



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:16 AM UTC

PDB ID : 7U2H / pdb_00007u2h
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNA_{gly}, aminoacylated P-site fMet-NH-tRNA_{met}, and deacylated E-site tRNA_{gly} at 2.55Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-02-24
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

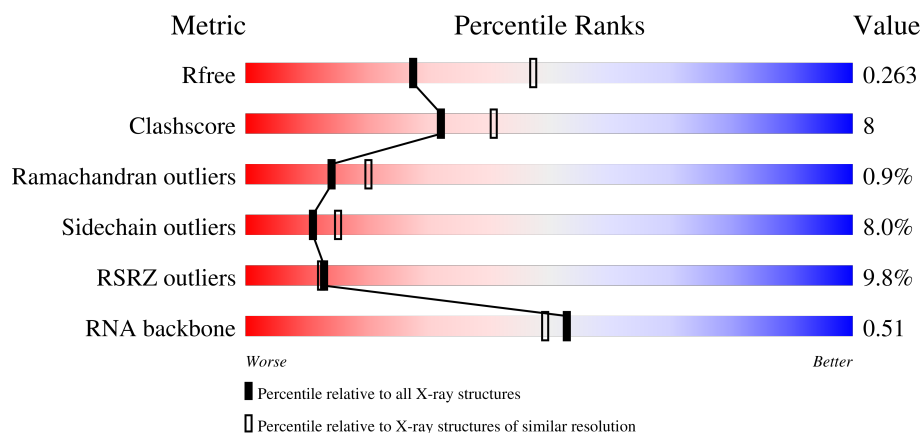
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



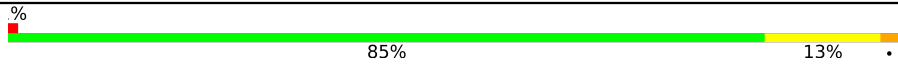
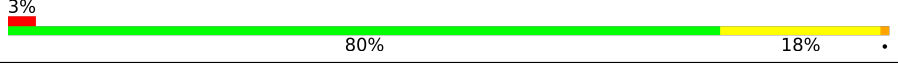
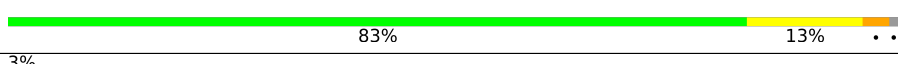
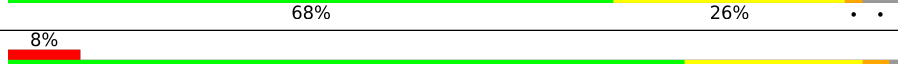
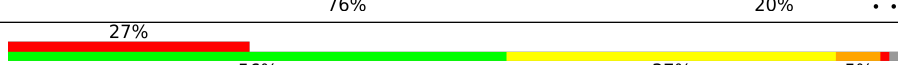
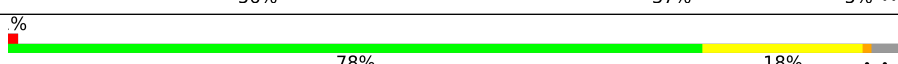
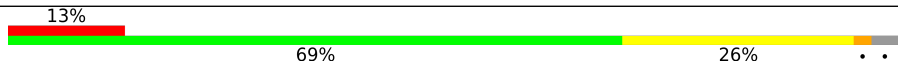
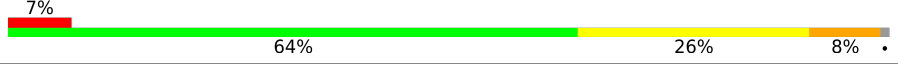
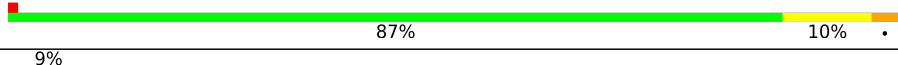
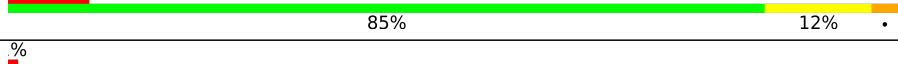
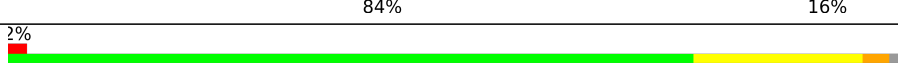
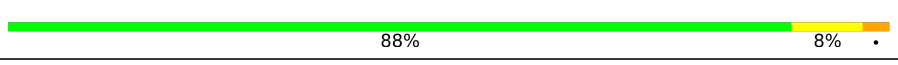
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 69% 23% 6% .
1	2A	2915	5% 62% 29% 6% .
2	1B	121	74% 24% ..
2	2B	121	3% 47% 42% 10% .

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

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

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

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	74	
54	2w	74	
55	1x	77	
55	2x	77	
56	1y	74	
56	2y	74	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	2A	3423	-	-	-	X
57	MG	2a	1725	-	-	-	X
57	MG	2a	1743	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	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 MG-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			
53	2v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Gly-NH-tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1556	695	275	512	73	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1536	686	273	504	72	1			

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-NH-tRNAmet.

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 tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1096	Total	Mg	0	0
			1096	1096		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	15	Total	Mg	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	4	Total 4	Mg 4	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	5	Total 5	Mg 5	0	0
57	1P	6	Total 6	Mg 6	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	2	Total 2	Mg 2	0	0
57	1U	9	Total 9	Mg 9	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	7	Total 7	Mg 7	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	9	Total 9	Mg 9	0	0
57	11	2	Total 2	Mg 2	0	0
57	12	1	Total 1	Mg 1	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	3	Total 3	Mg 3	0	0
57	17	5	Total 5	Mg 5	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	224	Total 224	Mg 224	0	0
57	1b	2	Total 2	Mg 2	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	2	Total 2	Mg 2	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1w	9	Total 9	Mg 9	0	0
57	1x	12	Total 12	Mg 12	0	0
57	2A	861	Total 861	Mg 861	0	0
57	2B	18	Total 18	Mg 18	0	0
57	2D	7	Total 7	Mg 7	0	0
57	2E	9	Total 9	Mg 9	0	0
57	2F	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	3	Total 3	Mg 3	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	3	Total 3	Mg 3	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	2Z	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	3	Total 3	Mg 3	0	0
57	25	5	Total 5	Mg 5	0	0
57	26	1	Total 1	Mg 1	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	3	Total 3	Mg 3	0	0
57	2a	226	Total 226	Mg 226	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2i	1	Total 1	Mg 1	0	0
57	2j	2	Total 2	Mg 2	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	3	Total 3	Mg 3	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2w	4	Total 4	Mg 4	0	0
57	2x	6	Total 6	Mg 6	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
58	2A	1	Total 1	K 1	0	0

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

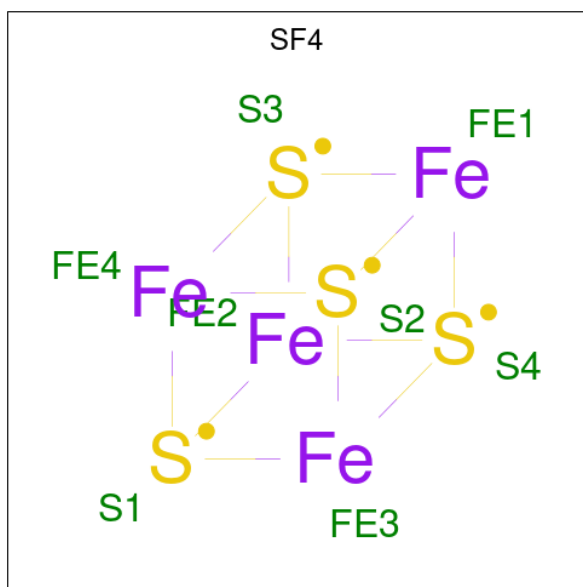
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total 1	Zn 1	0	0

