
57	MG	1A	3199	1/1	0.88	0.15	71,71,71,71	0
57	MG	2A	3253	1/1	0.88	0.13	72,72,72,72	0
57	MG	1A	3702	1/1	0.88	0.32	67,67,67,67	0
57	MG	1A	3373	1/1	0.88	0.28	69,69,69,69	0
57	MG	2A	3487	1/1	0.88	0.19	63,63,63,63	0
57	MG	1A	3950	1/1	0.88	0.10	58,58,58,58	0
57	MG	1A	3707	1/1	0.88	0.11	67,67,67,67	0
57	MG	2A	3065	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3508	1/1	0.88	0.19	76,76,76,76	0
57	MG	1A	3498	1/1	0.88	0.12	63,63,63,63	0
57	MG	2A	3071	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3073	1/1	0.88	0.19	49,49,49,49	0
57	MG	2a	1726	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3787	1/1	0.88	0.12	58,58,58,58	0
57	MG	2A	3791	1/1	0.88	0.27	71,71,71,71	0
57	MG	2a	1734	1/1	0.88	0.12	70,70,70,70	0
57	MG	1a	1692	1/1	0.88	0.23	69,69,69,69	0
57	MG	2A	3521	1/1	0.88	0.13	45,45,45,45	0
57	MG	2A	3522	1/1	0.88	0.21	69,69,69,69	0
57	MG	1B	231	1/1	0.88	0.22	63,63,63,63	0
57	MG	2A	3526	1/1	0.88	0.21	65,65,65,65	0
57	MG	1a	1697	1/1	0.88	0.11	49,49,49,49	0
57	MG	2A	3536	1/1	0.88	0.19	46,46,46,46	0
57	MG	1A	3259	1/1	0.88	0.09	40,40,40,40	0
57	MG	1E	305	1/1	0.88	0.11	28,28,28,28	0
57	MG	1E	307	1/1	0.88	0.14	67,67,67,67	0
57	MG	1A	3724	1/1	0.88	0.15	45,45,45,45	0
57	MG	1a	1720	1/1	0.88	0.15	44,44,44,44	0
57	MG	1a	1724	1/1	0.88	0.21	59,59,59,59	0
57	MG	2A	3286	1/1	0.88	0.17	61,61,61,61	0
57	MG	2A	3288	1/1	0.88	0.13	57,57,57,57	0
57	MG	2a	1782	1/1	0.88	0.22	70,70,70,70	0
57	MG	1A	3431	1/1	0.88	0.16	66,66,66,66	0
57	MG	1F	315	1/1	0.88	0.17	58,58,58,58	0
57	MG	2A	3101	1/1	0.88	0.18	50,50,50,50	0
57	MG	1A	3827	1/1	0.88	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3297	1/1	0.88	0.18	69,69,69,69	0
57	MG	1A	3282	1/1	0.88	0.17	46,46,46,46	0
57	MG	2A	3110	1/1	0.88	0.13	76,76,76,76	0
57	MG	1A	3742	1/1	0.88	0.09	35,35,35,35	0
57	MG	1A	3990	1/1	0.88	0.12	54,54,54,54	0
57	MG	2A	3304	1/1	0.88	0.27	62,62,62,62	0
57	MG	1A	3061	1/1	0.88	0.27	59,59,59,59	0
57	MG	1T	201	1/1	0.88	0.28	65,65,65,65	0
57	MG	2A	3140	1/1	0.88	0.17	73,73,73,73	0
57	MG	1T	202	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3849	1/1	0.88	0.08	35,35,35,35	0
57	MG	2A	3317	1/1	0.88	0.07	58,58,58,58	0
57	MG	1U	210	1/1	0.88	0.12	55,55,55,55	0
57	MG	1A	3999	1/1	0.88	0.14	34,34,34,34	0
57	MG	25	103	1/1	0.88	0.18	63,63,63,63	0
57	MG	1A	3348	1/1	0.88	0.24	61,61,61,61	0
57	MG	28	104	1/1	0.88	0.31	58,58,58,58	0
57	MG	2w	103	1/1	0.88	0.15	70,70,70,70	0
57	MG	10	103	1/1	0.88	0.14	52,52,52,52	0
57	MG	2A	3161	1/1	0.88	0.10	57,57,57,57	0
57	MG	10	105	1/1	0.88	0.27	43,43,43,43	0
57	MG	1A	3294	1/1	0.88	0.13	63,63,63,63	0
57	MG	1A	3401	1/1	0.88	0.23	56,56,56,56	0
57	MG	1A	3647	1/1	0.88	0.14	24,24,24,24	0
57	MG	1A	3653	1/1	0.88	0.10	37,37,37,37	0
57	MG	2A	3058	1/1	0.89	0.34	68,68,68,68	0
57	MG	1B	201	1/1	0.89	0.15	51,51,51,51	0
57	MG	2A	3267	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3067	1/1	0.89	0.14	51,51,51,51	0
57	MG	1B	204	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3203	1/1	0.89	0.06	40,40,40,40	0
57	MG	2V	201	1/1	0.89	0.34	51,51,51,51	0
57	MG	1A	3082	1/1	0.89	0.09	52,52,52,52	0
57	MG	1a	1679	1/1	0.89	0.32	47,47,47,47	0
57	MG	2A	3553	1/1	0.89	0.17	61,61,61,61	0
57	MG	1a	1682	1/1	0.89	0.27	62,62,62,62	0
57	MG	1A	3219	1/1	0.89	0.28	33,33,33,33	0
57	MG	1a	1688	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3082	1/1	0.89	0.14	78,78,78,78	0
57	MG	1A	3679	1/1	0.89	0.15	66,66,66,66	0
57	MG	1a	1694	1/1	0.89	0.36	63,63,63,63	0
57	MG	2A	3565	1/1	0.89	0.15	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	2a	1606	1/1	0.89	0.23	74,74,74,74	0
57	MG	1A	3023	1/1	0.89	0.26	55,55,55,55	0
57	MG	2A	3570	1/1	0.89	0.22	73,73,73,73	0
57	MG	1A	3934	1/1	0.89	0.09	61,61,61,61	0
57	MG	1A	3296	1/1	0.89	0.23	56,56,56,56	0
57	MG	1A	3223	1/1	0.89	0.11	57,57,57,57	0
57	MG	2A	3578	1/1	0.89	0.12	69,69,69,69	0
57	MG	2A	3579	1/1	0.89	0.16	58,58,58,58	0
57	MG	2a	1624	1/1	0.89	0.38	64,64,64,64	0
57	MG	1A	3388	1/1	0.89	0.48	70,70,70,70	0
57	MG	1A	3947	1/1	0.89	0.13	50,50,50,50	0
57	MG	1A	3151	1/1	0.89	0.23	39,39,39,39	0
57	MG	1A	3159	1/1	0.89	0.10	40,40,40,40	0
57	MG	1A	3805	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3302	1/1	0.89	0.26	57,57,57,57	0
57	MG	2a	1634	1/1	0.89	0.19	62,62,62,62	0
57	MG	2a	1636	1/1	0.89	0.32	69,69,69,69	0
57	MG	1A	3960	1/1	0.89	0.11	65,65,65,65	0
57	MG	1a	1734	1/1	0.89	0.14	76,76,76,76	0
57	MG	1A	3468	1/1	0.89	0.17	54,54,54,54	0
57	MG	1A	3576	1/1	0.89	0.11	41,41,41,41	0
57	MG	2A	3134	1/1	0.89	0.35	63,63,63,63	0
57	MG	2A	3135	1/1	0.89	0.23	44,44,44,44	0
57	MG	2a	1644	1/1	0.89	0.27	83,83,83,83	0
57	MG	2A	3609	1/1	0.89	0.16	40,40,40,40	0
57	MG	1A	3247	1/1	0.89	0.11	42,42,42,42	0
57	MG	2A	3316	1/1	0.89	0.24	75,75,75,75	0
57	MG	1A	3584	1/1	0.89	0.18	30,30,30,30	0
57	MG	2A	3144	1/1	0.89	0.30	44,44,44,44	0
57	MG	1A	3405	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3630	1/1	0.89	0.13	65,65,65,65	0
57	MG	1a	1760	1/1	0.89	0.13	49,49,49,49	0
57	MG	2A	3329	1/1	0.89	0.19	43,43,43,43	0
57	MG	2A	3153	1/1	0.89	0.14	48,48,48,48	0
57	MG	2A	3635	1/1	0.89	0.15	68,68,68,68	0
57	MG	1A	3723	1/1	0.89	0.13	26,26,26,26	0
57	MG	2a	1675	1/1	0.89	0.22	53,53,53,53	0
57	MG	1A	3982	1/1	0.89	0.10	55,55,55,55	0
57	MG	1S	201	1/1	0.89	0.18	44,44,44,44	0
57	MG	2a	1683	1/1	0.89	0.14	75,75,75,75	0
57	MG	1A	3985	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3648	1/1	0.89	0.10	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	2A	3652	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3345	1/1	0.89	0.26	56,56,56,56	0
57	MG	1A	3829	1/1	0.89	0.08	37,37,37,37	0
57	MG	1A	3478	1/1	0.89	0.20	74,74,74,74	0
57	MG	1A	3601	1/1	0.89	0.14	70,70,70,70	0
57	MG	2A	3352	1/1	0.89	0.25	63,63,63,63	0
57	MG	1A	3996	1/1	0.89	0.09	53,53,53,53	0
57	MG	1A	3248	1/1	0.89	0.08	32,32,32,32	0
57	MG	2A	3173	1/1	0.89	0.10	70,70,70,70	0
57	MG	1A	3484	1/1	0.89	0.30	44,44,44,44	0
57	MG	1A	4011	1/1	0.89	0.12	51,51,51,51	0
57	MG	10	107	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3364	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3852	1/1	0.89	0.11	23,23,23,23	0
57	MG	2A	3380	1/1	0.89	0.20	58,58,58,58	0
57	MG	1A	3853	1/1	0.89	0.12	77,77,77,77	0
57	MG	2a	1716	1/1	0.89	0.27	63,63,63,63	0
57	MG	2A	3713	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3385	1/1	0.89	0.30	73,73,73,73	0
57	MG	2A	3193	1/1	0.89	0.23	55,55,55,55	0
57	MG	11	102	1/1	0.89	0.17	60,60,60,60	0
57	MG	1A	3097	1/1	0.89	0.10	37,37,37,37	0
57	MG	2A	3198	1/1	0.89	0.14	69,69,69,69	0
57	MG	2A	3403	1/1	0.89	0.24	56,56,56,56	0
57	MG	1A	3257	1/1	0.89	0.26	58,58,58,58	0
57	MG	1A	3058	1/1	0.89	0.26	54,54,54,54	0
57	MG	2A	3209	1/1	0.89	0.16	47,47,47,47	0
57	MG	2a	1739	1/1	0.89	0.11	69,69,69,69	0
57	MG	2a	1748	1/1	0.89	0.14	78,78,78,78	0
57	MG	2A	3414	1/1	0.89	0.22	62,62,62,62	0
57	MG	1A	3861	1/1	0.89	0.21	37,37,37,37	0
57	MG	2A	3418	1/1	0.89	0.13	28,28,28,28	0
57	MG	2A	3759	1/1	0.89	0.16	64,64,64,64	0
57	MG	1A	4037	1/1	0.89	0.14	58,58,58,58	0
57	MG	1A	4038	1/1	0.89	0.12	62,62,62,62	0
57	MG	1A	3196	1/1	0.89	0.19	53,53,53,53	0
57	MG	1A	3872	1/1	0.89	0.11	41,41,41,41	0
57	MG	2a	1764	1/1	0.89	0.21	66,66,66,66	0
57	MG	2a	1765	1/1	0.89	0.13	67,67,67,67	0
57	MG	2A	3428	1/1	0.89	0.10	45,45,45,45	0
57	MG	2A	3430	1/1	0.89	0.09	39,39,39,39	0
57	MG	1a	1604	1/1	0.89	0.15	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	2a	1775	1/1	0.89	0.26	78,78,78,78	0
57	MG	1A	3879	1/1	0.89	0.10	68,68,68,68	0
57	MG	1A	3759	1/1	0.89	0.10	55,55,55,55	0
57	MG	2A	3449	1/1	0.89	0.10	49,49,49,49	0
57	MG	1A	4047	1/1	0.89	0.18	55,55,55,55	0
57	MG	1A	4051	1/1	0.89	0.23	57,57,57,57	0
57	MG	1a	1626	1/1	0.89	0.31	59,59,59,59	0
57	MG	1A	3885	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3470	1/1	0.89	0.10	39,39,39,39	0
57	MG	1a	1634	1/1	0.89	0.25	74,74,74,74	0
57	MG	1x	113	1/1	0.89	0.24	62,62,62,62	0
57	MG	1A	3338	1/1	0.89	0.32	48,48,48,48	0
57	MG	1A	3897	1/1	0.89	0.09	18,18,18,18	0
57	MG	1A	3347	1/1	0.89	0.10	47,47,47,47	0
57	MG	1A	3424	1/1	0.89	0.23	60,60,60,60	0
57	MG	2A	3026	1/1	0.89	0.14	43,43,43,43	0
57	MG	1A	3198	1/1	0.89	0.19	59,59,59,59	0
57	MG	1a	1651	1/1	0.89	0.16	54,54,54,54	0
57	MG	2A	3495	1/1	0.89	0.23	63,63,63,63	0
57	MG	1A	4084	1/1	0.89	0.18	73,73,73,73	0
57	MG	2A	3502	1/1	0.89	0.13	67,67,67,67	0
57	MG	2A	3503	1/1	0.89	0.08	40,40,40,40	0
57	MG	2j	201	1/1	0.89	0.14	74,74,74,74	0
57	MG	1A	3774	1/1	0.89	0.23	32,32,32,32	0
57	MG	1A	3124	1/1	0.89	0.14	37,37,37,37	0
57	MG	2A	3514	1/1	0.89	0.12	65,65,65,65	0
57	MG	2B	218	1/1	0.89	0.33	78,78,78,78	0
57	MG	1A	4088	1/1	0.89	0.22	75,75,75,75	0
57	MG	2w	102	1/1	0.89	0.15	84,84,84,84	0
57	MG	2A	3050	1/1	0.89	0.28	65,65,65,65	0
57	MG	2w	104	1/1	0.89	0.11	87,87,87,87	0
57	MG	2D	308	1/1	0.89	0.16	59,59,59,59	0
57	MG	2A	3257	1/1	0.89	0.10	68,68,68,68	0
57	MG	2E	304	1/1	0.89	0.13	34,34,34,34	0
57	MG	2E	306	1/1	0.89	0.14	54,54,54,54	0
57	MG	2x	107	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3259	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3916	1/1	0.89	0.07	23,23,23,23	0
57	MG	1A	3666	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3179	1/1	0.90	0.15	38,38,38,38	0
57	MG	1A	3656	1/1	0.90	0.08	31,31,31,31	0
57	MG	29	101	1/1	0.90	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3523	1/1	0.90	0.34	42,42,42,42	0
57	MG	1Q	207	1/1	0.90	0.11	49,49,49,49	0
57	MG	2a	1605	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3358	1/1	0.90	0.22	52,52,52,52	0
57	MG	1A	3786	1/1	0.90	0.21	47,47,47,47	0
57	MG	1a	1690	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3222	1/1	0.90	0.12	62,62,62,62	0
57	MG	2a	1612	1/1	0.90	0.17	60,60,60,60	0
57	MG	1A	4033	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3293	1/1	0.90	0.19	57,57,57,57	0
57	MG	2a	1618	1/1	0.90	0.29	71,71,71,71	0
57	MG	2A	3368	1/1	0.90	0.33	57,57,57,57	0
57	MG	2A	3374	1/1	0.90	0.10	40,40,40,40	0
57	MG	2A	3379	1/1	0.90	0.29	58,58,58,58	0
57	MG	2A	3226	1/1	0.90	0.19	59,59,59,59	0
57	MG	1S	203	1/1	0.90	0.22	67,67,67,67	0
57	MG	1A	3668	1/1	0.90	0.15	61,61,61,61	0
57	MG	2a	1630	1/1	0.90	0.19	68,68,68,68	0
57	MG	1A	3914	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3368	1/1	0.90	0.10	43,43,43,43	0
57	MG	2A	3398	1/1	0.90	0.39	62,62,62,62	0
57	MG	1A	3430	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3059	1/1	0.90	0.22	55,55,55,55	0
57	MG	2A	3640	1/1	0.90	0.16	68,68,68,68	0
57	MG	2A	3642	1/1	0.90	0.09	69,69,69,69	0
57	MG	1A	3018	1/1	0.90	0.31	50,50,50,50	0
57	MG	1A	3295	1/1	0.90	0.33	63,63,63,63	0
57	MG	2A	3647	1/1	0.90	0.12	54,54,54,54	0
57	MG	2A	3239	1/1	0.90	0.16	55,55,55,55	0
57	MG	2A	3408	1/1	0.90	0.12	65,65,65,65	0
57	MG	2A	3410	1/1	0.90	0.10	76,76,76,76	0
57	MG	2a	1648	1/1	0.90	0.09	66,66,66,66	0
57	MG	2a	1649	1/1	0.90	0.32	67,67,67,67	0
57	MG	2A	3242	1/1	0.90	0.16	66,66,66,66	0
57	MG	2A	3413	1/1	0.90	0.12	38,38,38,38	0
57	MG	2A	3659	1/1	0.90	0.16	69,69,69,69	0
57	MG	1A	4050	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3433	1/1	0.90	0.16	47,47,47,47	0
57	MG	1A	4059	1/1	0.90	0.18	61,61,61,61	0
57	MG	1a	1732	1/1	0.90	0.08	53,53,53,53	0
57	MG	1A	3242	1/1	0.90	0.22	57,57,57,57	0
57	MG	2A	3424	1/1	0.90	0.14	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	1737	1/1	0.90	0.11	56,56,56,56	0
57	MG	1A	3243	1/1	0.90	0.17	41,41,41,41	0
57	MG	1A	3193	1/1	0.90	0.09	47,47,47,47	0
57	MG	1A	3550	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3381	1/1	0.90	0.12	57,57,57,57	0
57	MG	2a	1680	1/1	0.90	0.21	66,66,66,66	0
57	MG	2A	3709	1/1	0.90	0.10	36,36,36,36	0
57	MG	2A	3439	1/1	0.90	0.27	68,68,68,68	0
57	MG	2A	3086	1/1	0.90	0.12	44,44,44,44	0
57	MG	2A	3717	1/1	0.90	0.12	64,64,64,64	0
57	MG	1a	1745	1/1	0.90	0.20	74,74,74,74	0
57	MG	2A	3091	1/1	0.90	0.30	70,70,70,70	0
57	MG	2A	3261	1/1	0.90	0.13	56,56,56,56	0
57	MG	1a	1748	1/1	0.90	0.14	71,71,71,71	0
57	MG	2A	3731	1/1	0.90	0.10	59,59,59,59	0
57	MG	1a	1752	1/1	0.90	0.09	63,63,63,63	0
57	MG	2A	3463	1/1	0.90	0.20	53,53,53,53	0
57	MG	2A	3737	1/1	0.90	0.14	48,48,48,48	0
57	MG	1A	3815	1/1	0.90	0.13	57,57,57,57	0
57	MG	2A	3739	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3266	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3743	1/1	0.90	0.21	70,70,70,70	0
57	MG	2A	3748	1/1	0.90	0.19	68,68,68,68	0
57	MG	2A	3473	1/1	0.90	0.22	54,54,54,54	0
57	MG	1A	3088	1/1	0.90	0.22	53,53,53,53	0
57	MG	2A	3100	1/1	0.90	0.23	70,70,70,70	0
57	MG	1A	3459	1/1	0.90	0.08	52,52,52,52	0