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1984	Total 1984	O 1984	0	0
61	1B	63	Total 63	O 63	0	0
61	1D	27	Total 27	O 27	0	0
61	1E	27	Total 27	O 27	0	0
61	1F	17	Total 17	O 17	0	0
61	1G	4	Total 4	O 4	0	0
61	1H	2	Total 2	O 2	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	4	Total 4	O 4	0	0
61	1O	5	Total 5	O 5	0	0
61	1P	17	Total 17	O 17	0	0
61	1Q	8	Total 8	O 8	0	0
61	1R	6	Total 6	O 6	0	0
61	1S	2	Total 2	O 2	0	0
61	1T	9	Total 9	O 9	0	0
61	1U	10	Total 10	O 10	0	0
61	1V	11	Total 11	O 11	0	0
61	1W	9	Total 9	O 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1X	6	Total 6	O 6	0	0
61	1Y	4	Total 4	O 4	0	0
61	10	12	Total 12	O 12	0	0
61	11	8	Total 8	O 8	0	0
61	12	3	Total 3	O 3	0	0
61	13	6	Total 6	O 6	0	0
61	15	7	Total 7	O 7	0	0
61	16	4	Total 4	O 4	0	0
61	17	9	Total 9	O 9	0	0
61	18	12	Total 12	O 12	0	0
61	1a	278	Total 278	O 278	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1v	4	Total 4	O 4	0	0
61	1w	7	Total 7	O 7	0	0
61	1x	12	Total 12	O 12	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1142	Total 1142	O 1142	0	0
61	2B	21	Total 21	O 21	0	0
61	2D	28	Total 28	O 28	0	0
61	2E	12	Total 12	O 12	0	0
61	2F	17	Total 17	O 17	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	8	Total 8	O 8	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	5	Total 5	O 5	0	0
61	2U	2	Total 2	O 2	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	3	Total 3	O 3	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	1	Total 1	O 1	0	0

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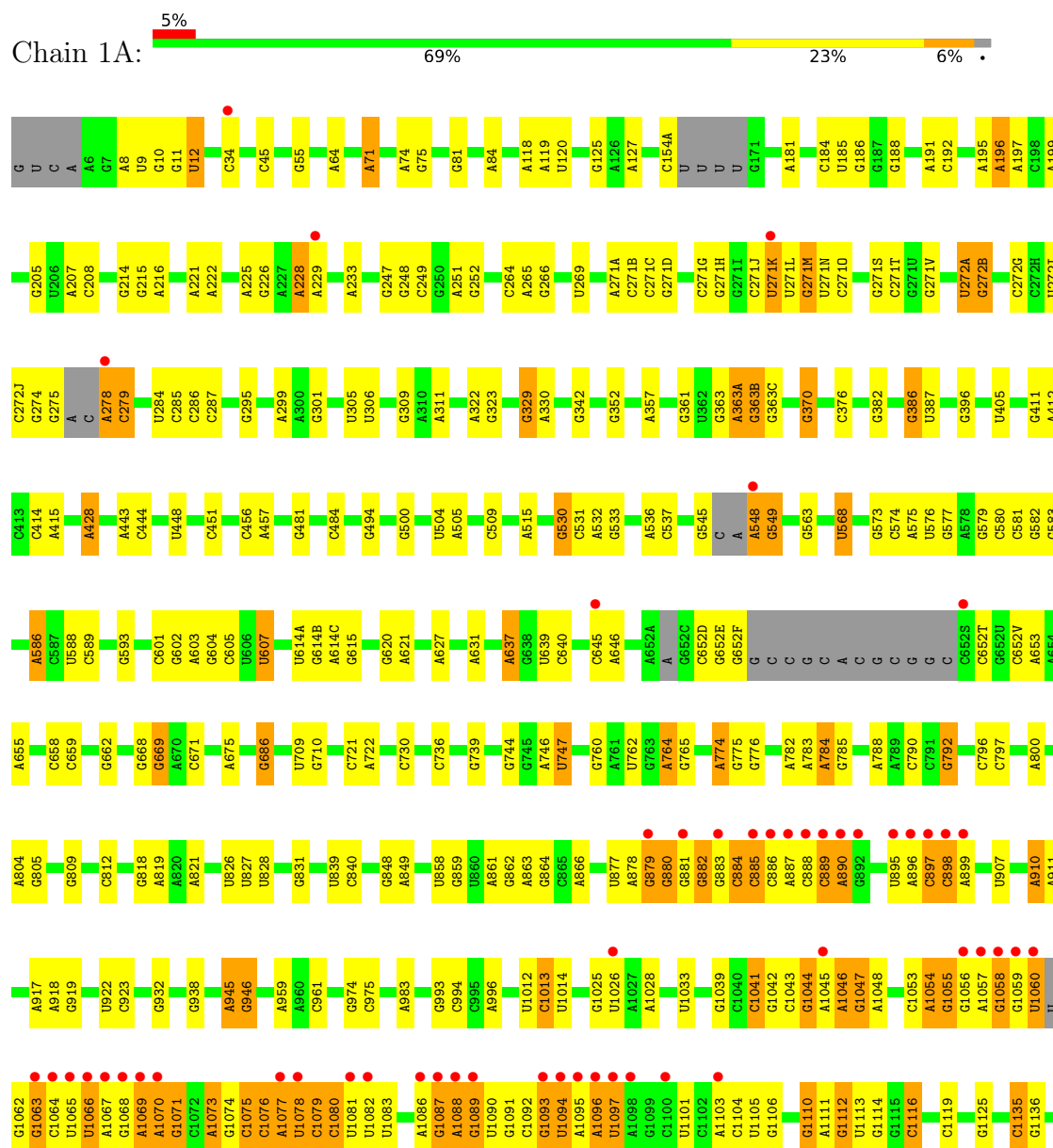
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	20	3	Total 3	O 3	0	0
61	21	9	Total 9	O 9	0	0
61	23	2	Total 2	O 2	0	0
61	25	2	Total 2	O 2	0	0
61	27	4	Total 4	O 4	0	0
61	28	6	Total 6	O 6	0	0
61	29	1	Total 1	O 1	0	0
61	2a	210	Total 210	O 210	0	0
61	2d	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	3	Total 3	O 3	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	1	Total 1	O 1	0	0
61	2x	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

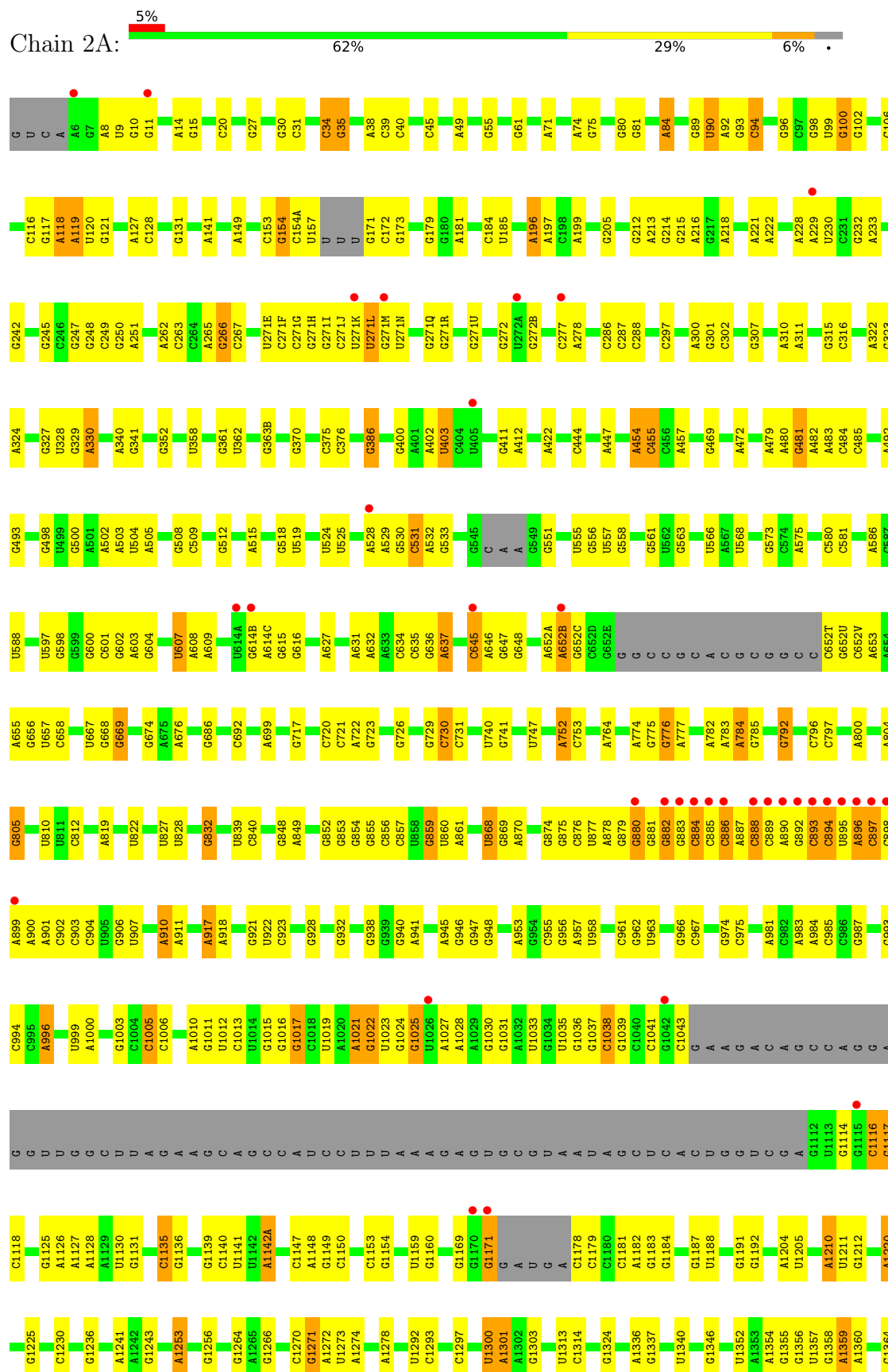
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



U2887	A2764	U2611	A2448	G2321	G2182	U2123	A2020	C1866	G1746	G1581	A1445	U1292	G1139
C2888	A2765	C2612	A2449	G2325	C2183	G2123	A2021	A1876	G1747	C1582	A1446	U1293	C1140
G2889	C2771	U2615	G2468	G2326	C2184	G2124	U2022	A1877	G1753	A1583	G1448	C1293	U1141
A2892	C2772	C2616	A2469	A2327	C2185	G2125	G2023	A1878	G1754	C1584	G1449	U1142	U1142
G2893	G2773	G2617	A2470	A2328	G2186	A2126	G2024	A1879	G1755	A1585	G1450	U1300	A1142A
U2894	A2774	A2629	A2471	G2329	C2187	G2127	G2025	A1880	G1756	A1586	A1451	A1301	A1143
C2895	A2775	G2630	C2472	G2330	C2188	C2128	G2026	A1881	A1762	A1587	A1452	A1302	A1144
U2897	A2776	C2631	A2473	G2331	U2189	U2129	A2031	A1882	A1763	C1588	U1453	G1303	
U	C2787	G2646	C2474	G2332	G2190	U2130	G2032	A1883	G1764	C1589	G1455	C1315	C1161
G	C2788	U2491	A2475	G2333	G2191	U2131	A2033	A1884	A1773	G1594	A1460	G1332	G1164
A	A2790	U2492	U2493	G2334	G2192	U2132	A2034	A1885	A1774	G1595	C1467	G1333	U1165
C	C2791	U2493	U2494	G2335	G2193	U2133	G2035	A1886	C1775	A1608	C1468	G1334	C1166
C	G2792	C2498	C2499	G2336	G2194	A2134	G2036	A1887	C1776	A1609	A1469	G1335	U1167
C	G2793	C2500	C2501	G2337	A2198	A2135	G2037	A1888	U1778	A1489	A1342	A1342	G1168
C	C2794	C2502	C2503	G2338	G2206	C2137	C2043	A1889	U1779	G1630	A1343	U1352	G1171
C	G2795	C2504	A2503	G2339	G2207	U2138	G2044	A1890	A1780	C1631	A1477	U1353	G1172
C	C2796	U2504	G2505	G2340	U2218	C2139	G2045	A1891	A1781	U1354	G1482	A1354	A1174
C	G2797	U2506	U2507	G2341	G2219	G2140	A2054	A1892	C1782	A1355	G1483	A1355	U1175
C	U2801A	U2508	U2509	G2342	G2220	G2141	G2055	A1893	A1783	U1639	U1489	A1356	U1176
C	G2802	U2510	U2511	G2343	G2221	C2142	G2056	A1894	A1784	C1640	A1490	A1357	A1177
C	C2803	U2512	U2513	G2344	G2222	U2143	G2057	A1895	A1785	A1641	A1491	A1358	C1178
C	C2804	U2514	U2515	G2345	G2223	U2144	A2060	A1896	A1786	G1642	C1493	A1359	C1179
C	G2805	A2516	U2516	G2346	C2224	C2145	G2061	A1897	A1787	G1643	A1494	G1364	C1180
C	A2810	U2517	U2518	G2347	C2225	C2146	G2062	A1898	A1788	C1644	A1495	A1365	C1181
C	C2811	U2519	U2520	G2348	G2226	G2147	G2063	A1899	G1792	C1645	C1496	G1371	C1185
C	G2812	U2521	U2522	G2349	G2227	U2148	U2079	A1900	C1793	G1646	C1497	U1372	G1186
C	C2813	U2523	U2524	G2350	G2228	C2149	G2080	A1901	U1794	G1647	C1498	A1373	G1187
C	G2814	U2525	U2526	G2351	U2243	U2150	G2081	A1902	C1795	A1664	U1503	U1374	U1188
C	C2815	U2527	U2528	G2352	U2244	U2151	G2082	A1903	U1796	A1665	C1504	A1375	
C	U2816	U2529	U2530	G2353	U2245	U2152	U2083	A1904	U1797	G1666	A1508	G1377	C1201
C	C2817	U2531	U2532	G2354	U2246	G2153	U2084	A1905	C1798	G1667	C1509	A1378	
C	A2820	U2533	U2534	G2355	G2251	U2154	G2085	A1906	G1799	G1668	A1509A	A1379	C1202
C	G2821	U2535	U2536	G2356	G2252	G2155	G2086	A1907	A1800	A1669	A1509B	A1380	A1220
C	C2822	U2537	U2538	G2357	G2253	G2156	U2096	A1908	A1801	C1670	G1515	G1384	
C	U2823	U2539	U2540	G2358	G2254	G2157	U2097	A1909	A1802	C1671	U1516	A1385	G1244
C	A2835	U2541	U2542	G2359	G2255	U2158	U2098	A1910	A1803	G1672	U1517	G1386	
C	G2836	U2543	U2544	G2360	G2256	G2159	G2100	A1911	G1811	C1673	U1518	U1387	A1247
C	U2837	U2545	U2546	G2361	G2257	G2160	G2101	A1912	G1812	C1674	U1519	U1388	
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● Molecule 1: 23S Ribosomal RNA





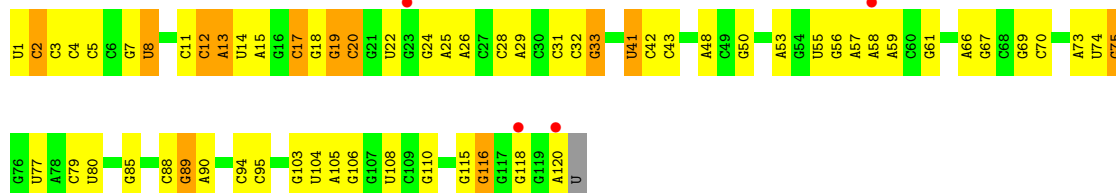
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 



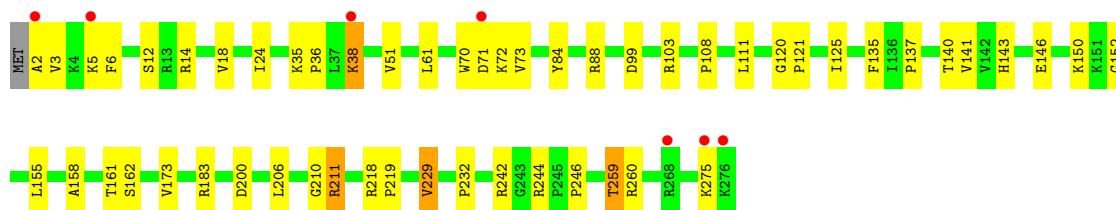
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 



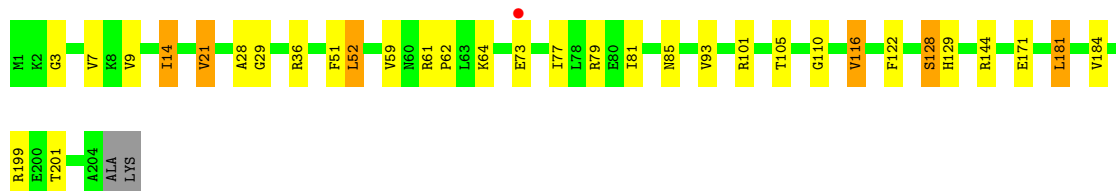
- Molecule 3: 50S ribosomal protein L2

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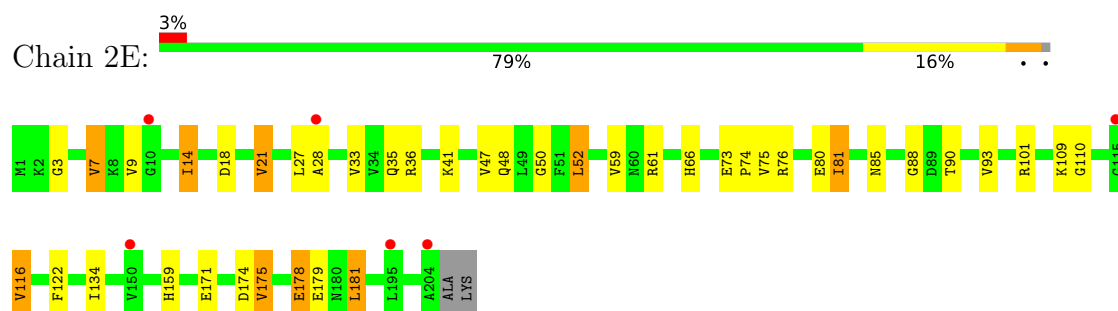