57	MG	1A	3461	1/1	0.90	0.12	62,62,62,62	0
57	MG	15	104	1/1	0.90	0.25	40,40,40,40	0
57	MG	1A	3089	1/1	0.90	0.08	76,76,76,76	0
57	MG	2A	3764	1/1	0.90	0.11	73,73,73,73	0
57	MG	2A	3765	1/1	0.90	0.09	63,63,63,63	0
57	MG	17	104	1/1	0.90	0.10	51,51,51,51	0
57	MG	1A	4089	1/1	0.90	0.13	58,58,58,58	0
57	MG	1a	1603	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3771	1/1	0.90	0.28	61,61,61,61	0
57	MG	1A	4092	1/1	0.90	0.10	72,72,72,72	0
57	MG	1A	3309	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3501	1/1	0.90	0.20	63,63,63,63	0
57	MG	1A	3830	1/1	0.90	0.18	45,45,45,45	0
57	MG	1A	3400	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3506	1/1	0.90	0.19	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	1A	3840	1/1	0.90	0.09	48,48,48,48	0
57	MG	1a	1623	1/1	0.90	0.28	58,58,58,58	0
57	MG	2A	3513	1/1	0.90	0.19	76,76,76,76	0
57	MG	2A	3292	1/1	0.90	0.12	58,58,58,58	0
57	MG	2A	3792	1/1	0.90	0.09	77,77,77,77	0
57	MG	2A	3515	1/1	0.90	0.09	34,34,34,34	0
57	MG	1a	1625	1/1	0.90	0.27	52,52,52,52	0
57	MG	2a	1769	1/1	0.90	0.21	64,64,64,64	0
57	MG	1A	3966	1/1	0.90	0.13	40,40,40,40	0
57	MG	2A	3296	1/1	0.90	0.25	75,75,75,75	0
57	MG	2a	1772	1/1	0.90	0.20	62,62,62,62	0
57	MG	1A	3591	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3025	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3152	1/1	0.90	0.12	42,42,42,42	0
57	MG	1A	3319	1/1	0.90	0.23	67,67,67,67	0
57	MG	1A	3213	1/1	0.90	0.29	45,45,45,45	0
57	MG	2A	3530	1/1	0.90	0.16	39,39,39,39	0
57	MG	2A	3531	1/1	0.90	0.12	64,64,64,64	0
57	MG	1a	1642	1/1	0.90	0.31	64,64,64,64	0
57	MG	2A	3538	1/1	0.90	0.08	41,41,41,41	0
57	MG	1p	101	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3158	1/1	0.90	0.23	62,62,62,62	0
57	MG	1A	3049	1/1	0.90	0.17	32,32,32,32	0
57	MG	1A	3278	1/1	0.90	0.09	53,53,53,53	0
57	MG	2a	1804	1/1	0.90	0.25	65,65,65,65	0
57	MG	2D	302	1/1	0.90	0.23	66,66,66,66	0
57	MG	2a	1807	1/1	0.90	0.17	69,69,69,69	0
57	MG	2A	3549	1/1	0.90	0.11	53,53,53,53	0
57	MG	1B	229	1/1	0.90	0.10	75,75,75,75	0
57	MG	2A	3174	1/1	0.90	0.21	60,60,60,60	0
57	MG	2A	3554	1/1	0.90	0.21	63,63,63,63	0
57	MG	1a	1658	1/1	0.90	0.23	65,65,65,65	0
57	MG	2a	1818	1/1	0.90	0.11	72,72,72,72	0
57	MG	1A	3859	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3319	1/1	0.90	0.10	73,73,73,73	0
57	MG	2A	3180	1/1	0.90	0.15	60,60,60,60	0
57	MG	2F	305	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3165	1/1	0.90	0.29	45,45,45,45	0
57	MG	2A	3322	1/1	0.90	0.09	57,57,57,57	0
57	MG	1A	3494	1/1	0.90	0.32	69,69,69,69	0
57	MG	1A	3422	1/1	0.90	0.17	48,48,48,48	0
57	MG	2A	3190	1/1	0.90	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1E	309	1/1	0.90	0.10	51,51,51,51	0
57	MG	1x	112	1/1	0.90	0.14	72,72,72,72	0
57	MG	1A	3646	1/1	0.90	0.14	34,34,34,34	0
57	MG	1A	3056	1/1	0.90	0.11	37,37,37,37	0
57	MG	2A	3013	1/1	0.90	0.43	78,78,78,78	0
57	MG	2A	3200	1/1	0.90	0.26	60,60,60,60	0
57	MG	2A	3017	1/1	0.90	0.16	61,61,61,61	0
57	MG	2I	102	1/1	0.90	0.21	68,68,68,68	0
57	MG	2A	3349	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3511	1/1	0.90	0.36	58,58,58,58	0
57	MG	25	104	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3825	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	4008	1/1	0.91	0.07	18,18,18,18	0
57	MG	2D	305	1/1	0.91	0.30	52,52,52,52	0
57	MG	1A	4009	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3240	1/1	0.91	0.13	63,63,63,63	0
57	MG	2A	3504	1/1	0.91	0.29	72,72,72,72	0
57	MG	1A	4010	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3507	1/1	0.91	0.09	61,61,61,61	0
57	MG	2E	307	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3243	1/1	0.91	0.15	77,77,77,77	0
57	MG	1A	3283	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	3675	1/1	0.91	0.23	49,49,49,49	0
57	MG	1A	3364	1/1	0.91	0.19	34,34,34,34	0
57	MG	1A	3529	1/1	0.91	0.17	56,56,56,56	0
57	MG	1A	4024	1/1	0.91	0.10	22,22,22,22	0
57	MG	2A	3517	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3367	1/1	0.91	0.08	47,47,47,47	0
57	MG	1A	3238	1/1	0.91	0.17	41,41,41,41	0
57	MG	2T	201	1/1	0.91	0.14	70,70,70,70	0
57	MG	2T	202	1/1	0.91	0.26	64,64,64,64	0
57	MG	1x	103	1/1	0.91	0.19	55,55,55,55	0
57	MG	15	101	1/1	0.91	0.18	39,39,39,39	0
57	MG	1x	106	1/1	0.91	0.27	61,61,61,61	0
57	MG	1A	3371	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3258	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3848	1/1	0.91	0.07	22,22,22,22	0
57	MG	1A	4035	1/1	0.91	0.27	58,58,58,58	0
57	MG	1A	3439	1/1	0.91	0.14	46,46,46,46	0
57	MG	1a	1601	1/1	0.91	0.24	55,55,55,55	0
57	MG	2A	3539	1/1	0.91	0.15	47,47,47,47	0
57	MG	28	101	1/1	0.91	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1602	1/1	0.91	0.25	71,71,71,71	0
57	MG	2A	3007	1/1	0.91	0.13	59,59,59,59	0
57	MG	1A	3442	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	3545	1/1	0.91	0.41	61,61,61,61	0
57	MG	2A	3268	1/1	0.91	0.08	44,44,44,44	0
57	MG	1A	3444	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	3019	1/1	0.91	0.22	48,48,48,48	0
57	MG	1a	1614	1/1	0.91	0.30	56,56,56,56	0
57	MG	2a	1609	1/1	0.91	0.22	71,71,71,71	0
57	MG	1A	3084	1/1	0.91	0.25	45,45,45,45	0
57	MG	1A	3552	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3711	1/1	0.91	0.07	27,27,27,27	0
57	MG	2A	3039	1/1	0.91	0.13	56,56,56,56	0
57	MG	1a	1624	1/1	0.91	0.07	46,46,46,46	0
57	MG	1A	3718	1/1	0.91	0.09	20,20,20,20	0
57	MG	1A	3868	1/1	0.91	0.28	33,33,33,33	0
57	MG	2A	3567	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3106	1/1	0.91	0.21	40,40,40,40	0
57	MG	1A	3876	1/1	0.91	0.10	61,61,61,61	0
57	MG	1a	1636	1/1	0.91	0.29	57,57,57,57	0
57	MG	1A	4066	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3454	1/1	0.91	0.16	36,36,36,36	0
57	MG	1A	4072	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3062	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3295	1/1	0.91	0.23	70,70,70,70	0
57	MG	1A	4073	1/1	0.91	0.12	66,66,66,66	0
57	MG	2A	3066	1/1	0.91	0.19	68,68,68,68	0
57	MG	1a	1646	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3245	1/1	0.91	0.17	77,77,77,77	0
57	MG	1A	3246	1/1	0.91	0.20	28,28,28,28	0
57	MG	1A	3561	1/1	0.91	0.12	39,39,39,39	0
57	MG	1a	1652	1/1	0.91	0.08	45,45,45,45	0
57	MG	1A	3565	1/1	0.91	0.08	23,23,23,23	0
57	MG	1A	3568	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3899	1/1	0.91	0.12	66,66,66,66	0
57	MG	1a	1660	1/1	0.91	0.15	60,60,60,60	0
57	MG	1A	3900	1/1	0.91	0.14	65,65,65,65	0
57	MG	1A	3748	1/1	0.91	0.14	51,51,51,51	0
57	MG	1a	1663	1/1	0.91	0.22	68,68,68,68	0
57	MG	2A	3614	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	3570	1/1	0.91	0.18	50,50,50,50	0
57	MG	1A	3908	1/1	0.91	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1663	1/1	0.91	0.19	67,67,67,67	0
57	MG	2A	3620	1/1	0.91	0.24	71,71,71,71	0
57	MG	2A	3626	1/1	0.91	0.15	62,62,62,62	0
57	MG	1A	3162	1/1	0.91	0.17	42,42,42,42	0
57	MG	1A	4099	1/1	0.91	0.26	53,53,53,53	0
57	MG	1A	3463	1/1	0.91	0.14	55,55,55,55	0
57	MG	1B	203	1/1	0.91	0.34	66,66,66,66	0
57	MG	2A	3326	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3328	1/1	0.91	0.20	61,61,61,61	0
57	MG	1a	1678	1/1	0.91	0.32	54,54,54,54	0
57	MG	1A	3204	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3589	1/1	0.91	0.10	32,32,32,32	0
57	MG	1A	3251	1/1	0.91	0.20	64,64,64,64	0
57	MG	2A	3643	1/1	0.91	0.10	71,71,71,71	0
57	MG	1a	1686	1/1	0.91	0.29	62,62,62,62	0
57	MG	1A	3769	1/1	0.91	0.08	57,57,57,57	0
57	MG	2A	3114	1/1	0.91	0.07	62,62,62,62	0
57	MG	1A	3210	1/1	0.91	0.11	49,49,49,49	0
57	MG	2a	1692	1/1	0.91	0.13	73,73,73,73	0
57	MG	1B	218	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3472	1/1	0.91	0.31	35,35,35,35	0
57	MG	2A	3128	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3131	1/1	0.91	0.18	53,53,53,53	0
57	MG	2a	1699	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3474	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3776	1/1	0.91	0.08	46,46,46,46	0
57	MG	1a	1698	1/1	0.91	0.29	63,63,63,63	0
57	MG	2A	3671	1/1	0.91	0.09	73,73,73,73	0
57	MG	2A	3357	1/1	0.91	0.15	58,58,58,58	0
57	MG	2A	3676	1/1	0.91	0.09	61,61,61,61	0
57	MG	1A	3933	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	1713	1/1	0.91	0.33	68,68,68,68	0
57	MG	2A	3679	1/1	0.91	0.09	71,71,71,71	0
57	MG	1A	3163	1/1	0.91	0.25	59,59,59,59	0
57	MG	2a	1717	1/1	0.91	0.30	75,75,75,75	0
57	MG	2A	3146	1/1	0.91	0.16	66,66,66,66	0
57	MG	2a	1719	1/1	0.91	0.15	69,69,69,69	0
57	MG	1A	3617	1/1	0.91	0.09	25,25,25,25	0
57	MG	1a	1718	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3365	1/1	0.91	0.12	69,69,69,69	0
57	MG	2A	3697	1/1	0.91	0.08	72,72,72,72	0
57	MG	1A	3085	1/1	0.91	0.17	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	3155	1/1	0.91	0.10	67,67,67,67	0
57	MG	2a	1728	1/1	0.91	0.12	64,64,64,64	0
57	MG	2A	3707	1/1	0.91	0.11	51,51,51,51	0
57	MG	2A	3369	1/1	0.91	0.15	70,70,70,70	0
57	MG	1B	232	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3157	1/1	0.91	0.15	76,76,76,76	0
57	MG	2a	1740	1/1	0.91	0.11	56,56,56,56	0
57	MG	2a	1747	1/1	0.91	0.12	72,72,72,72	0
57	MG	1B	233	1/1	0.91	0.15	61,61,61,61	0
57	MG	1A	3125	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3722	1/1	0.91	0.20	61,61,61,61	0
57	MG	2A	3160	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3386	1/1	0.91	0.16	56,56,56,56	0
57	MG	2a	1757	1/1	0.91	0.27	69,69,69,69	0
57	MG	2a	1758	1/1	0.91	0.12	67,67,67,67	0
57	MG	1E	302	1/1	0.91	0.19	36,36,36,36	0
57	MG	2A	3163	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3394	1/1	0.91	0.19	57,57,57,57	0
57	MG	1A	3621	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3220	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3481	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3326	1/1	0.91	0.29	62,62,62,62	0
57	MG	2A	3168	1/1	0.91	0.11	49,49,49,49	0
57	MG	1a	1739	1/1	0.91	0.15	67,67,67,67	0
57	MG	1A	3271	1/1	0.91	0.41	40,40,40,40	0
57	MG	1F	314	1/1	0.91	0.13	55,55,55,55	0
57	MG	2a	1773	1/1	0.91	0.14	68,68,68,68	0
57	MG	1A	3798	1/1	0.91	0.20	51,51,51,51	0
57	MG	1G	203	1/1	0.91	0.16	68,68,68,68	0
57	MG	2A	3756	1/1	0.91	0.19	48,48,48,48	0
57	MG	1a	1747	1/1	0.91	0.10	59,59,59,59	0
57	MG	1I	201	1/1	0.91	0.10	65,65,65,65	0
57	MG	2A	3417	1/1	0.91	0.17	63,63,63,63	0
57	MG	1A	3331	1/1	0.91	0.12	56,56,56,56	0
57	MG	2a	1785	1/1	0.91	0.28	66,66,66,66	0
57	MG	2a	1787	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3184	1/1	0.91	0.27	66,66,66,66	0
57	MG	1A	3276	1/1	0.91	0.15	45,45,45,45	0
57	MG	1A	3026	1/1	0.91	0.34	65,65,65,65	0
57	MG	1P	205	1/1	0.91	0.14	41,41,41,41	0
57	MG	2A	3194	1/1	0.91	0.13	59,59,59,59	0
57	MG	2a	1794	1/1	0.91	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1795	1/1	0.91	0.31	72,72,72,72	0
57	MG	1a	1763	1/1	0.91	0.16	64,64,64,64	0
57	MG	2a	1800	1/1	0.91	0.17	56,56,56,56	0
57	MG	2a	1801	1/1	0.91	0.13	83,83,83,83	0
57	MG	1A	3495	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3977	1/1	0.91	0.14	56,56,56,56	0
57	MG	1a	1772	1/1	0.91	0.09	77,77,77,77	0
57	MG	1a	1778	1/1	0.91	0.09	78,78,78,78	0
57	MG	2A	3444	1/1	0.91	0.25	70,70,70,70	0
57	MG	1A	3340	1/1	0.91	0.13	49,49,49,49	0
57	MG	2A	3207	1/1	0.91	0.32	56,56,56,56	0
57	MG	2a	1814	1/1	0.91	0.11	60,60,60,60	0
57	MG	1a	1780	1/1	0.91	0.09	64,64,64,64	0
57	MG	1a	1789	1/1	0.91	0.30	60,60,60,60	0
57	MG	2A	3788	1/1	0.91	0.12	64,64,64,64	0
57	MG	2e	201	1/1	0.91	0.07	73,73,73,73	0
57	MG	2f	201	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3345	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	3808	1/1	0.91	0.09	22,22,22,22	0
57	MG	2A	3464	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3663	1/1	0.91	0.11	28,28,28,28	0
57	MG	1A	3814	1/1	0.91	0.09	41,41,41,41	0
57	MG	1T	203	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	1799	1/1	0.91	0.13	73,73,73,73	0
57	MG	1U	202	1/1	0.91	0.12	36,36,36,36	0
57	MG	2v	103	1/1	0.91	0.20	60,60,60,60	0
57	MG	2v	104	1/1	0.91	0.20	62,62,62,62	0
57	MG	1U	205	1/1	0.91	0.14	36,36,36,36	0
57	MG	2A	3481	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3064	1/1	0.91	0.15	48,48,48,48	0
57	MG	1A	3992	1/1	0.91	0.13	53,53,53,53	0
57	MG	2x	101	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3484	1/1	0.91	0.10	32,32,32,32	0
57	MG	2x	103	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3667	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3486	1/1	0.91	0.18	60,60,60,60	0
57	MG	1W	201	1/1	0.91	0.24	49,49,49,49	0
57	MG	1A	3235	1/1	0.91	0.24	71,71,71,71	0
57	MG	1A	3001	1/1	0.91	0.07	43,43,43,43	0
57	MG	1a	1811	1/1	0.91	0.18	61,61,61,61	0
57	MG	2A	3064	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3276	1/1	0.92	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3118	1/1	0.92	0.23	52,52,52,52	0
57	MG	1A	3184	1/1	0.92	0.13	30,30,30,30	0
57	MG	1A	3493	1/1	0.92	0.25	49,49,49,49	0
57	MG	2P	201	1/1	0.92	0.08	63,63,63,63	0
57	MG	1A	3832	1/1	0.92	0.12	37,37,37,37	0
57	MG	1A	3321	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3218	1/1	0.92	0.20	36,36,36,36	0
57	MG	2A	3537	1/1	0.92	0.20	52,52,52,52	0
57	MG	2A	3284	1/1	0.92	0.11	66,66,66,66	0
57	MG	1F	305	1/1	0.92	0.10	60,60,60,60	0
57	MG	2A	3541	1/1	0.92	0.22	63,63,63,63	0
57	MG	1a	1691	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3991	1/1	0.92	0.07	56,56,56,56	0
57	MG	2A	3290	1/1	0.92	0.07	64,64,64,64	0
57	MG	1A	3598	1/1	0.92	0.07	19,19,19,19	0
57	MG	1G	202	1/1	0.92	0.32	67,67,67,67	0
57	MG	2A	3550	1/1	0.92	0.15	68,68,68,68	0
57	MG	25	102	1/1	0.92	0.20	45,45,45,45	0
57	MG	2A	3551	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3123	1/1	0.92	0.22	52,52,52,52	0
57	MG	1H	201	1/1	0.92	0.18	48,48,48,48	0
57	MG	1a	1700	1/1	0.92	0.19	50,50,50,50	0
57	MG	28	103	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3087	1/1	0.92	0.24	69,69,69,69	0
57	MG	2A	3558	1/1	0.92	0.12	46,46,46,46	0
57	MG	1a	1703	1/1	0.92	0.32	53,53,53,53	0
57	MG	1A	3380	1/1	0.92	0.14	68,68,68,68	0
57	MG	2a	1603	1/1	0.92	0.21	58,58,58,58	0
57	MG	1a	1710	1/1	0.92	0.10	57,57,57,57	0
57	MG	1N	204	1/1	0.92	0.19	44,44,44,44	0
57	MG	1A	3736	1/1	0.92	0.11	33,33,33,33	0
57	MG	2A	3097	1/1	0.92	0.31	50,50,50,50	0
57	MG	2A	3566	1/1	0.92	0.08	33,33,33,33	0
57	MG	1A	3739	1/1	0.92	0.09	27,27,27,27	0
57	MG	1O	205	1/1	0.92	0.09	48,48,48,48	0
57	MG	2a	1613	1/1	0.92	0.20	53,53,53,53	0
57	MG	1A	4007	1/1	0.92	0.17	77,77,77,77	0
57	MG	2a	1616	1/1	0.92	0.19	79,79,79,79	0
57	MG	1a	1723	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3740	1/1	0.92	0.06	71,71,71,71	0
57	MG	2A	3313	1/1	0.92	0.10	63,63,63,63	0
57	MG	2A	3314	1/1	0.92	0.43	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1623	1/1	0.92	0.09	63,63,63,63	0
57	MG	1Q	204	1/1	0.92	0.13	54,54,54,54	0
57	MG	1A	3507	1/1	0.92	0.32	53,53,53,53	0
57	MG	1a	1731	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3318	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3116	1/1	0.92	0.17	65,65,65,65	0
57	MG	1A	3746	1/1	0.92	0.08	16,16,16,16	0
57	MG	2A	3591	1/1	0.92	0.08	66,66,66,66	0
57	MG	1A	3608	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3596	1/1	0.92	0.13	56,56,56,56	0
57	MG	2a	1635	1/1	0.92	0.21	69,69,69,69	0
57	MG	1A	3509	1/1	0.92	0.17	35,35,35,35	0
57	MG	2A	3598	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3323	1/1	0.92	0.11	67,67,67,67	0
57	MG	2A	3324	1/1	0.92	0.28	55,55,55,55	0
57	MG	1A	4013	1/1	0.92	0.18	41,41,41,41	0
57	MG	1A	3754	1/1	0.92	0.08	19,19,19,19	0
57	MG	1A	4020	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3510	1/1	0.92	0.20	54,54,54,54	0
57	MG	2A	3137	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3138	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3334	1/1	0.92	0.36	54,54,54,54	0
57	MG	2A	3139	1/1	0.92	0.24	61,61,61,61	0
57	MG	2A	3340	1/1	0.92	0.36	56,56,56,56	0
57	MG	1A	3865	1/1	0.92	0.10	47,47,47,47	0
57	MG	2a	1655	1/1	0.92	0.09	68,68,68,68	0
57	MG	2a	1657	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3866	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3627	1/1	0.92	0.16	61,61,61,61	0
57	MG	2A	3344	1/1	0.92	0.21	63,63,63,63	0
57	MG	1A	3867	1/1	0.92	0.11	33,33,33,33	0
57	MG	1A	3190	1/1	0.92	0.12	46,46,46,46	0
57	MG	2a	1668	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3382	1/1	0.92	0.20	59,59,59,59	0
57	MG	2A	3348	1/1	0.92	0.28	58,58,58,58	0
57	MG	1A	3874	1/1	0.92	0.14	52,52,52,52	0
57	MG	1a	1758	1/1	0.92	0.08	63,63,63,63	0
57	MG	2A	3638	1/1	0.92	0.07	68,68,68,68	0
57	MG	2a	1676	1/1	0.92	0.29	61,61,61,61	0
57	MG	2A	3351	1/1	0.92	0.24	57,57,57,57	0
57	MG	1Y	201	1/1	0.92	0.26	69,69,69,69	0
57	MG	1Y	202	1/1	0.92	0.35	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	1Z	301	1/1	0.92	0.15	67,67,67,67	0
57	MG	2A	3355	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3384	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3632	1/1	0.92	0.10	29,29,29,29	0
57	MG	2a	1687	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3385	1/1	0.92	0.11	63,63,63,63	0
57	MG	2A	3650	1/1	0.92	0.27	47,47,47,47	0
57	MG	2a	1690	1/1	0.92	0.12	66,66,66,66	0
57	MG	1a	1777	1/1	0.92	0.07	85,85,85,85	0
57	MG	1A	3639	1/1	0.92	0.18	61,61,61,61	0
57	MG	1A	4041	1/1	0.92	0.07	53,53,53,53	0
57	MG	2A	3656	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3333	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3157	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3532	1/1	0.92	0.20	46,46,46,46	0
57	MG	2A	3663	1/1	0.92	0.12	66,66,66,66	0
57	MG	2a	1702	1/1	0.92	0.13	64,64,64,64	0
57	MG	1A	3016	1/1	0.92	0.20	66,66,66,66	0
57	MG	2A	3665	1/1	0.92	0.13	70,70,70,70	0
57	MG	2A	3666	1/1	0.92	0.15	72,72,72,72	0
57	MG	2A	3668	1/1	0.92	0.16	56,56,56,56	0
57	MG	1a	1794	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3396	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3376	1/1	0.92	0.21	62,62,62,62	0
57	MG	1A	3537	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3175	1/1	0.92	0.23	65,65,65,65	0
57	MG	1A	3398	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3685	1/1	0.92	0.13	88,88,88,88	0
57	MG	1A	4063	1/1	0.92	0.10	71,71,71,71	0
57	MG	2A	3689	1/1	0.92	0.16	54,54,54,54	0
57	MG	1A	3233	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3388	1/1	0.92	0.25	66,66,66,66	0
57	MG	1A	3787	1/1	0.92	0.33	62,62,62,62	0
57	MG	2A	3696	1/1	0.92	0.13	73,73,73,73	0
57	MG	1A	3788	1/1	0.92	0.20	59,59,59,59	0
57	MG	1A	3341	1/1	0.92	0.15	35,35,35,35	0
57	MG	2a	1729	1/1	0.92	0.16	74,74,74,74	0
57	MG	2A	3395	1/1	0.92	0.20	58,58,58,58	0
57	MG	2A	3396	1/1	0.92	0.18	48,48,48,48	0
57	MG	2A	3397	1/1	0.92	0.28	62,62,62,62	0
57	MG	1a	1805	1/1	0.92	0.25	53,53,53,53	0
57	MG	2A	3187	1/1	0.92	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1745	1/1	0.92	0.11	75,75,75,75	0
57	MG	2A	3714	1/1	0.92	0.09	52,52,52,52	0
57	MG	2A	3188	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	3790	1/1	0.92	0.11	70,70,70,70	0
57	MG	2A	3192	1/1	0.92	0.14	45,45,45,45	0
57	MG	2a	1753	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	4074	1/1	0.92	0.12	62,62,62,62	0
57	MG	1A	3918	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3920	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	4077	1/1	0.92	0.07	61,61,61,61	0
57	MG	1A	3791	1/1	0.92	0.12	40,40,40,40	0
57	MG	1a	1606	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	4083	1/1	0.92	0.17	31,31,31,31	0
57	MG	1e	201	1/1	0.92	0.16	72,72,72,72	0
57	MG	1h	201	1/1	0.92	0.07	66,66,66,66	0
57	MG	2A	3740	1/1	0.92	0.10	62,62,62,62	0
57	MG	2a	1766	1/1	0.92	0.26	61,61,61,61	0
57	MG	1A	3197	1/1	0.92	0.14	39,39,39,39	0
57	MG	2A	3210	1/1	0.92	0.19	63,63,63,63	0
57	MG	2A	3746	1/1	0.92	0.11	55,55,55,55	0
57	MG	1l	3201	1/1	0.92	0.18	60,60,60,60	0
57	MG	1A	3406	1/1	0.92	0.29	41,41,41,41	0
57	MG	2A	3752	1/1	0.92	0.19	71,71,71,71	0
57	MG	2a	1774	1/1	0.92	0.18	68,68,68,68	0
57	MG	1A	3302	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3093	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3126	1/1	0.92	0.17	48,48,48,48	0
57	MG	2a	1778	1/1	0.92	0.21	56,56,56,56	0
57	MG	2A	3218	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3220	1/1	0.92	0.10	63,63,63,63	0
57	MG	1A	4091	1/1	0.92	0.17	40,40,40,40	0
57	MG	1A	3275	1/1	0.92	0.07	53,53,53,53	0
57	MG	2a	1784	1/1	0.92	0.25	65,65,65,65	0
57	MG	1A	3416	1/1	0.92	0.23	67,67,67,67	0
57	MG	1A	4094	1/1	0.92	0.21	42,42,42,42	0
57	MG	1a	1635	1/1	0.92	0.12	49,49,49,49	0
57	MG	1A	3417	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3458	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3938	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3133	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	3942	1/1	0.92	0.09	31,31,31,31	0
57	MG	1a	1641	1/1	0.92	0.16	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	1A	3943	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	1799	1/1	0.92	0.25	60,60,60,60	0
57	MG	1a	1645	1/1	0.92	0.21	54,54,54,54	0
57	MG	2A	3780	1/1	0.92	0.18	67,67,67,67	0
57	MG	2A	3004	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3475	1/1	0.92	0.07	46,46,46,46	0
57	MG	2a	1806	1/1	0.92	0.17	53,53,53,53	0
57	MG	2A	3476	1/1	0.92	0.12	71,71,71,71	0
57	MG	2A	3005	1/1	0.92	0.20	56,56,56,56	0
57	MG	1B	206	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3681	1/1	0.92	0.16	62,62,62,62	0
57	MG	1B	209	1/1	0.92	0.25	57,57,57,57	0
57	MG	1A	3946	1/1	0.92	0.10	28,28,28,28	0
57	MG	1A	3104	1/1	0.92	0.26	29,29,29,29	0
57	MG	1A	3563	1/1	0.92	0.10	25,25,25,25	0
57	MG	1A	3480	1/1	0.92	0.11	52,52,52,52	0
57	MG	2d	301	1/1	0.92	0.10	69,69,69,69	0
57	MG	2A	3027	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3489	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3042	1/1	0.92	0.23	35,35,35,35	0
57	MG	2B	205	1/1	0.92	0.25	57,57,57,57	0
57	MG	2A	3033	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3957	1/1	0.92	0.06	26,26,26,26	0
57	MG	2A	3036	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3038	1/1	0.92	0.18	70,70,70,70	0
57	MG	1A	3698	1/1	0.92	0.08	25,25,25,25	0
57	MG	2B	212	1/1	0.92	0.23	65,65,65,65	0
57	MG	2A	3040	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3041	1/1	0.92	0.16	62,62,62,62	0
57	MG	2A	3505	1/1	0.92	0.19	59,59,59,59	0
57	MG	1A	3816	1/1	0.92	0.32	41,41,41,41	0
57	MG	1A	3817	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3369	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3315	1/1	0.92	0.17	61,61,61,61	0
57	MG	1A	3974	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3051	1/1	0.92	0.20	56,56,56,56	0
57	MG	1a	1669	1/1	0.92	0.21	64,64,64,64	0
57	MG	1A	3579	1/1	0.92	0.08	34,34,34,34	0
57	MG	1A	3582	1/1	0.92	0.11	51,51,51,51	0
57	MG	1D	312	1/1	0.92	0.14	39,39,39,39	0
57	MG	2x	109	1/1	0.92	0.13	70,70,70,70	0
57	MG	1a	1674	1/1	0.92	0.24	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	3520	1/1	0.92	0.12	41,41,41,41	0
57	MG	2E	308	1/1	0.93	0.11	61,61,61,61	0
57	MG	2A	3016	1/1	0.93	0.20	39,39,39,39	0
57	MG	1A	3361	1/1	0.93	0.29	33,33,33,33	0
57	MG	1A	3813	1/1	0.93	0.12	32,32,32,32	0
57	MG	2F	307	1/1	0.93	0.25	51,51,51,51	0
57	MG	1B	205	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	3691	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3948	1/1	0.93	0.13	40,40,40,40	0
57	MG	1a	1643	1/1	0.93	0.23	67,67,67,67	0
57	MG	2A	3029	1/1	0.93	0.22	48,48,48,48	0
57	MG	2Q	201	1/1	0.93	0.08	65,65,65,65	0
57	MG	1a	1644	1/1	0.93	0.12	49,49,49,49	0
57	MG	2R	201	1/1	0.93	0.33	50,50,50,50	0
57	MG	1A	3567	1/1	0.93	0.09	30,30,30,30	0
57	MG	1B	210	1/1	0.93	0.17	51,51,51,51	0
57	MG	1B	211	1/1	0.93	0.27	64,64,64,64	0
57	MG	1B	212	1/1	0.93	0.18	60,60,60,60	0
57	MG	1A	3002	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3951	1/1	0.93	0.15	52,52,52,52	0
57	MG	1a	1653	1/1	0.93	0.23	50,50,50,50	0
57	MG	1a	1656	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3272	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3273	1/1	0.93	0.18	70,70,70,70	0
57	MG	1A	3569	1/1	0.93	0.11	39,39,39,39	0
57	MG	1A	3820	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3059	1/1	0.93	0.19	44,44,44,44	0
57	MG	2A	3049	1/1	0.93	0.15	67,67,67,67	0
57	MG	27	102	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3182	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3578	1/1	0.93	0.17	35,35,35,35	0
57	MG	2A	3052	1/1	0.93	0.16	59,59,59,59	0
57	MG	1A	3487	1/1	0.93	0.18	41,41,41,41	0
57	MG	1A	3581	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3555	1/1	0.93	0.18	50,50,50,50	0
57	MG	2A	3556	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3421	1/1	0.93	0.18	52,52,52,52	0
57	MG	2a	1604	1/1	0.93	0.28	73,73,73,73	0
57	MG	1B	230	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3287	1/1	0.93	0.28	58,58,58,58	0
57	MG	2a	1607	1/1	0.93	0.43	69,69,69,69	0
57	MG	1a	1667	1/1	0.93	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	3063	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3712	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3831	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3978	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3715	1/1	0.93	0.06	20,20,20,20	0