- Molecule 4: 50S ribosomal protein L3

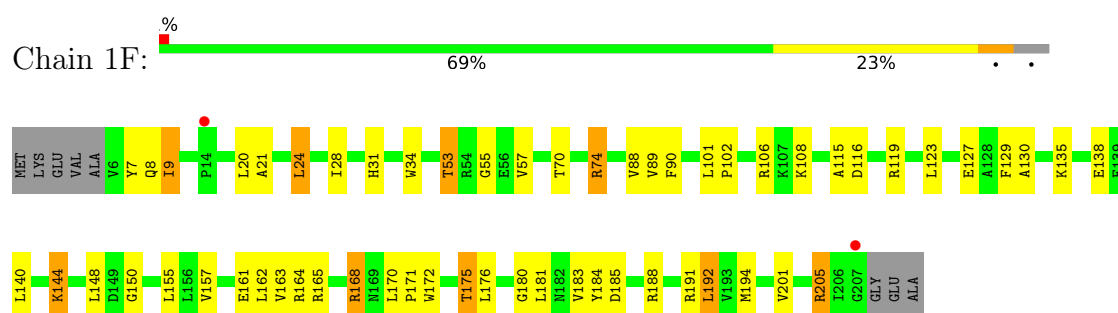
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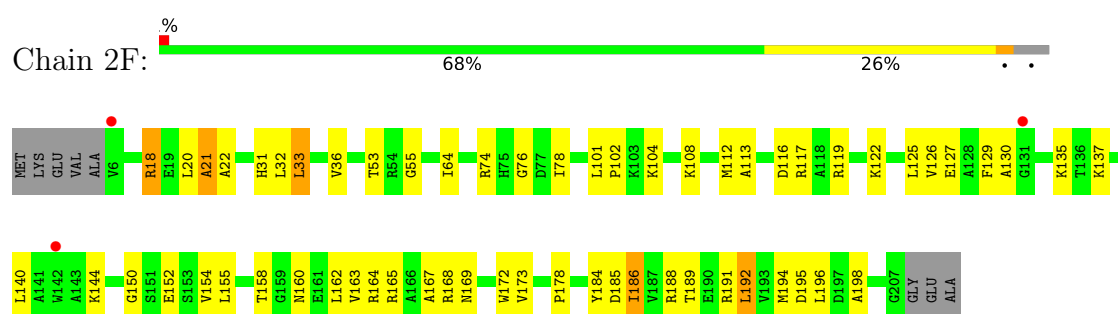
- Molecule 4: 50S ribosomal protein L3



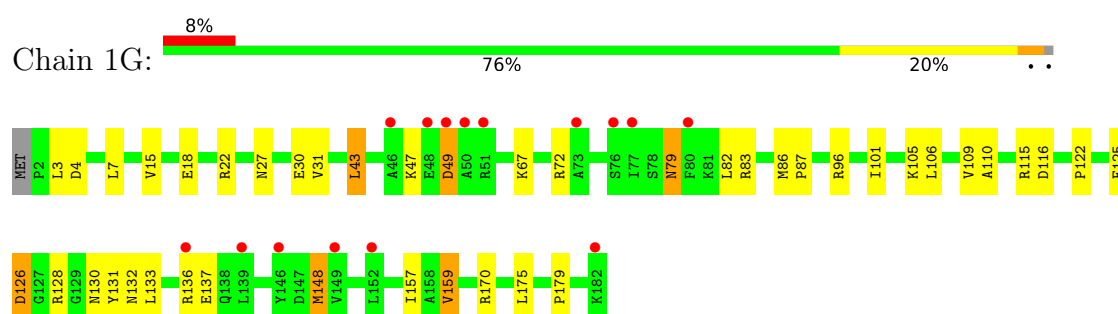
- Molecule 5: 50S ribosomal protein L4



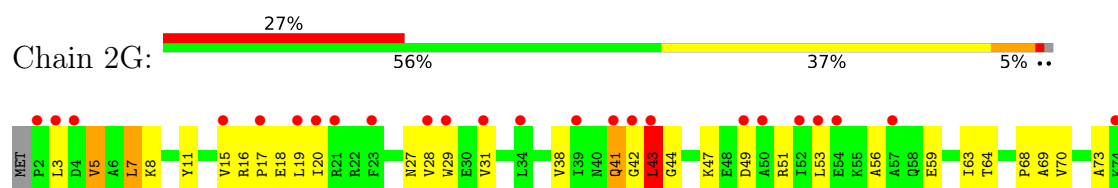
- Molecule 5: 50S ribosomal protein L4

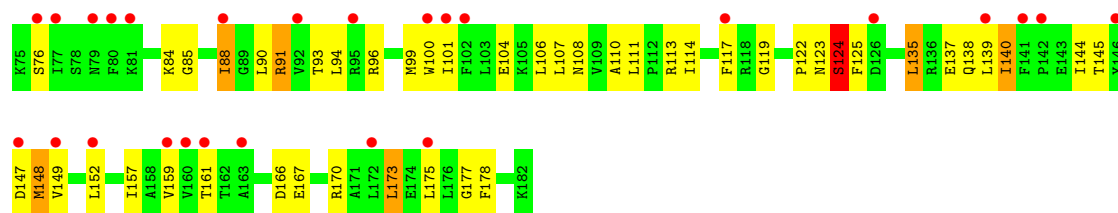


- Molecule 6: 50S ribosomal protein L5

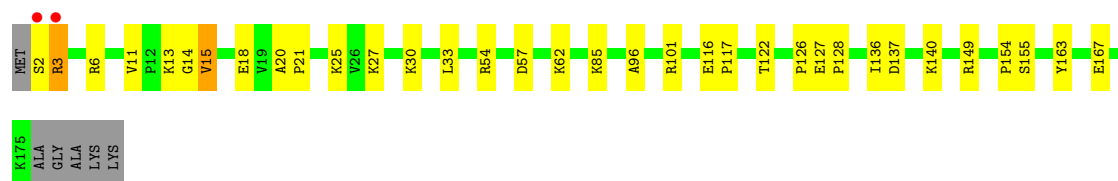
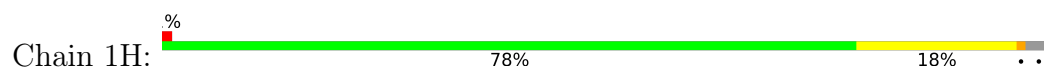


- Molecule 6: 50S ribosomal protein L5

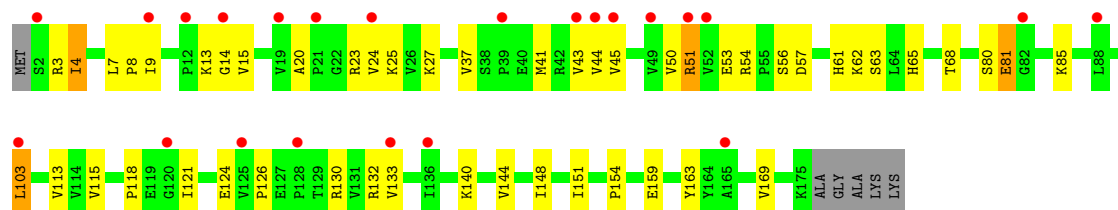




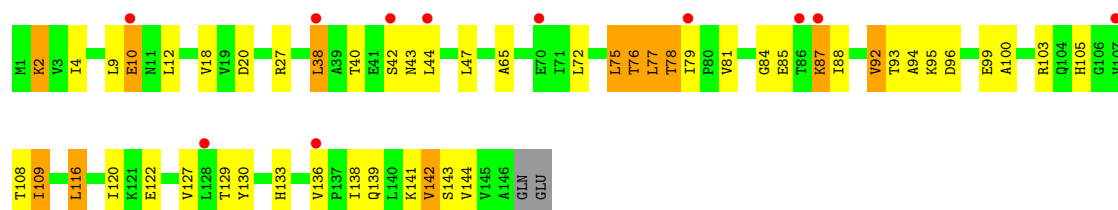
• Molecule 7: 50S ribosomal protein L6



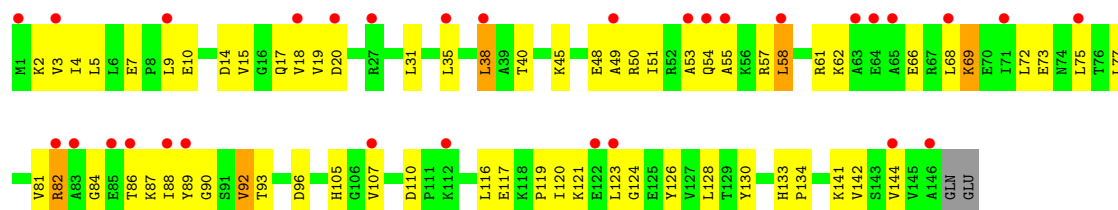
• Molecule 7: 50S ribosomal protein L6



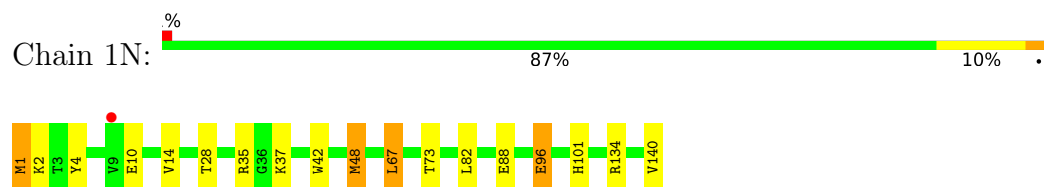
• Molecule 8: 50S ribosomal protein L9



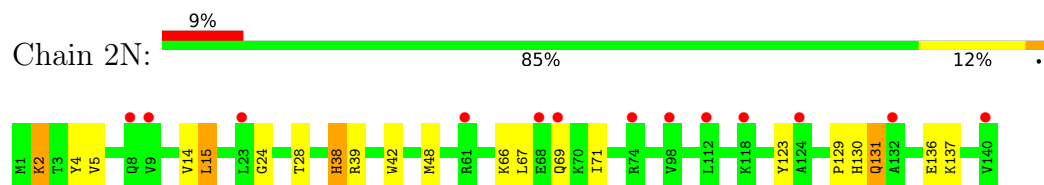
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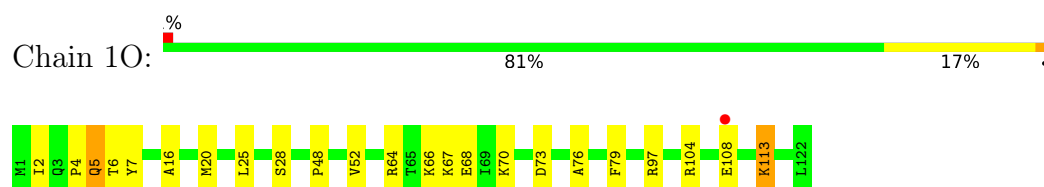
- Molecule 9: 50S ribosomal protein L13



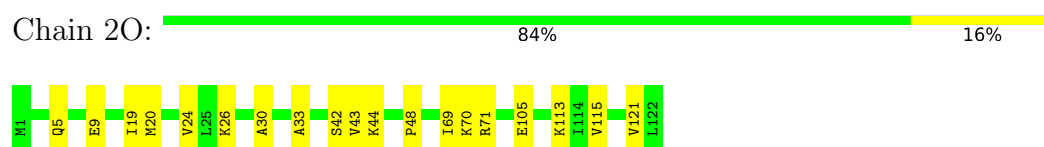
- Molecule 9: 50S ribosomal protein L13



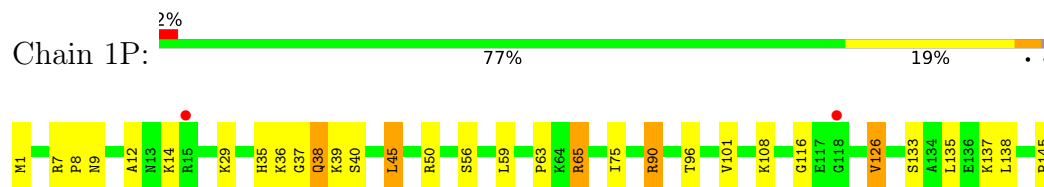
- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

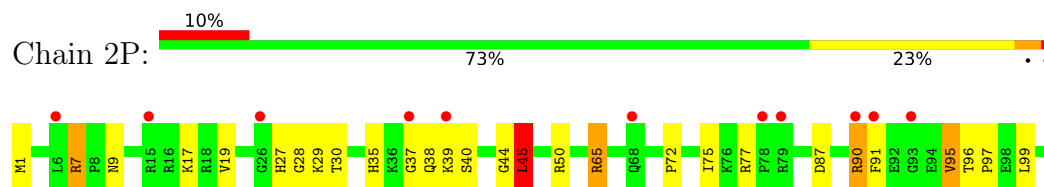


- Molecule 11: 50S ribosomal protein L15

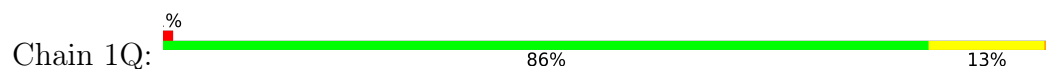


ALA

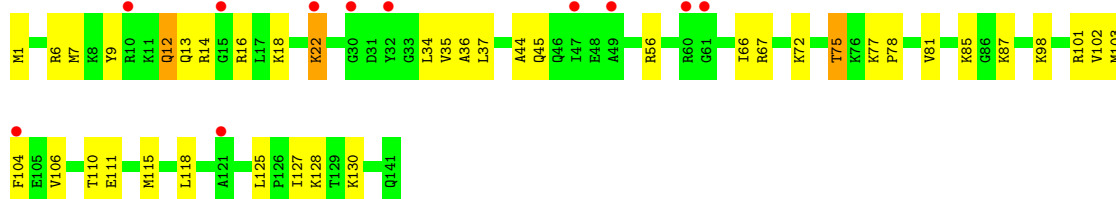
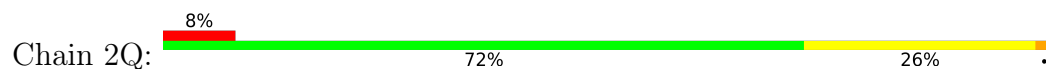
- Molecule 11: 50S ribosomal protein L15



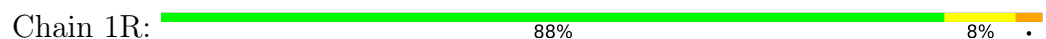
- Molecule 12: 50S ribosomal protein L16



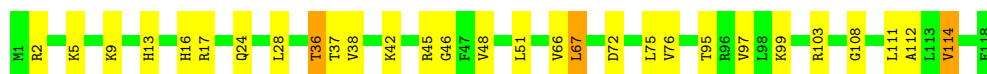
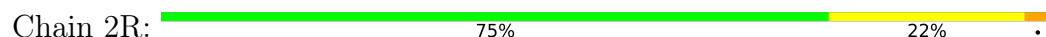
- Molecule 12: 50S ribosomal protein L16



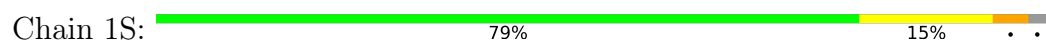
- Molecule 13: 50S ribosomal protein L17



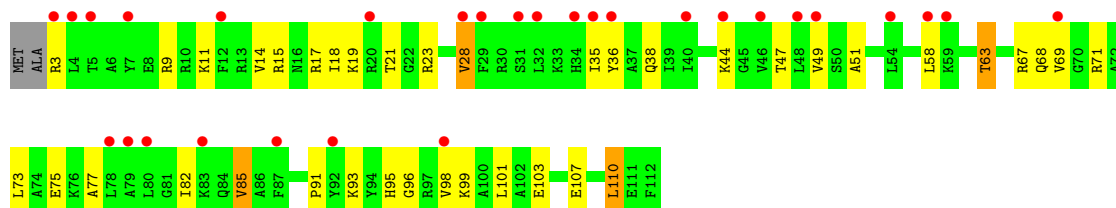
- Molecule 13: 50S ribosomal protein L17