57	MG	1a	1672	1/1	0.93	0.27	70,70,70,70	0
57	MG	1A	3834	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3836	1/1	0.93	0.21	40,40,40,40	0
57	MG	1A	3716	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3075	1/1	0.93	0.15	57,57,57,57	0
57	MG	2A	3076	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3577	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3986	1/1	0.93	0.09	41,41,41,41	0
57	MG	1E	308	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3094	1/1	0.93	0.21	66,66,66,66	0
57	MG	2A	3081	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3583	1/1	0.93	0.09	43,43,43,43	0
57	MG	1a	1685	1/1	0.93	0.23	61,61,61,61	0
57	MG	2A	3585	1/1	0.93	0.27	57,57,57,57	0
57	MG	1A	3006	1/1	0.93	0.17	55,55,55,55	0
57	MG	2A	3589	1/1	0.93	0.12	54,54,54,54	0
57	MG	2A	3308	1/1	0.93	0.25	70,70,70,70	0
57	MG	2A	3084	1/1	0.93	0.09	41,41,41,41	0
57	MG	1a	1687	1/1	0.93	0.32	55,55,55,55	0
57	MG	2A	3595	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3311	1/1	0.93	0.11	65,65,65,65	0
57	MG	1F	303	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3843	1/1	0.93	0.09	31,31,31,31	0
57	MG	1A	3586	1/1	0.93	0.06	33,33,33,33	0
57	MG	2A	3602	1/1	0.93	0.08	31,31,31,31	0
57	MG	1F	307	1/1	0.93	0.09	38,38,38,38	0
57	MG	1a	1693	1/1	0.93	0.13	61,61,61,61	0
57	MG	1F	309	1/1	0.93	0.22	29,29,29,29	0
57	MG	1F	311	1/1	0.93	0.09	46,46,46,46	0
57	MG	2a	1651	1/1	0.93	0.15	67,67,67,67	0
57	MG	2A	3096	1/1	0.93	0.12	62,62,62,62	0
57	MG	1F	312	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	3253	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3590	1/1	0.93	0.08	24,24,24,24	0
57	MG	1A	3316	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3595	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3104	1/1	0.93	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1664	1/1	0.93	0.15	64,64,64,64	0
57	MG	1a	1708	1/1	0.93	0.17	60,60,60,60	0
57	MG	2A	3109	1/1	0.93	0.16	45,45,45,45	0
57	MG	1G	204	1/1	0.93	0.14	62,62,62,62	0
57	MG	2A	3629	1/1	0.93	0.12	61,61,61,61	0
57	MG	2A	3332	1/1	0.93	0.21	39,39,39,39	0
57	MG	1A	4000	1/1	0.93	0.09	33,33,33,33	0
57	MG	2A	3113	1/1	0.93	0.11	52,52,52,52	0
57	MG	2a	1674	1/1	0.93	0.27	59,59,59,59	0
57	MG	2A	3335	1/1	0.93	0.30	62,62,62,62	0
57	MG	2A	3336	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	4006	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3637	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3115	1/1	0.93	0.11	61,61,61,61	0
57	MG	1N	201	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3342	1/1	0.93	0.31	54,54,54,54	0
57	MG	1A	3285	1/1	0.93	0.28	52,52,52,52	0
57	MG	2A	3120	1/1	0.93	0.09	53,53,53,53	0
57	MG	1N	205	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3256	1/1	0.93	0.07	56,56,56,56	0
57	MG	2A	3646	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3124	1/1	0.93	0.25	46,46,46,46	0
57	MG	1A	3505	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3129	1/1	0.93	0.16	41,41,41,41	0
57	MG	2a	1693	1/1	0.93	0.22	65,65,65,65	0
57	MG	1A	3288	1/1	0.93	0.18	42,42,42,42	0
57	MG	2A	3132	1/1	0.93	0.21	64,64,64,64	0
57	MG	1A	3603	1/1	0.93	0.10	32,32,32,32	0
57	MG	1P	203	1/1	0.93	0.27	32,32,32,32	0
57	MG	2A	3657	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3377	1/1	0.93	0.12	37,37,37,37	0
57	MG	1a	1733	1/1	0.93	0.21	71,71,71,71	0
57	MG	2A	3660	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3325	1/1	0.93	0.12	39,39,39,39	0
57	MG	1Q	206	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3142	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	4014	1/1	0.93	0.18	29,29,29,29	0
57	MG	1R	204	1/1	0.93	0.11	30,30,30,30	0
57	MG	2a	1712	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3612	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3147	1/1	0.93	0.08	56,56,56,56	0
57	MG	2A	3674	1/1	0.93	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1741	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3292	1/1	0.93	0.28	47,47,47,47	0
57	MG	1A	3513	1/1	0.93	0.17	50,50,50,50	0
57	MG	1S	202	1/1	0.93	0.10	54,54,54,54	0
57	MG	1a	1746	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3681	1/1	0.93	0.06	40,40,40,40	0
57	MG	1A	3211	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3378	1/1	0.93	0.16	59,59,59,59	0
57	MG	2a	1725	1/1	0.93	0.06	84,84,84,84	0
57	MG	1A	3873	1/1	0.93	0.19	42,42,42,42	0
57	MG	1a	1751	1/1	0.93	0.12	64,64,64,64	0
57	MG	1A	3518	1/1	0.93	0.12	54,54,54,54	0
57	MG	2A	3383	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3875	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3440	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3878	1/1	0.93	0.07	48,48,48,48	0
57	MG	2A	3389	1/1	0.93	0.28	54,54,54,54	0
57	MG	2a	1742	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3703	1/1	0.93	0.09	63,63,63,63	0
57	MG	1A	4036	1/1	0.93	0.15	50,50,50,50	0
57	MG	1A	3767	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3710	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1750	1/1	0.93	0.23	63,63,63,63	0
57	MG	2A	3393	1/1	0.93	0.17	43,43,43,43	0
57	MG	1A	3880	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3330	1/1	0.93	0.17	39,39,39,39	0
57	MG	2A	3170	1/1	0.93	0.18	62,62,62,62	0
57	MG	1a	1770	1/1	0.93	0.09	53,53,53,53	0
57	MG	1X	104	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3116	1/1	0.93	0.26	45,45,45,45	0
57	MG	2A	3727	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3156	1/1	0.93	0.31	35,35,35,35	0
57	MG	1A	3895	1/1	0.93	0.08	53,53,53,53	0
57	MG	10	101	1/1	0.93	0.20	43,43,43,43	0
57	MG	1A	3334	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	4046	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3409	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3389	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	4049	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3780	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3782	1/1	0.93	0.08	34,34,34,34	0
57	MG	2A	3742	1/1	0.93	0.17	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	10	110	1/1	0.93	0.06	42,42,42,42	0
57	MG	1A	3904	1/1	0.93	0.08	74,74,74,74	0
57	MG	2A	3191	1/1	0.93	0.20	56,56,56,56	0
57	MG	1A	3534	1/1	0.93	0.07	40,40,40,40	0
57	MG	1A	3391	1/1	0.93	0.12	36,36,36,36	0
57	MG	1A	3648	1/1	0.93	0.09	20,20,20,20	0
57	MG	2a	1780	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3215	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3910	1/1	0.93	0.19	67,67,67,67	0
57	MG	2A	3197	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	4069	1/1	0.93	0.08	63,63,63,63	0
57	MG	2A	3434	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	4071	1/1	0.93	0.13	59,59,59,59	0
57	MG	2A	3763	1/1	0.93	0.11	60,60,60,60	0
57	MG	2A	3438	1/1	0.93	0.11	69,69,69,69	0
57	MG	15	102	1/1	0.93	0.15	36,36,36,36	0
57	MG	2A	3440	1/1	0.93	0.14	55,55,55,55	0
57	MG	2A	3201	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3203	1/1	0.93	0.23	54,54,54,54	0
57	MG	2A	3445	1/1	0.93	0.11	36,36,36,36	0
57	MG	2A	3204	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3337	1/1	0.93	0.28	36,36,36,36	0
57	MG	2A	3206	1/1	0.93	0.26	45,45,45,45	0
57	MG	1A	3297	1/1	0.93	0.21	58,58,58,58	0
57	MG	2A	3778	1/1	0.93	0.07	60,60,60,60	0
57	MG	16	101	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3166	1/1	0.93	0.18	60,60,60,60	0
57	MG	18	105	1/1	0.93	0.16	50,50,50,50	0
57	MG	18	106	1/1	0.93	0.17	53,53,53,53	0
57	MG	2A	3466	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3544	1/1	0.93	0.13	27,27,27,27	0
57	MG	1A	3919	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3472	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3665	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	3792	1/1	0.93	0.07	28,28,28,28	0
57	MG	1A	3465	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3300	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3925	1/1	0.93	0.14	56,56,56,56	0
57	MG	2B	201	1/1	0.93	0.18	69,69,69,69	0
57	MG	1a	1608	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3224	1/1	0.93	0.34	65,65,65,65	0
57	MG	1A	3342	1/1	0.93	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3343	1/1	0.93	0.11	45,45,45,45	0
57	MG	1x	102	1/1	0.93	0.17	70,70,70,70	0
57	MG	1A	3469	1/1	0.93	0.24	29,29,29,29	0
57	MG	1A	3273	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3407	1/1	0.93	0.17	43,43,43,43	0
57	MG	2A	3232	1/1	0.93	0.12	66,66,66,66	0
57	MG	1A	3303	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	3304	1/1	0.93	0.21	45,45,45,45	0
57	MG	1x	109	1/1	0.93	0.29	71,71,71,71	0
57	MG	1A	3176	1/1	0.93	0.17	48,48,48,48	0
57	MG	1a	1627	1/1	0.93	0.27	63,63,63,63	0
57	MG	1A	4097	1/1	0.93	0.08	46,46,46,46	0
57	MG	1y	101	1/1	0.93	0.13	55,55,55,55	0
57	MG	1a	1630	1/1	0.93	0.48	71,71,71,71	0
57	MG	1a	1633	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3359	1/1	0.93	0.27	36,36,36,36	0
57	MG	2x	106	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	4100	1/1	0.93	0.26	53,53,53,53	0
57	MG	2A	3008	1/1	0.93	0.21	49,49,49,49	0
57	MG	1A	3686	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3251	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3015	1/1	0.93	0.21	58,58,58,58	0
59	TYK	2A	3798	64/64	0.93	0.11	32,46,61,66	0
57	MG	1A	3554	1/1	0.94	0.19	63,63,63,63	0
57	MG	2A	3172	1/1	0.94	0.10	56,56,56,56	0
57	MG	27	101	1/1	0.94	0.24	59,59,59,59	0
57	MG	1e	202	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3682	1/1	0.94	0.10	57,57,57,57	0
57	MG	1B	219	1/1	0.94	0.09	34,34,34,34	0
57	MG	1a	1631	1/1	0.94	0.19	59,59,59,59	0
57	MG	2A	3601	1/1	0.94	0.11	68,68,68,68	0
57	MG	1A	3241	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3178	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3195	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3362	1/1	0.94	0.08	50,50,50,50	0
57	MG	1B	222	1/1	0.94	0.12	56,56,56,56	0
57	MG	1B	223	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3611	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3070	1/1	0.94	0.06	33,33,33,33	0
57	MG	1B	226	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3471	1/1	0.94	0.32	40,40,40,40	0
57	MG	1A	3826	1/1	0.94	0.11	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	2A	3372	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3189	1/1	0.94	0.16	64,64,64,64	0
57	MG	2A	3622	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3625	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3375	1/1	0.94	0.09	69,69,69,69	0
57	MG	1A	3403	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3828	1/1	0.94	0.22	38,38,38,38	0
57	MG	1A	3695	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3244	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3344	1/1	0.94	0.21	45,45,45,45	0
57	MG	1D	309	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3566	1/1	0.94	0.07	52,52,52,52	0
57	MG	2a	1627	1/1	0.94	0.23	45,45,45,45	0
57	MG	1a	1649	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3476	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3077	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	3408	1/1	0.94	0.21	46,46,46,46	0
57	MG	2A	3391	1/1	0.94	0.19	61,61,61,61	0
57	MG	2A	3003	1/1	0.94	0.23	57,57,57,57	0
57	MG	1a	1655	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3838	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3022	1/1	0.94	0.04	17,17,17,17	0
57	MG	1A	3571	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3011	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3411	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3014	1/1	0.94	0.11	50,50,50,50	0
57	MG	2A	3212	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3401	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3402	1/1	0.94	0.24	71,71,71,71	0
57	MG	2a	1646	1/1	0.94	0.26	61,61,61,61	0
57	MG	1A	3994	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3050	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3845	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3353	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3202	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	3719	1/1	0.94	0.08	38,38,38,38	0
57	MG	2a	1653	1/1	0.94	0.12	47,47,47,47	0
57	MG	2A	3661	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3219	1/1	0.94	0.14	49,49,49,49	0
57	MG	2a	1656	1/1	0.94	0.26	63,63,63,63	0