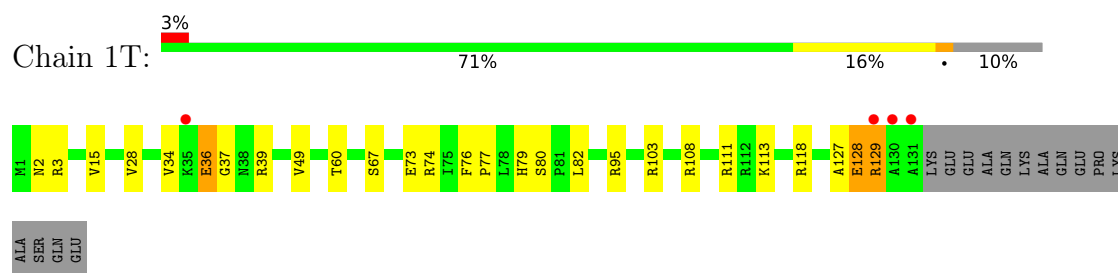
- Molecule 14: 50S ribosomal protein L18



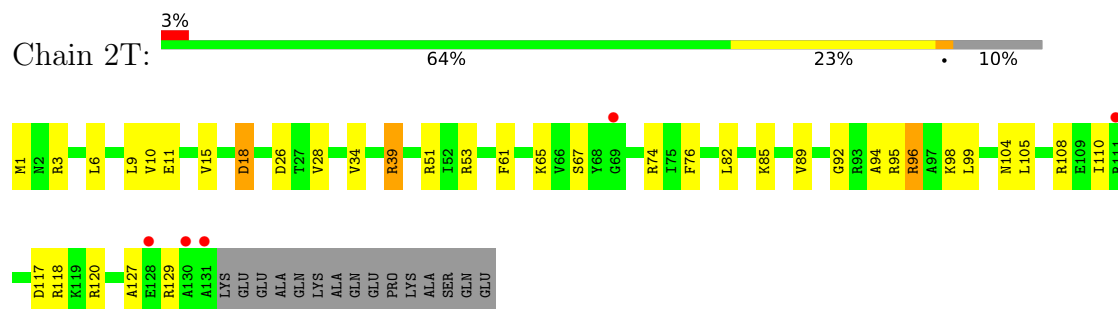
- Molecule 14: 50S ribosomal protein L18



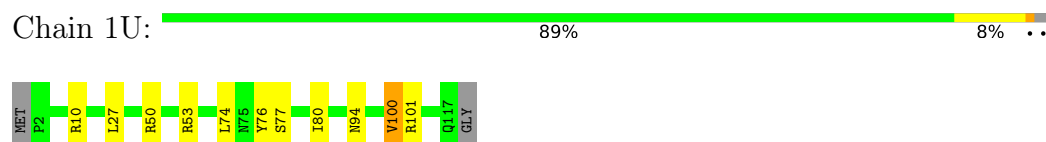
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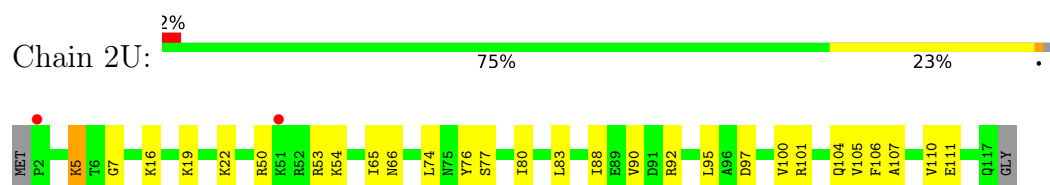
• Molecule 15: 50S ribosomal protein L19



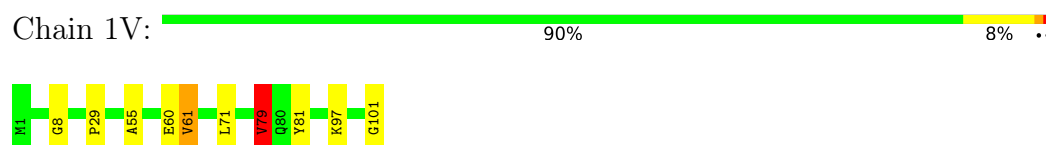
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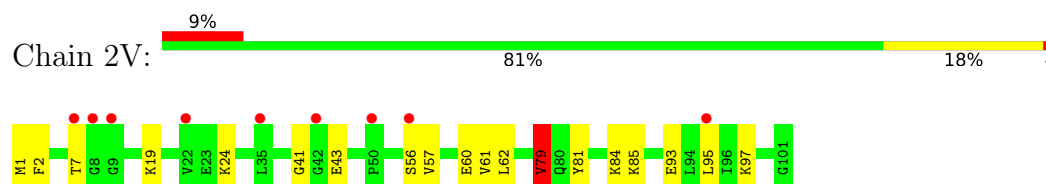
• Molecule 16: 50S ribosomal protein L20



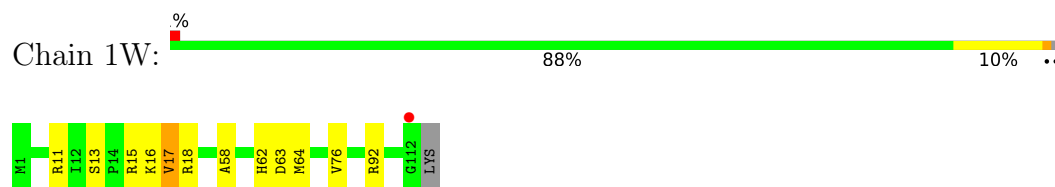
• Molecule 17: 50S ribosomal protein L21



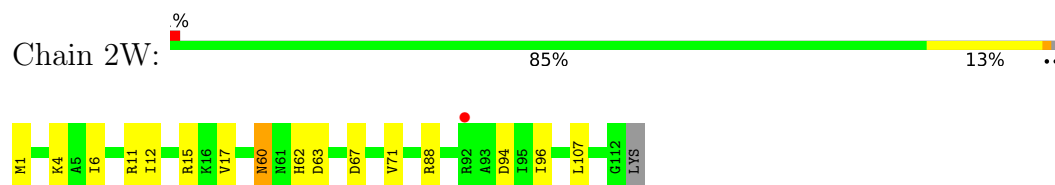
• Molecule 17: 50S ribosomal protein L21



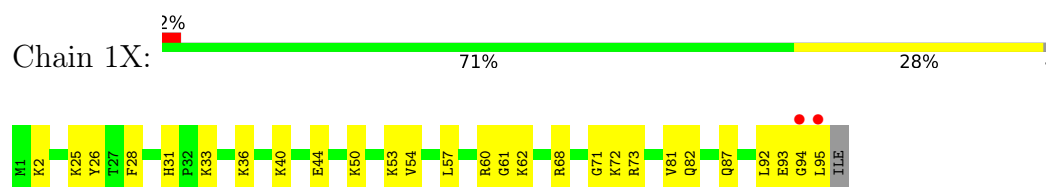
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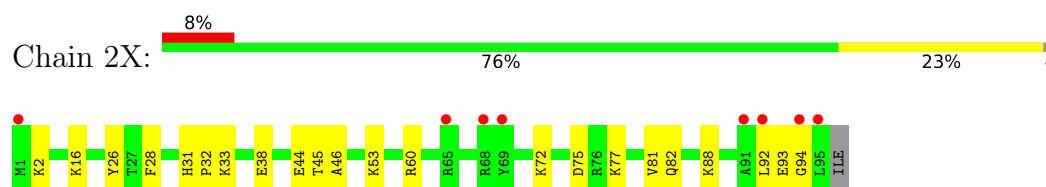
• Molecule 18: 50S ribosomal protein L22



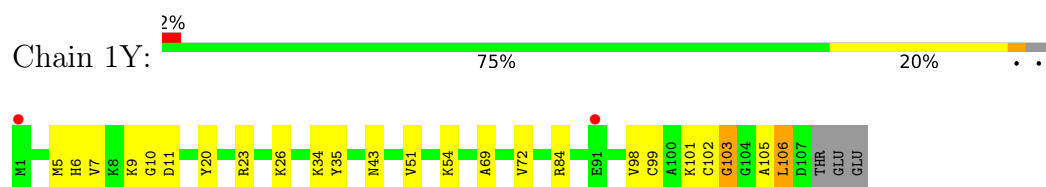
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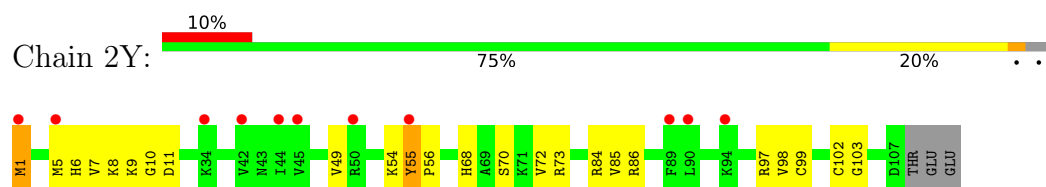
• Molecule 19: 50S ribosomal protein L23