57	MG	1A	3486	1/1	0.94	0.25	43,43,43,43	0
57	MG	2a	1658	1/1	0.94	0.21	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	313	1/1	0.94	0.16	32,32,32,32	0
57	MG	2A	3028	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3052	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3360	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3856	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3725	1/1	0.94	0.12	27,27,27,27	0
57	MG	2a	1667	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3490	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3103	1/1	0.94	0.29	34,34,34,34	0
57	MG	1a	1675	1/1	0.94	0.36	58,58,58,58	0
57	MG	1a	1676	1/1	0.94	0.07	73,73,73,73	0
57	MG	1a	1677	1/1	0.94	0.22	41,41,41,41	0
57	MG	2A	3432	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3683	1/1	0.94	0.13	72,72,72,72	0
57	MG	2A	3684	1/1	0.94	0.19	50,50,50,50	0
57	MG	2A	3433	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3042	1/1	0.94	0.21	36,36,36,36	0
57	MG	2A	3435	1/1	0.94	0.17	69,69,69,69	0
57	MG	2a	1681	1/1	0.94	0.19	35,35,35,35	0
57	MG	2a	1682	1/1	0.94	0.35	60,60,60,60	0
57	MG	1A	3492	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3208	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3694	1/1	0.94	0.12	64,64,64,64	0
57	MG	1a	1680	1/1	0.94	0.24	40,40,40,40	0
57	MG	1a	1681	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3254	1/1	0.94	0.13	34,34,34,34	0
57	MG	2A	3442	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3443	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3255	1/1	0.94	0.13	46,46,46,46	0
57	MG	2A	3704	1/1	0.94	0.07	72,72,72,72	0
57	MG	1A	3127	1/1	0.94	0.24	41,41,41,41	0
57	MG	1A	4025	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3053	1/1	0.94	0.17	58,58,58,58	0
57	MG	1A	4027	1/1	0.94	0.14	49,49,49,49	0
57	MG	2A	3712	1/1	0.94	0.11	40,40,40,40	0
57	MG	2A	3452	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3056	1/1	0.94	0.16	73,73,73,73	0
57	MG	1A	3499	1/1	0.94	0.07	58,58,58,58	0
57	MG	2a	1703	1/1	0.94	0.18	64,64,64,64	0
57	MG	2A	3719	1/1	0.94	0.07	56,56,56,56	0
57	MG	2a	1706	1/1	0.94	0.17	61,61,61,61	0
57	MG	2A	3249	1/1	0.94	0.16	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	1P	201	1/1	0.94	0.27	32,32,32,32	0
57	MG	1A	3167	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3060	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3061	1/1	0.94	0.09	37,37,37,37	0
57	MG	1P	204	1/1	0.94	0.35	28,28,28,28	0
57	MG	1A	3750	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3501	1/1	0.94	0.24	32,32,32,32	0
57	MG	2a	1715	1/1	0.94	0.45	60,60,60,60	0
57	MG	1Q	205	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3174	1/1	0.94	0.10	32,32,32,32	0
57	MG	1A	3129	1/1	0.94	0.11	39,39,39,39	0
57	MG	2A	3068	1/1	0.94	0.25	44,44,44,44	0
57	MG	1A	3610	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3611	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3072	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3763	1/1	0.94	0.06	32,32,32,32	0
57	MG	1A	3882	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3429	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3613	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3177	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3216	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3004	1/1	0.94	0.10	25,25,25,25	0
57	MG	2A	3755	1/1	0.94	0.17	62,62,62,62	0
57	MG	2a	1733	1/1	0.94	0.13	72,72,72,72	0
57	MG	1A	4048	1/1	0.94	0.13	61,61,61,61	0
57	MG	2a	1735	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3771	1/1	0.94	0.18	73,73,73,73	0
57	MG	2A	3758	1/1	0.94	0.19	50,50,50,50	0
57	MG	2a	1741	1/1	0.94	0.10	77,77,77,77	0
57	MG	1A	3038	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3499	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3903	1/1	0.94	0.10	61,61,61,61	0
57	MG	1V	201	1/1	0.94	0.13	28,28,28,28	0
57	MG	1a	1729	1/1	0.94	0.26	45,45,45,45	0
57	MG	1V	204	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3516	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3627	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3779	1/1	0.94	0.08	30,30,30,30	0
57	MG	1a	1736	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3180	1/1	0.94	0.13	50,50,50,50	0
57	MG	2A	3510	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3511	1/1	0.94	0.12	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	3435	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3524	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3912	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3525	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3782	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3379	1/1	0.94	0.25	47,47,47,47	0
57	MG	1A	3645	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3917	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3110	1/1	0.94	0.17	35,35,35,35	0
57	MG	2A	3107	1/1	0.94	0.10	70,70,70,70	0
57	MG	2A	3790	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3327	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3531	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3793	1/1	0.94	0.07	64,64,64,64	0
57	MG	2A	3524	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3111	1/1	0.94	0.23	57,57,57,57	0
57	MG	2A	3300	1/1	0.94	0.11	64,64,64,64	0
57	MG	1a	1749	1/1	0.94	0.08	73,73,73,73	0
57	MG	1A	3649	1/1	0.94	0.05	28,28,28,28	0
57	MG	2A	3532	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	4079	1/1	0.94	0.08	48,48,48,48	0
57	MG	1a	1754	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	4082	1/1	0.94	0.29	33,33,33,33	0
57	MG	2A	3118	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1786	1/1	0.94	0.18	68,68,68,68	0
57	MG	2B	207	1/1	0.94	0.09	65,65,65,65	0
57	MG	1l	105	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3147	1/1	0.94	0.26	38,38,38,38	0
57	MG	1A	3224	1/1	0.94	0.20	50,50,50,50	0
57	MG	2A	3545	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3111	1/1	0.94	0.16	39,39,39,39	0
57	MG	1A	3447	1/1	0.94	0.23	50,50,50,50	0
57	MG	1A	4087	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3660	1/1	0.94	0.06	16,16,16,16	0
57	MG	1A	3929	1/1	0.94	0.08	65,65,65,65	0
57	MG	2B	217	1/1	0.94	0.32	71,71,71,71	0
57	MG	1A	3661	1/1	0.94	0.13	46,46,46,46	0
57	MG	2a	1802	1/1	0.94	0.19	55,55,55,55	0
57	MG	2B	219	1/1	0.94	0.13	62,62,62,62	0
57	MG	2D	301	1/1	0.94	0.08	42,42,42,42	0
57	MG	1A	3797	1/1	0.94	0.06	36,36,36,36	0
57	MG	1A	3332	1/1	0.94	0.32	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	2A	3136	1/1	0.94	0.11	32,32,32,32	0
57	MG	2a	1809	1/1	0.94	0.13	78,78,78,78	0
57	MG	1A	3234	1/1	0.94	0.09	52,52,52,52	0
57	MG	1a	1783	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3390	1/1	0.94	0.22	37,37,37,37	0
57	MG	2E	302	1/1	0.94	0.11	55,55,55,55	0
57	MG	1a	1790	1/1	0.94	0.25	74,74,74,74	0
57	MG	2a	1817	1/1	0.94	0.14	54,54,54,54	0
57	MG	2E	305	1/1	0.94	0.10	63,63,63,63	0
57	MG	2A	3141	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	4096	1/1	0.94	0.09	50,50,50,50	0
57	MG	2d	302	1/1	0.94	0.22	56,56,56,56	0
57	MG	2A	3327	1/1	0.94	0.17	39,39,39,39	0
57	MG	19	101	1/1	0.94	0.20	52,52,52,52	0
57	MG	2F	301	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3458	1/1	0.94	0.07	55,55,55,55	0
57	MG	2F	303	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3940	1/1	0.94	0.17	51,51,51,51	0
57	MG	2F	306	1/1	0.94	0.16	48,48,48,48	0
57	MG	2q	201	1/1	0.94	0.09	77,77,77,77	0
57	MG	1A	3941	1/1	0.94	0.13	18,18,18,18	0
57	MG	2t	201	1/1	0.94	0.12	58,58,58,58	0
57	MG	1a	1797	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3187	1/1	0.94	0.35	37,37,37,37	0
57	MG	1A	3460	1/1	0.94	0.06	51,51,51,51	0
57	MG	1A	3672	1/1	0.94	0.18	63,63,63,63	0
57	MG	2A	3575	1/1	0.94	0.13	60,60,60,60	0
57	MG	1A	3673	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3809	1/1	0.94	0.19	45,45,45,45	0
57	MG	2w	105	1/1	0.94	0.20	51,51,51,51	0
57	MG	1a	1612	1/1	0.94	0.16	66,66,66,66	0
57	MG	1a	1613	1/1	0.94	0.11	62,62,62,62	0
57	MG	1A	3392	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3189	1/1	0.94	0.35	38,38,38,38	0
57	MG	1a	1808	1/1	0.94	0.13	67,67,67,67	0
57	MG	1a	1616	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3549	1/1	0.94	0.38	59,59,59,59	0
57	MG	1A	3112	1/1	0.94	0.18	30,30,30,30	0
57	MG	2A	3588	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3953	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3115	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3956	1/1	0.94	0.18	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	1A	3512	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3592	1/1	0.94	0.12	36,36,36,36	0
60	ZN	24	501	1/1	0.94	0.14	126,126,126,126	0
57	MG	1A	3024	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3075	1/1	0.95	0.13	33,33,33,33	0
57	MG	2A	3669	1/1	0.95	0.13	73,73,73,73	0
57	MG	2A	3670	1/1	0.95	0.10	48,48,48,48	0
57	MG	1a	1750	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3672	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3226	1/1	0.95	0.19	31,31,31,31	0
57	MG	2A	3456	1/1	0.95	0.16	51,51,51,51	0
57	MG	2A	3265	1/1	0.95	0.11	60,60,60,60	0
57	MG	2A	3677	1/1	0.95	0.06	60,60,60,60	0
57	MG	17	105	1/1	0.95	0.09	50,50,50,50	0
57	MG	18	103	1/1	0.95	0.16	33,33,33,33	0
57	MG	1A	3231	1/1	0.95	0.22	42,42,42,42	0
57	MG	2a	1641	1/1	0.95	0.16	67,67,67,67	0
57	MG	2A	3269	1/1	0.95	0.16	66,66,66,66	0
57	MG	1a	1756	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3833	1/1	0.95	0.15	32,32,32,32	0
57	MG	2a	1645	1/1	0.95	0.13	70,70,70,70	0
57	MG	1A	3968	1/1	0.95	0.05	37,37,37,37	0
57	MG	2A	3686	1/1	0.95	0.06	55,55,55,55	0
57	MG	2A	3471	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3688	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3098	1/1	0.95	0.15	49,49,49,49	0
57	MG	1A	3415	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3972	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3835	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3076	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3103	1/1	0.95	0.38	68,68,68,68	0
57	MG	1A	3289	1/1	0.95	0.38	56,56,56,56	0
57	MG	2A	3698	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3291	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3130	1/1	0.95	0.08	42,42,42,42	0
57	MG	1A	3503	1/1	0.95	0.10	44,44,44,44	0
57	MG	1a	1609	1/1	0.95	0.32	56,56,56,56	0
57	MG	2A	3705	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3706	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3734	1/1	0.95	0.06	27,27,27,27	0
57	MG	1a	1782	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3983	1/1	0.95	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3606	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3737	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3493	1/1	0.95	0.07	64,64,64,64	0
57	MG	1A	3351	1/1	0.95	0.23	47,47,47,47	0
57	MG	2A	3117	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3352	1/1	0.95	0.07	47,47,47,47	0
57	MG	1a	1793	1/1	0.95	0.17	65,65,65,65	0
57	MG	1a	1620	1/1	0.95	0.07	50,50,50,50	0
57	MG	2a	1678	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3851	1/1	0.95	0.06	24,24,24,24	0
57	MG	1A	3508	1/1	0.95	0.18	36,36,36,36	0
57	MG	1A	3745	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3126	1/1	0.95	0.15	61,61,61,61	0
57	MG	1A	3101	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3186	1/1	0.95	0.27	33,33,33,33	0
57	MG	2A	3734	1/1	0.95	0.07	24,24,24,24	0
57	MG	1D	302	1/1	0.95	0.23	40,40,40,40	0
57	MG	1a	1628	1/1	0.95	0.11	43,43,43,43	0
57	MG	1D	303	1/1	0.95	0.17	39,39,39,39	0
57	MG	1D	305	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3512	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3102	1/1	0.95	0.20	40,40,40,40	0
57	MG	1A	3998	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3143	1/1	0.95	0.24	39,39,39,39	0
57	MG	1A	3753	1/1	0.95	0.10	22,22,22,22	0
57	MG	1E	303	1/1	0.95	0.17	36,36,36,36	0
57	MG	2A	3312	1/1	0.95	0.25	69,69,69,69	0
57	MG	2A	3751	1/1	0.95	0.07	65,65,65,65	0
57	MG	1A	4005	1/1	0.95	0.08	26,26,26,26	0
57	MG	1A	3035	1/1	0.95	0.07	29,29,29,29	0
57	MG	2a	1701	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3862	1/1	0.95	0.13	47,47,47,47	0
57	MG	1a	1813	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3145	1/1	0.95	0.38	39,39,39,39	0
57	MG	1A	3146	1/1	0.95	0.16	34,34,34,34	0
57	MG	1F	301	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3527	1/1	0.95	0.12	59,59,59,59	0
57	MG	1F	302	1/1	0.95	0.11	33,33,33,33	0
57	MG	1A	3366	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3626	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3760	1/1	0.95	0.07	24,24,24,24	0
57	MG	2A	3533	1/1	0.95	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3534	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3871	1/1	0.95	0.10	24,24,24,24	0
57	MG	1r	101	1/1	0.95	0.11	69,69,69,69	0
57	MG	1F	308	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3773	1/1	0.95	0.14	70,70,70,70	0
57	MG	1A	3081	1/1	0.95	0.18	37,37,37,37	0
57	MG	2A	3540	1/1	0.95	0.08	48,48,48,48	0
57	MG	1w	102	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	4017	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3764	1/1	0.95	0.36	30,30,30,30	0
57	MG	2A	3331	1/1	0.95	0.32	48,48,48,48	0
57	MG	2A	3546	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3048	1/1	0.95	0.10	27,27,27,27	0
57	MG	2a	1727	1/1	0.95	0.09	71,71,71,71	0
57	MG	1A	3108	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3370	1/1	0.95	0.15	52,52,52,52	0
57	MG	1A	3768	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3036	1/1	0.95	0.15	28,28,28,28	0
57	MG	1x	105	1/1	0.95	0.16	63,63,63,63	0
57	MG	2A	3789	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3306	1/1	0.95	0.29	58,58,58,58	0
57	MG	2a	1738	1/1	0.95	0.06	75,75,75,75	0
57	MG	1G	205	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3443	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3200	1/1	0.95	0.10	36,36,36,36	0
57	MG	1x	110	1/1	0.95	0.07	22,22,22,22	0
57	MG	1a	1664	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	4031	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3179	1/1	0.95	0.37	65,65,65,65	0
57	MG	1A	3249	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3775	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3892	1/1	0.95	0.12	62,62,62,62	0
57	MG	1O	203	1/1	0.95	0.18	55,55,55,55	0
57	MG	1A	3201	1/1	0.95	0.14	49,49,49,49	0
57	MG	2a	1755	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3186	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3777	1/1	0.95	0.06	26,26,26,26	0
57	MG	2A	3569	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3310	1/1	0.95	0.12	51,51,51,51	0
57	MG	2a	1760	1/1	0.95	0.19	54,54,54,54	0
57	MG	1A	3312	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3010	1/1	0.95	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3781	1/1	0.95	0.08	31,31,31,31	0
57	MG	1A	3452	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3060	1/1	0.95	0.18	39,39,39,39	0
57	MG	1A	3029	1/1	0.95	0.28	31,31,31,31	0
57	MG	1A	3457	1/1	0.95	0.17	39,39,39,39	0
57	MG	1A	3113	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3581	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3160	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3020	1/1	0.95	0.14	49,49,49,49	0
57	MG	2A	3022	1/1	0.95	0.28	47,47,47,47	0
57	MG	1R	202	1/1	0.95	0.19	37,37,37,37	0
57	MG	1A	3548	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3202	1/1	0.95	0.18	50,50,50,50	0
57	MG	2D	307	1/1	0.95	0.15	68,68,68,68	0
57	MG	1a	1683	1/1	0.95	0.17	55,55,55,55	0
57	MG	1A	3911	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3383	1/1	0.95	0.24	54,54,54,54	0
57	MG	1A	3318	1/1	0.95	0.25	54,54,54,54	0
57	MG	1A	3209	1/1	0.95	0.30	44,44,44,44	0
57	MG	2A	3381	1/1	0.95	0.18	50,50,50,50	0
57	MG	2A	3208	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3031	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3384	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	3669	1/1	0.95	0.07	61,61,61,61	0
57	MG	2A	3211	1/1	0.95	0.11	49,49,49,49	0
57	MG	2a	1789	1/1	0.95	0.10	60,60,60,60	0
57	MG	2A	3387	1/1	0.95	0.14	53,53,53,53	0
57	MG	2F	304	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3386	1/1	0.95	0.06	48,48,48,48	0
57	MG	1A	3555	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	3114	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	4070	1/1	0.95	0.10	45,45,45,45	0
57	MG	2a	1796	1/1	0.95	0.22	63,63,63,63	0
57	MG	1A	3051	1/1	0.95	0.08	54,54,54,54	0
57	MG	1a	1695	1/1	0.95	0.20	43,43,43,43	0
57	MG	2O	201	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3322	1/1	0.95	0.32	39,39,39,39	0
57	MG	1A	3676	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3091	1/1	0.95	0.09	32,32,32,32	0
57	MG	2Q	202	1/1	0.95	0.22	47,47,47,47	0
57	MG	1V	203	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3092	1/1	0.95	0.15	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	2A	3618	1/1	0.95	0.08	47,47,47,47	0
57	MG	2A	3619	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3562	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	1707	1/1	0.95	0.14	65,65,65,65	0
57	MG	1A	3393	1/1	0.95	0.17	47,47,47,47	0
57	MG	1W	204	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3267	1/1	0.95	0.16	34,34,34,34	0
57	MG	20	101	1/1	0.95	0.07	63,63,63,63	0
57	MG	1a	1712	1/1	0.95	0.06	31,31,31,31	0
57	MG	1a	1716	1/1	0.95	0.07	69,69,69,69	0
57	MG	1A	3806	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	4080	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3632	1/1	0.95	0.06	61,61,61,61	0
57	MG	1A	3931	1/1	0.95	0.07	72,72,72,72	0
57	MG	2A	3234	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3119	1/1	0.95	0.20	32,32,32,32	0
57	MG	1a	1721	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3237	1/1	0.95	0.30	53,53,53,53	0
57	MG	1A	3329	1/1	0.95	0.17	54,54,54,54	0
57	MG	1A	3397	1/1	0.95	0.16	42,42,42,42	0
57	MG	1a	1726	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3241	1/1	0.95	0.23	63,63,63,63	0
57	MG	1A	3272	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3812	1/1	0.95	0.12	18,18,18,18	0
57	MG	1A	3173	1/1	0.95	0.08	20,20,20,20	0
57	MG	1A	3217	1/1	0.95	0.10	22,22,22,22	0
57	MG	2A	3429	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3574	1/1	0.95	0.13	13,13,13,13	0
57	MG	2A	3649	1/1	0.95	0.07	51,51,51,51	0
57	MG	11	101	1/1	0.95	0.41	39,39,39,39	0
57	MG	2A	3651	1/1	0.95	0.12	51,51,51,51	0
57	MG	2w	107	1/1	0.95	0.21	70,70,70,70	0
57	MG	1A	3402	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	3577	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3654	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3120	1/1	0.95	0.25	35,35,35,35	0
57	MG	1A	3066	1/1	0.95	0.18	31,31,31,31	0
57	MG	1A	3705	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3005	1/1	0.95	0.09	45,45,45,45	0
57	MG	13	103	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3824	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3336	1/1	0.95	0.08	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	3280	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3095	1/1	0.95	0.06	42,42,42,42	0
59	TYK	1A	4101	64/64	0.95	0.09	16,30,46,51	0
57	MG	1A	3713	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3447	1/1	0.95	0.10	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.18	33,33,33,33	0
57	MG	1a	1699	1/1	0.96	0.20	51,51,51,51	0
57	MG	2A	3048	1/1	0.96	0.09	48,48,48,48	0
57	MG	1U	207	1/1	0.96	0.24	38,38,38,38	0
57	MG	2a	1625	1/1	0.96	0.07	86,86,86,86	0
57	MG	2A	3437	1/1	0.96	0.05	33,33,33,33	0
57	MG	1a	1701	1/1	0.96	0.17	38,38,38,38	0
57	MG	1A	3453	1/1	0.96	0.27	48,48,48,48	0
57	MG	1A	3175	1/1	0.96	0.06	38,38,38,38	0
57	MG	1a	1705	1/1	0.96	0.11	55,55,55,55	0
57	MG	2A	3054	1/1	0.96	0.11	45,45,45,45	0
57	MG	1a	1706	1/1	0.96	0.31	63,63,63,63	0
57	MG	1A	3932	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3818	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3078	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3298	1/1	0.96	0.21	39,39,39,39	0
57	MG	1A	3937	1/1	0.96	0.10	53,53,53,53	0
57	MG	1a	1713	1/1	0.96	0.12	37,37,37,37	0
57	MG	2A	3451	1/1	0.96	0.09	42,42,42,42	0
57	MG	1a	1715	1/1	0.96	0.14	57,57,57,57	0
57	MG	2A	3250	1/1	0.96	0.21	57,57,57,57	0
57	MG	1A	3720	1/1	0.96	0.07	29,29,29,29	0
57	MG	1W	205	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3682	1/1	0.96	0.07	67,67,67,67	0
57	MG	2A	3459	1/1	0.96	0.13	38,38,38,38	0
57	MG	1W	206	1/1	0.96	0.13	28,28,28,28	0
57	MG	2A	3461	1/1	0.96	0.10	57,57,57,57	0
57	MG	2A	3462	1/1	0.96	0.07	31,31,31,31	0
57	MG	1X	102	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3721	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3465	1/1	0.96	0.06	60,60,60,60	0
57	MG	1X	105	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3530	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3693	1/1	0.96	0.13	71,71,71,71	0
57	MG	2A	3468	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3117	1/1	0.96	0.22	37,37,37,37	0
57	MG	1a	1725	1/1	0.96	0.07	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	3614	1/1	0.96	0.16	50,50,50,50	0
57	MG	1Z	302	1/1	0.96	0.25	47,47,47,47	0
57	MG	1A	3615	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3701	1/1	0.96	0.04	46,46,46,46	0
57	MG	1A	3726	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3616	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3080	1/1	0.96	0.11	34,34,34,34	0
57	MG	10	106	1/1	0.96	0.27	64,64,64,64	0
57	MG	1A	3733	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3399	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	3619	1/1	0.96	0.08	19,19,19,19	0
57	MG	1A	4090	1/1	0.96	0.31	31,31,31,31	0
57	MG	2a	1672	1/1	0.96	0.14	56,56,56,56	0
57	MG	1A	3346	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3301	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3148	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3488	1/1	0.96	0.10	52,52,52,52	0
57	MG	2A	3715	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3955	1/1	0.96	0.08	16,16,16,16	0
57	MG	2A	3089	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3090	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3625	1/1	0.96	0.05	21,21,21,21	0
57	MG	1A	3021	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3726	1/1	0.96	0.06	61,61,61,61	0
57	MG	1A	3181	1/1	0.96	0.15	39,39,39,39	0
57	MG	2A	3280	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	4098	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3631	1/1	0.96	0.05	17,17,17,17	0
57	MG	1A	3009	1/1	0.96	0.04	22,22,22,22	0
57	MG	1A	3963	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3964	1/1	0.96	0.10	24,24,24,24	0
57	MG	2A	3736	1/1	0.96	0.05	56,56,56,56	0
57	MG	1A	3965	1/1	0.96	0.05	32,32,32,32	0
57	MG	15	105	1/1	0.96	0.13	43,43,43,43	0
57	MG	2a	1694	1/1	0.96	0.16	63,63,63,63	0
57	MG	1A	3749	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3543	1/1	0.96	0.18	55,55,55,55	0
57	MG	17	101	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3105	1/1	0.96	0.23	55,55,55,55	0
57	MG	1A	3847	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3744	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3354	1/1	0.96	0.20	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	2A	3747	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3108	1/1	0.96	0.12	40,40,40,40	0
57	MG	18	101	1/1	0.96	0.18	53,53,53,53	0
57	MG	2a	1705	1/1	0.96	0.16	44,44,44,44	0
57	MG	2A	3750	1/1	0.96	0.07	59,59,59,59	0
57	MG	18	102	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3973	1/1	0.96	0.04	54,54,54,54	0
57	MG	18	104	1/1	0.96	0.18	41,41,41,41	0
57	MG	1a	1771	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3183	1/1	0.96	0.19	45,45,45,45	0
57	MG	1a	1775	1/1	0.96	0.06	62,62,62,62	0
57	MG	1A	3154	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3473	1/1	0.96	0.30	38,38,38,38	0
57	MG	1A	3155	1/1	0.96	0.14	27,27,27,27	0
57	MG	2A	3525	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3260	1/1	0.96	0.29	47,47,47,47	0
57	MG	1A	3980	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3063	1/1	0.96	0.04	31,31,31,31	0
57	MG	2A	3122	1/1	0.96	0.09	44,44,44,44	0
57	MG	1a	1784	1/1	0.96	0.07	46,46,46,46	0
57	MG	1a	1785	1/1	0.96	0.10	59,59,59,59	0
57	MG	1a	1788	1/1	0.96	0.20	50,50,50,50	0
57	MG	2A	3770	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3761	1/1	0.96	0.10	20,20,20,20	0
57	MG	1A	3762	1/1	0.96	0.05	37,37,37,37	0
57	MG	2A	3130	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3984	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3311	1/1	0.96	0.13	54,54,54,54	0
57	MG	2A	3133	1/1	0.96	0.15	60,60,60,60	0
57	MG	1A	3650	1/1	0.96	0.07	61,61,61,61	0