• Molecule 20: 50S ribosomal protein L24

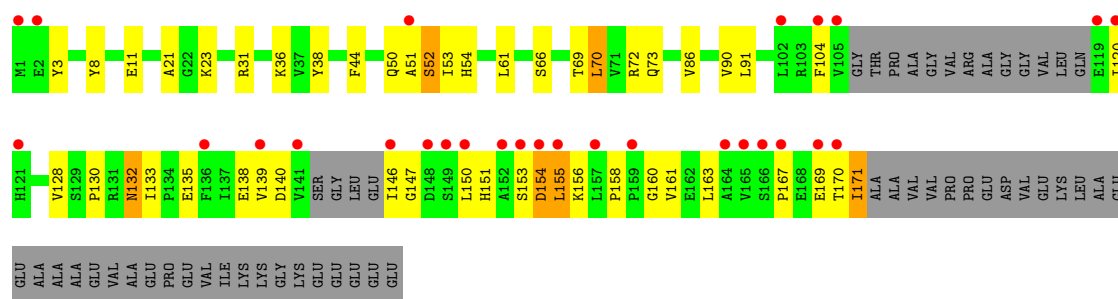


• Molecule 20: 50S ribosomal protein L24

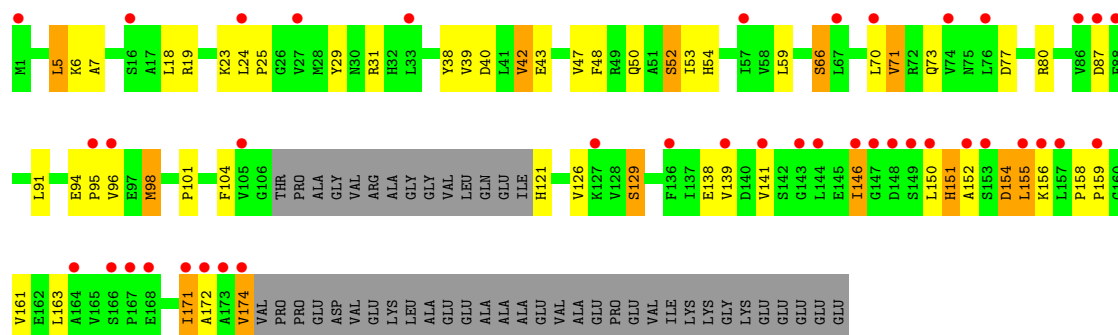


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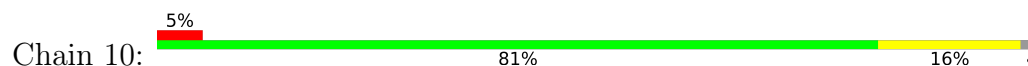




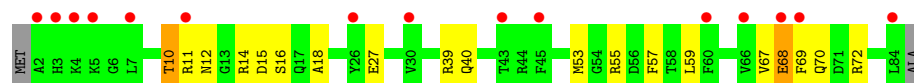
- Molecule 21: 50S ribosomal protein L25



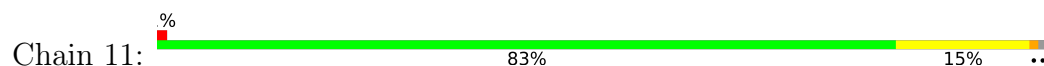
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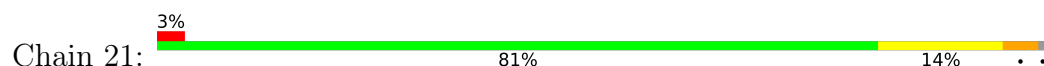
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

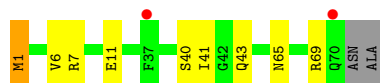
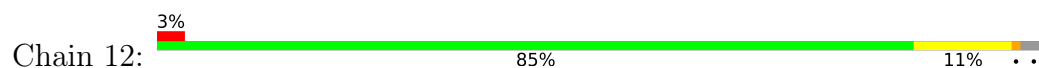


- Molecule 23: 50S ribosomal protein L28

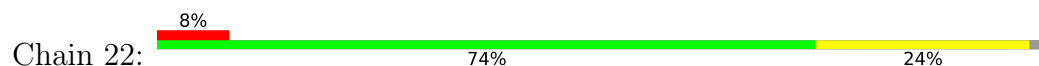




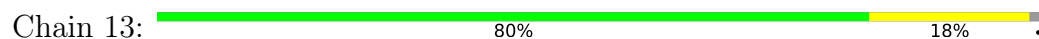
- Molecule 24: 50S ribosomal protein L29



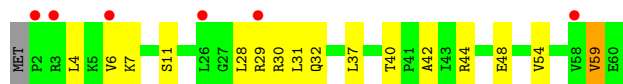
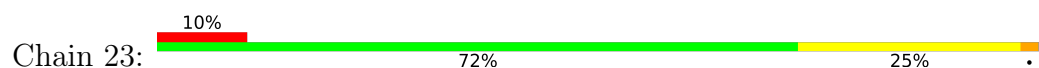
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



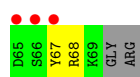
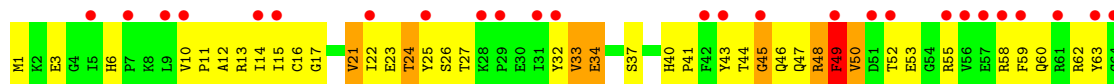
- Molecule 25: 50S ribosomal protein L30



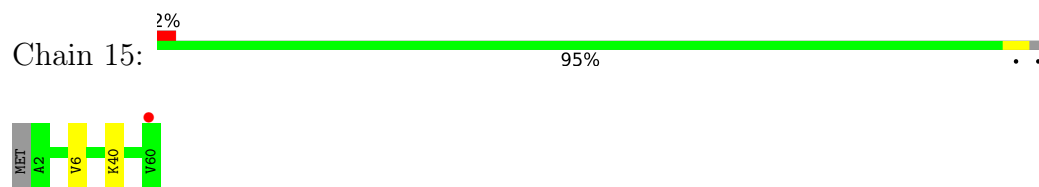
- Molecule 26: 50S ribosomal protein L31



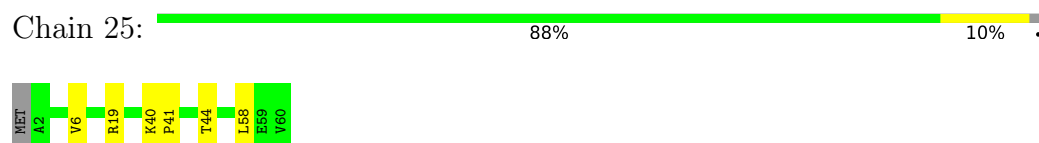
- Molecule 26: 50S ribosomal protein L31



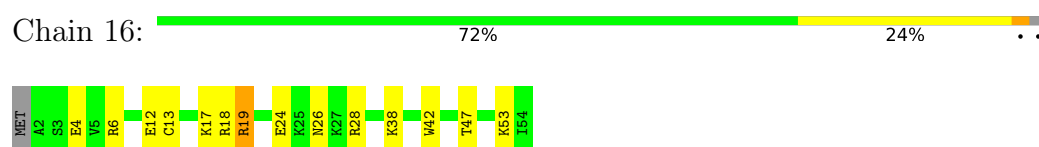
- Molecule 27: 50S ribosomal protein L32



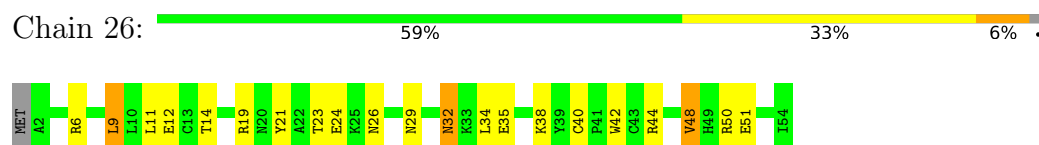
- Molecule 27: 50S ribosomal protein L32



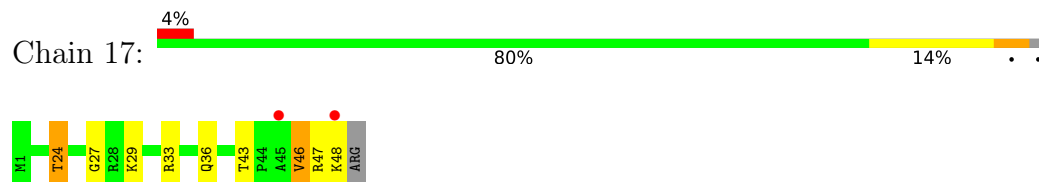
- Molecule 28: 50S ribosomal protein L33