57	MG	1B	225	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3988	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3781	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3263	1/1	0.96	0.20	39,39,39,39	0
57	MG	1A	3266	1/1	0.96	0.23	28,28,28,28	0
57	MG	1A	3041	1/1	0.96	0.16	30,30,30,30	0
57	MG	1A	3017	1/1	0.96	0.15	28,28,28,28	0
57	MG	1A	3658	1/1	0.96	0.12	31,31,31,31	0
57	MG	2a	1744	1/1	0.96	0.17	64,64,64,64	0
57	MG	1a	1621	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3659	1/1	0.96	0.04	23,23,23,23	0
57	MG	1a	1803	1/1	0.96	0.07	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	3145	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3483	1/1	0.96	0.14	35,35,35,35	0
57	MG	1B	234	1/1	0.96	0.06	37,37,37,37	0
57	MG	2a	1752	1/1	0.96	0.09	53,53,53,53	0
57	MG	2A	3148	1/1	0.96	0.25	46,46,46,46	0
57	MG	1D	301	1/1	0.96	0.16	36,36,36,36	0
57	MG	2A	3150	1/1	0.96	0.13	63,63,63,63	0
57	MG	2A	3338	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3772	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3054	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3662	1/1	0.96	0.06	27,27,27,27	0
57	MG	1D	308	1/1	0.96	0.11	47,47,47,47	0
57	MG	1A	3420	1/1	0.96	0.17	43,43,43,43	0
57	MG	1D	310	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	4001	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	4003	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3191	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3877	1/1	0.96	0.14	33,33,33,33	0
57	MG	2a	1767	1/1	0.96	0.39	69,69,69,69	0
57	MG	2A	3571	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3274	1/1	0.96	0.07	37,37,37,37	0
57	MG	1E	306	1/1	0.96	0.11	23,23,23,23	0
57	MG	1A	3778	1/1	0.96	0.09	28,28,28,28	0
57	MG	1a	1640	1/1	0.96	0.34	61,61,61,61	0
57	MG	1m	3001	1/1	0.96	0.13	58,58,58,58	0
57	MG	2A	3169	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3228	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3230	1/1	0.96	0.23	28,28,28,28	0
57	MG	1A	3192	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3883	1/1	0.96	0.09	45,45,45,45	0
57	MG	1w	101	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3376	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3323	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3888	1/1	0.96	0.06	70,70,70,70	0
57	MG	2A	3587	1/1	0.96	0.15	68,68,68,68	0
57	MG	1A	3891	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3232	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3366	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3893	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3109	1/1	0.96	0.05	33,33,33,33	0
57	MG	1A	3573	1/1	0.96	0.07	35,35,35,35	0
57	MG	2A	3370	1/1	0.96	0.16	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	2A	3183	1/1	0.96	0.19	56,56,56,56	0
57	MG	1a	1654	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3194	1/1	0.96	0.07	22,22,22,22	0
57	MG	1A	3161	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3600	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3027	1/1	0.96	0.32	32,32,32,32	0
57	MG	1A	3902	1/1	0.96	0.06	47,47,47,47	0
57	MG	1G	201	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3071	1/1	0.96	0.33	47,47,47,47	0
57	MG	1A	4032	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3436	1/1	0.96	0.14	46,46,46,46	0
57	MG	2A	3607	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	4034	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3610	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3504	1/1	0.96	0.22	37,37,37,37	0
57	MG	1A	3132	1/1	0.96	0.15	29,29,29,29	0
57	MG	2Q	203	1/1	0.96	0.05	48,48,48,48	0
57	MG	1A	3506	1/1	0.96	0.17	34,34,34,34	0
57	MG	1A	3689	1/1	0.96	0.08	56,56,56,56	0
57	MG	2A	3006	1/1	0.96	0.06	40,40,40,40	0
57	MG	2a	1813	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	3073	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3046	1/1	0.96	0.06	35,35,35,35	0
57	MG	1O	202	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3387	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	1819	1/1	0.96	0.07	69,69,69,69	0
57	MG	1A	3290	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3623	1/1	0.96	0.12	69,69,69,69	0
57	MG	2X	101	1/1	0.96	0.06	65,65,65,65	0
57	MG	1A	3169	1/1	0.96	0.26	29,29,29,29	0
57	MG	1A	4045	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3593	1/1	0.96	0.07	22,22,22,22	0
57	MG	1P	202	1/1	0.96	0.22	26,26,26,26	0
57	MG	23	102	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3172	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3596	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3047	1/1	0.96	0.17	34,34,34,34	0
57	MG	1Q	201	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3028	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3706	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	4052	1/1	0.96	0.05	50,50,50,50	0
57	MG	1A	4054	1/1	0.96	0.12	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	1A	4056	1/1	0.96	0.07	50,50,50,50	0
57	MG	2w	101	1/1	0.96	0.22	66,66,66,66	0
57	MG	1A	4057	1/1	0.96	0.07	51,51,51,51	0
57	MG	28	105	1/1	0.96	0.08	63,63,63,63	0
57	MG	2A	3411	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	4058	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3032	1/1	0.96	0.07	25,25,25,25	0
57	MG	1A	3450	1/1	0.96	0.05	43,43,43,43	0
57	MG	2A	3034	1/1	0.96	0.21	60,60,60,60	0
57	MG	2A	3416	1/1	0.96	0.09	35,35,35,35	0
57	MG	1a	1689	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3522	1/1	0.96	0.28	38,38,38,38	0
57	MG	1A	4061	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3420	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	4062	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3451	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3926	1/1	0.96	0.14	61,61,61,61	0
57	MG	2A	3228	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3604	1/1	0.96	0.07	29,29,29,29	0
57	MG	2a	1615	1/1	0.96	0.32	62,62,62,62	0
57	MG	1A	3207	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3714	1/1	0.96	0.08	51,51,51,51	0
60	ZN	2Y	202	1/1	0.96	0.05	105,105,105,105	0
57	MG	2A	3045	1/1	0.96	0.12	55,55,55,55	0
57	MG	1U	201	1/1	0.97	0.13	30,30,30,30	0
57	MG	2A	3422	1/1	0.97	0.11	59,59,59,59	0
57	MG	1A	3521	1/1	0.97	0.14	40,40,40,40	0
57	MG	1U	203	1/1	0.97	0.16	53,53,53,53	0
57	MG	1U	204	1/1	0.97	0.13	35,35,35,35	0
57	MG	2A	3426	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3137	1/1	0.97	0.13	51,51,51,51	0
57	MG	1A	3339	1/1	0.97	0.16	48,48,48,48	0
57	MG	1A	3592	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3125	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3431	1/1	0.97	0.07	53,53,53,53	0
57	MG	1n	101	1/1	0.97	0.15	46,46,46,46	0
57	MG	2A	3127	1/1	0.97	0.18	44,44,44,44	0
57	MG	1A	3138	1/1	0.97	0.12	57,57,57,57	0
57	MG	1A	3594	1/1	0.97	0.11	58,58,58,58	0
57	MG	1A	3087	1/1	0.97	0.10	27,27,27,27	0
57	MG	1V	202	1/1	0.97	0.16	36,36,36,36	0
57	MG	1A	3470	1/1	0.97	0.20	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	1A	3212	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3684	1/1	0.97	0.15	50,50,50,50	0
57	MG	1A	3685	1/1	0.97	0.08	44,44,44,44	0
57	MG	1W	202	1/1	0.97	0.09	57,57,57,57	0
57	MG	1W	203	1/1	0.97	0.19	33,33,33,33	0
57	MG	2A	3285	1/1	0.97	0.07	58,58,58,58	0
57	MG	1B	202	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3188	1/1	0.97	0.28	31,31,31,31	0
57	MG	1A	3599	1/1	0.97	0.04	16,16,16,16	0
57	MG	2A	3621	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3020	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3425	1/1	0.97	0.20	37,37,37,37	0
57	MG	1B	207	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3693	1/1	0.97	0.07	52,52,52,52	0
57	MG	2A	3453	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3884	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3065	1/1	0.97	0.06	14,14,14,14	0
57	MG	1A	3168	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3605	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3697	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3090	1/1	0.97	0.19	37,37,37,37	0
57	MG	10	104	1/1	0.97	0.11	44,44,44,44	0
57	MG	1B	215	1/1	0.97	0.05	55,55,55,55	0
57	MG	2A	3154	1/1	0.97	0.09	60,60,60,60	0
57	MG	1A	3699	1/1	0.97	0.11	29,29,29,29	0
57	MG	1A	4002	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3700	1/1	0.97	0.07	24,24,24,24	0
57	MG	2D	304	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3535	1/1	0.97	0.15	28,28,28,28	0
57	MG	2A	3469	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3171	1/1	0.97	0.07	34,34,34,34	0
57	MG	1a	1702	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3349	1/1	0.97	0.09	40,40,40,40	0
57	MG	2A	3162	1/1	0.97	0.06	34,34,34,34	0
57	MG	2E	303	1/1	0.97	0.10	43,43,43,43	0
57	MG	1A	3350	1/1	0.97	0.17	24,24,24,24	0
57	MG	1A	3032	1/1	0.97	0.38	27,27,27,27	0
57	MG	1A	3801	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3482	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3905	1/1	0.97	0.07	62,62,62,62	0
57	MG	2A	3479	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3480	1/1	0.97	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1736	1/1	0.97	0.21	56,56,56,56	0
57	MG	1A	3542	1/1	0.97	0.08	37,37,37,37	0
57	MG	12	103	1/1	0.97	0.10	43,43,43,43	0
57	MG	2A	3021	1/1	0.97	0.08	44,44,44,44	0
57	MG	13	101	1/1	0.97	0.05	36,36,36,36	0
57	MG	13	102	1/1	0.97	0.10	39,39,39,39	0
57	MG	2A	3024	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3250	1/1	0.97	0.15	51,51,51,51	0
57	MG	2a	1746	1/1	0.97	0.09	64,64,64,64	0
57	MG	1A	4016	1/1	0.97	0.04	25,25,25,25	0
57	MG	13	105	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3317	1/1	0.97	0.26	41,41,41,41	0
57	MG	1A	3286	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3107	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3043	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3667	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3441	1/1	0.97	0.12	64,64,64,64	0
57	MG	1A	3913	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3489	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3811	1/1	0.97	0.06	64,64,64,64	0
57	MG	17	102	1/1	0.97	0.11	33,33,33,33	0
57	MG	2A	3673	1/1	0.97	0.06	49,49,49,49	0
57	MG	1D	306	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3037	1/1	0.97	0.16	32,32,32,32	0
57	MG	1a	1730	1/1	0.97	0.08	54,54,54,54	0
57	MG	1A	3624	1/1	0.97	0.05	29,29,29,29	0
57	MG	2W	202	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3551	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3010	1/1	0.97	0.08	31,31,31,31	0
57	MG	1A	3225	1/1	0.97	0.10	61,61,61,61	0
57	MG	1A	3324	1/1	0.97	0.20	30,30,30,30	0
57	MG	1A	3365	1/1	0.97	0.18	42,42,42,42	0
57	MG	1A	3819	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3083	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3637	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3730	1/1	0.97	0.05	22,22,22,22	0
57	MG	1A	3638	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3496	1/1	0.97	0.26	54,54,54,54	0
57	MG	1A	3640	1/1	0.97	0.07	22,22,22,22	0
57	MG	1A	4043	1/1	0.97	0.15	55,55,55,55	0
57	MG	2A	3691	1/1	0.97	0.08	57,57,57,57	0
57	MG	1a	1607	1/1	0.97	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3735	1/1	0.97	0.09	25,25,25,25	0
57	MG	1A	3497	1/1	0.97	0.11	47,47,47,47	0
57	MG	1A	3560	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3644	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3448	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3404	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3528	1/1	0.97	0.04	36,36,36,36	0
57	MG	1F	310	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3743	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3361	1/1	0.97	0.20	54,54,54,54	0
57	MG	1a	1617	1/1	0.97	0.13	45,45,45,45	0
57	MG	1a	1759	1/1	0.97	0.05	67,67,67,67	0
57	MG	1a	1619	1/1	0.97	0.05	51,51,51,51	0
57	MG	1A	3128	1/1	0.97	0.04	36,36,36,36	0
57	MG	1A	3564	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	4053	1/1	0.97	0.13	24,24,24,24	0
57	MG	2A	3070	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3229	1/1	0.97	0.09	45,45,45,45	0
57	MG	1a	1766	1/1	0.97	0.11	64,64,64,64	0
57	MG	2A	3371	1/1	0.97	0.07	24,24,24,24	0
57	MG	1a	1768	1/1	0.97	0.06	53,53,53,53	0
57	MG	2A	3544	1/1	0.97	0.13	50,50,50,50	0
57	MG	2a	1803	1/1	0.97	0.12	61,61,61,61	0
57	MG	2A	3373	1/1	0.97	0.40	42,42,42,42	0
57	MG	2a	1621	1/1	0.97	0.19	61,61,61,61	0
57	MG	2a	1622	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	4055	1/1	0.97	0.08	58,58,58,58	0
57	MG	2A	3721	1/1	0.97	0.13	64,64,64,64	0
57	MG	1A	3502	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3015	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3724	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3055	1/1	0.97	0.22	49,49,49,49	0
57	MG	1A	3839	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3079	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3751	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3655	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3732	1/1	0.97	0.07	64,64,64,64	0
57	MG	1A	3842	1/1	0.97	0.05	23,23,23,23	0
57	MG	1a	1781	1/1	0.97	0.09	53,53,53,53	0
57	MG	2a	1821	1/1	0.97	0.06	66,66,66,66	0
57	MG	1A	3409	1/1	0.97	0.26	39,39,39,39	0
57	MG	1A	3455	1/1	0.97	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4065	1/1	0.97	0.11	51,51,51,51	0
57	MG	1A	3952	1/1	0.97	0.04	48,48,48,48	0
57	MG	1a	1786	1/1	0.97	0.05	53,53,53,53	0
57	MG	1a	1787	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3756	1/1	0.97	0.05	39,39,39,39	0
57	MG	2A	3563	1/1	0.97	0.09	71,71,71,71	0
57	MG	1A	4068	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3261	1/1	0.97	0.17	33,33,33,33	0
57	MG	2A	3745	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3131	1/1	0.97	0.08	28,28,28,28	0
57	MG	1A	3086	1/1	0.97	0.09	59,59,59,59	0
57	MG	1A	3850	1/1	0.97	0.09	21,21,21,21	0
57	MG	1A	3959	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3264	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3265	1/1	0.97	0.18	40,40,40,40	0
57	MG	2A	3572	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3205	1/1	0.97	0.06	48,48,48,48	0
57	MG	1Q	203	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3664	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3100	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3515	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3857	1/1	0.97	0.06	34,34,34,34	0
57	MG	2a	1660	1/1	0.97	0.17	42,42,42,42	0
57	MG	1R	201	1/1	0.97	0.18	43,43,43,43	0
57	MG	2a	1662	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	4081	1/1	0.97	0.07	57,57,57,57	0
57	MG	1R	203	1/1	0.97	0.36	38,38,38,38	0
57	MG	1A	3967	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3464	1/1	0.97	0.19	29,29,29,29	0
57	MG	1A	3969	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3517	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3134	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3520	1/1	0.97	0.22	40,40,40,40	0
57	MG	1A	3587	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3588	1/1	0.97	0.04	18,18,18,18	0
60	ZN	14	102	1/1	0.97	0.07	100,100,100,100	0
57	MG	2A	3772	1/1	0.97	0.04	49,49,49,49	0
57	MG	1A	3976	1/1	0.97	0.06	57,57,57,57	0
57	MG	1D	307	1/1	0.98	0.16	36,36,36,36	0
57	MG	1A	3692	1/1	0.98	0.05	46,46,46,46	0
57	MG	1U	208	1/1	0.98	0.29	37,37,37,37	0
57	MG	2A	3446	1/1	0.98	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	1a	1618	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3074	1/1	0.98	0.11	42,42,42,42	0
57	MG	1A	3752	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3642	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3008	1/1	0.98	0.04	26,26,26,26	0
57	MG	1E	301	1/1	0.98	0.24	36,36,36,36	0
57	MG	1A	3236	1/1	0.98	0.18	36,36,36,36	0
57	MG	2A	3454	1/1	0.98	0.09	35,35,35,35	0
57	MG	2A	3455	1/1	0.98	0.10	35,35,35,35	0
57	MG	2A	3152	1/1	0.98	0.10	58,58,58,58	0
57	MG	1a	1709	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3003	1/1	0.98	0.04	22,22,22,22	0
57	MG	1E	304	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3149	1/1	0.98	0.11	37,37,37,37	0
57	MG	1A	3519	1/1	0.98	0.17	35,35,35,35	0
57	MG	1A	3150	1/1	0.98	0.16	48,48,48,48	0
57	MG	1A	3240	1/1	0.98	0.06	48,48,48,48	0
57	MG	1A	3007	1/1	0.98	0.05	35,35,35,35	0
57	MG	1X	101	1/1	0.98	0.22	40,40,40,40	0
57	MG	1A	3945	1/1	0.98	0.07	26,26,26,26	0
57	MG	1X	103	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3651	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3602	1/1	0.98	0.14	24,24,24,24	0
57	MG	1f	201	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	4015	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3011	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3269	1/1	0.98	0.08	30,30,30,30	0
57	MG	1F	306	1/1	0.98	0.20	36,36,36,36	0
57	MG	1A	3355	1/1	0.98	0.31	27,27,27,27	0
57	MG	1A	4019	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3710	1/1	0.98	0.07	19,19,19,19	0
57	MG	1A	4021	1/1	0.98	0.09	19,19,19,19	0
57	MG	1A	3270	1/1	0.98	0.17	33,33,33,33	0
57	MG	1A	3527	1/1	0.98	0.23	34,34,34,34	0
57	MG	1A	3890	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	4026	1/1	0.98	0.05	46,46,46,46	0
57	MG	2A	3594	1/1	0.98	0.05	65,65,65,65	0
57	MG	2A	3708	1/1	0.98	0.11	39,39,39,39	0
57	MG	2A	3377	1/1	0.98	0.04	37,37,37,37	0
57	MG	1a	1650	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3357	1/1	0.98	0.23	27,27,27,27	0
57	MG	1A	3609	1/1	0.98	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3358	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3958	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3894	1/1	0.98	0.03	54,54,54,54	0
57	MG	1A	3153	1/1	0.98	0.11	32,32,32,32	0
57	MG	1a	1744	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3896	1/1	0.98	0.03	36,36,36,36	0
57	MG	1A	3079	1/1	0.98	0.30	33,33,33,33	0
57	MG	2A	3497	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3105	1/1	0.98	0.06	40,40,40,40	0
57	MG	2a	1797	1/1	0.98	0.17	54,54,54,54	0
57	MG	1N	202	1/1	0.98	0.04	45,45,45,45	0
57	MG	2A	3725	1/1	0.98	0.06	42,42,42,42	0
57	MG	2A	3500	1/1	0.98	0.08	59,59,59,59	0
57	MG	2A	3093	1/1	0.98	0.05	28,28,28,28	0
57	MG	2A	3728	1/1	0.98	0.07	36,36,36,36	0
57	MG	1N	203	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3362	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3221	1/1	0.98	0.13	42,42,42,42	0
57	MG	1A	3901	1/1	0.98	0.04	53,53,53,53	0
57	MG	1a	1753	1/1	0.98	0.05	66,66,66,66	0
57	MG	2A	3002	1/1	0.98	0.27	49,49,49,49	0
57	MG	1A	3013	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3135	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3069	1/1	0.98	0.06	27,27,27,27	0
57	MG	1a	1757	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3121	1/1	0.98	0.16	33,33,33,33	0
57	MG	2A	3624	1/1	0.98	0.06	33,33,33,33	0
57	MG	2a	1815	1/1	0.98	0.05	67,67,67,67	0
57	MG	1A	3971	1/1	0.98	0.07	38,38,38,38	0
57	MG	2A	3009	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3404	1/1	0.98	0.07	63,63,63,63	0
57	MG	1A	3671	1/1	0.98	0.06	21,21,21,21	0
57	MG	2X	102	1/1	0.98	0.12	48,48,48,48	0
57	MG	2Y	201	1/1	0.98	0.16	60,60,60,60	0
57	MG	1A	3539	1/1	0.98	0.19	49,49,49,49	0
57	MG	2A	3012	1/1	0.98	0.06	48,48,48,48	0
57	MG	2A	3306	1/1	0.98	0.06	43,43,43,43	0
57	MG	1a	1762	1/1	0.98	0.06	64,64,64,64	0
57	MG	23	101	1/1	0.98	0.06	58,58,58,58	0
57	MG	1A	3728	1/1	0.98	0.05	54,54,54,54	0
57	MG	1B	216	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3729	1/1	0.98	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3580	1/1	0.98	0.07	27,27,27,27	0
57	MG	2A	3018	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3731	1/1	0.98	0.05	40,40,40,40	0
57	MG	1a	1769	1/1	0.98	0.09	58,58,58,58	0
57	MG	1A	3622	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3641	1/1	0.98	0.20	41,41,41,41	0
57	MG	1A	3846	1/1	0.98	0.07	46,46,46,46	0
57	MG	1A	3044	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3421	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3761	1/1	0.98	0.06	57,57,57,57	0
57	MG	1a	1773	1/1	0.98	0.04	63,63,63,63	0
57	MG	1A	3227	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3141	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3142	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3585	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3738	1/1	0.98	0.09	48,48,48,48	0
57	MG	1A	3628	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3629	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3741	1/1	0.98	0.09	47,47,47,47	0
57	MG	1A	3437	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3438	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3744	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3284	1/1	0.98	0.14	41,41,41,41	0
57	MG	2a	1731	1/1	0.98	0.04	70,70,70,70	0
57	MG	2A	3037	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3030	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3995	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3164	1/1	0.98	0.10	17,17,17,17	0
57	MG	1a	1611	1/1	0.98	0.05	29,29,29,29	0
57	MG	1D	304	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3072	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3053	1/1	0.98	0.07	33,33,33,33	0
60	ZN	29	102	1/1	0.98	0.04	78,78,78,78	0
60	ZN	2n	501	1/1	0.98	0.04	86,86,86,86	0
61	SF4	2d	303	8/8	0.98	0.04	67,73,84,84	0
57	MG	1A	3268	1/1	0.99	0.14	33,33,33,33	0
57	MG	2A	3490	1/1	0.99	0.06	35,35,35,35	0
57	MG	2A	3716	1/1	0.99	0.07	37,37,37,37	0
57	MG	1Q	202	1/1	0.99	0.03	35,35,35,35	0
57	MG	2a	1743	1/1	0.99	0.09	69,69,69,69	0
57	MG	2A	3718	1/1	0.99	0.04	51,51,51,51	0
57	MG	2A	3492	1/1	0.99	0.04	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	3921	1/1	0.99	0.03	27,27,27,27	0
57	MG	2A	3337	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3031	1/1	0.99	0.11	23,23,23,23	0
57	MG	1X	106	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3886	1/1	0.99	0.03	12,12,12,12	0
57	MG	1a	1735	1/1	0.99	0.10	58,58,58,58	0
57	MG	2A	3786	1/1	0.99	0.03	64,64,64,64	0
57	MG	1A	3067	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3098	1/1	0.99	0.21	35,35,35,35	0
57	MG	1A	3553	1/1	0.99	0.29	31,31,31,31	0
57	MG	1A	3426	1/1	0.99	0.07	43,43,43,43	0
57	MG	1A	3703	1/1	0.99	0.07	46,46,46,46	0
57	MG	2A	3616	1/1	0.99	0.04	49,49,49,49	0
57	MG	1A	4004	1/1	0.99	0.03	41,41,41,41	0
57	MG	1A	3652	1/1	0.99	0.05	40,40,40,40	0
57	MG	1A	3572	1/1	0.99	0.04	21,21,21,21	0
57	MG	1A	3678	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3630	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3860	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3708	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3935	1/1	0.99	0.04	39,39,39,39	0
57	MG	2A	3406	1/1	0.99	0.06	65,65,65,65	0
57	MG	1A	3799	1/1	0.99	0.06	32,32,32,32	0
57	MG	1A	3136	1/1	0.99	0.06	16,16,16,16	0
57	MG	1A	3062	1/1	0.99	0.11	30,30,30,30	0
57	MG	1A	3633	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3634	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3635	1/1	0.99	0.02	26,26,26,26	0
57	MG	1A	3869	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3870	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3575	1/1	0.99	0.06	29,29,29,29	0
57	MG	1A	3012	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	4022	1/1	0.99	0.05	22,22,22,22	0
57	MG	1A	3687	1/1	0.99	0.06	21,21,21,21	0
57	MG	1A	3717	1/1	0.99	0.07	41,41,41,41	0
57	MG	1a	1714	1/1	0.99	0.08	45,45,45,45	0
57	MG	1A	3688	1/1	0.99	0.05	21,21,21,21	0
57	MG	1A	3122	1/1	0.99	0.18	32,32,32,32	0
57	MG	1A	3987	1/1	0.99	0.03	21,21,21,21	0
57	MG	15	103	1/1	0.99	0.32	28,28,28,28	0
57	MG	2A	3700	1/1	0.99	0.03	47,47,47,47	0
57	MG	1a	1767	1/1	0.99	0.04	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	3170	1/1	0.99	0.14	27,27,27,27	0
57	MG	1A	3462	1/1	0.99	0.19	39,39,39,39	0
57	MG	2A	3535	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3140	1/1	0.99	0.12	32,32,32,32	0
57	MG	1a	1722	1/1	0.99	0.05	35,35,35,35	0
57	MG	2A	3766	1/1	0.99	0.05	54,54,54,54	0
57	MG	1A	3014	1/1	0.99	0.04	28,28,28,28	0
57	MG	1a	1632	1/1	0.99	0.09	23,23,23,23	0
60	ZN	1Y	203	1/1	0.99	0.03	68,68,68,68	0
57	MG	1a	1774	1/1	0.99	0.03	44,44,44,44	0
60	ZN	15	107	1/1	0.99	0.03	43,43,43,43	0
60	ZN	16	102	1/1	0.99	0.03	44,44,44,44	0
60	ZN	19	102	1/1	0.99	0.04	42,42,42,42	0
60	ZN	1n	102	1/1	0.99	0.03	57,57,57,57	0
57	MG	1A	3279	1/1	0.99	0.20	30,30,30,30	0
57	MG	1A	3206	1/1	0.99	0.11	39,39,39,39	0
60	ZN	25	105	1/1	0.99	0.04	57,57,57,57	0
60	ZN	26	501	1/1	0.99	0.03	61,61,61,61	0
57	MG	17	103	1/1	0.99	0.05	29,29,29,29	0
57	MG	2a	1737	1/1	0.99	0.03	52,52,52,52	0
61	SF4	1d	501	8/8	0.99	0.06	56,62,68,68	0
57	MG	1A	3040	1/1	0.99	0.06	35,35,35,35	0
57	MG	2A	3608	1/1	1.00	0.02	32,32,32,32	0
57	MG	2A	3496	1/1	1.00	0.05	33,33,33,33	0
57	MG	1A	3889	1/1	1.00	0.04	23,23,23,23	0
57	MG	1a	1776	1/1	1.00	0.05	49,49,49,49	0
57	MG	1A	3864	1/1	1.00	0.06	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.