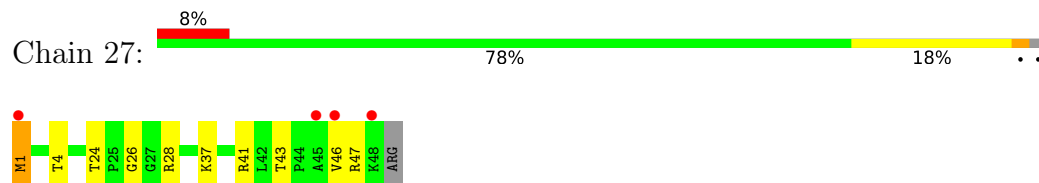
- Molecule 28: 50S ribosomal protein L33



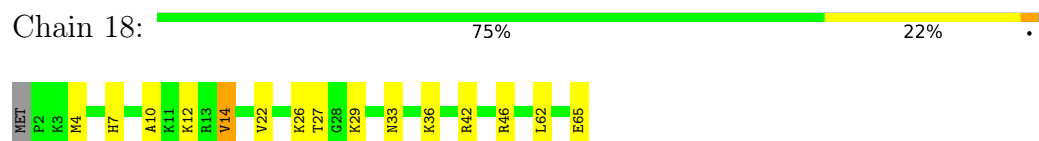
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

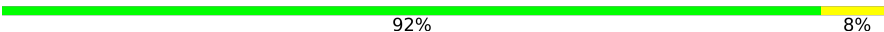


- Molecule 30: 50S ribosomal protein L35

Chain 28:  75% 23% .



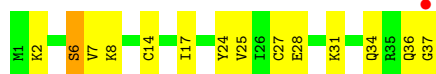
- Molecule 31: 50S ribosomal protein L36

Chain 19:  92% 8%



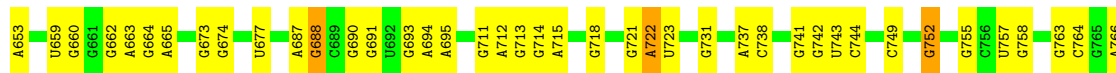
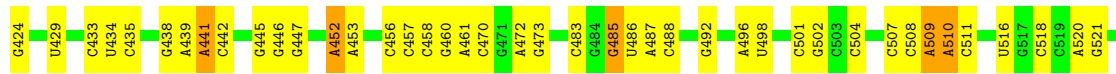
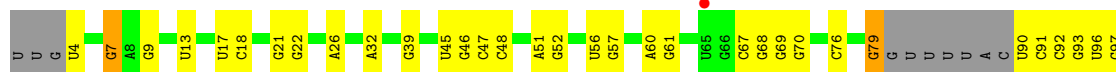
- Molecule 31: 50S ribosomal protein L36

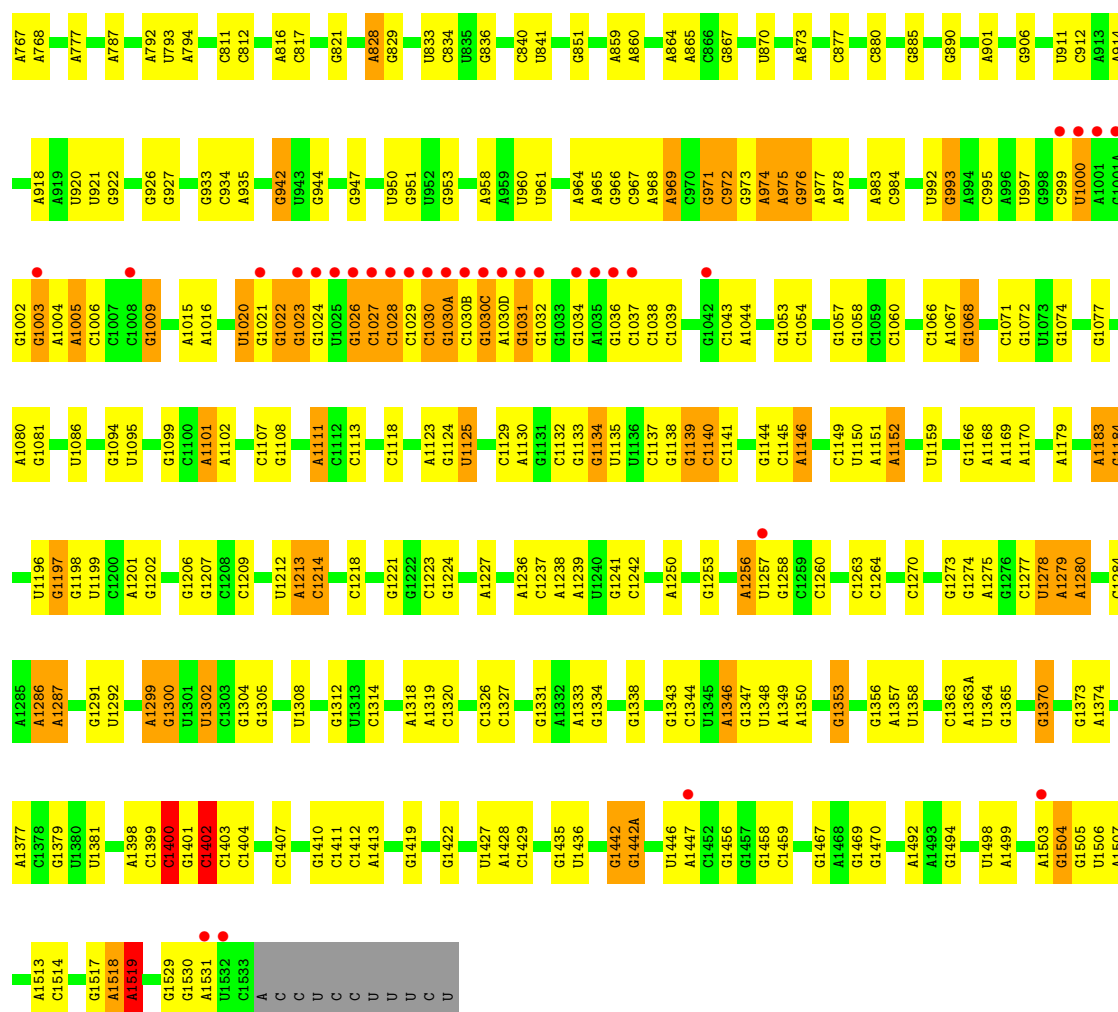
Chain 29:  3% 62% 35% .



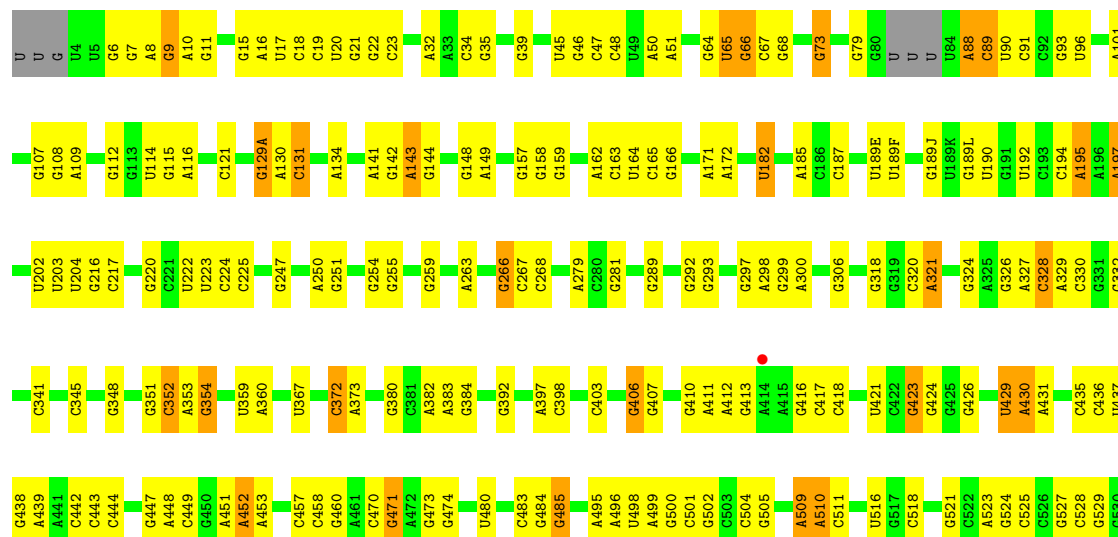
- Molecule 32: 16S Ribosomal RNA

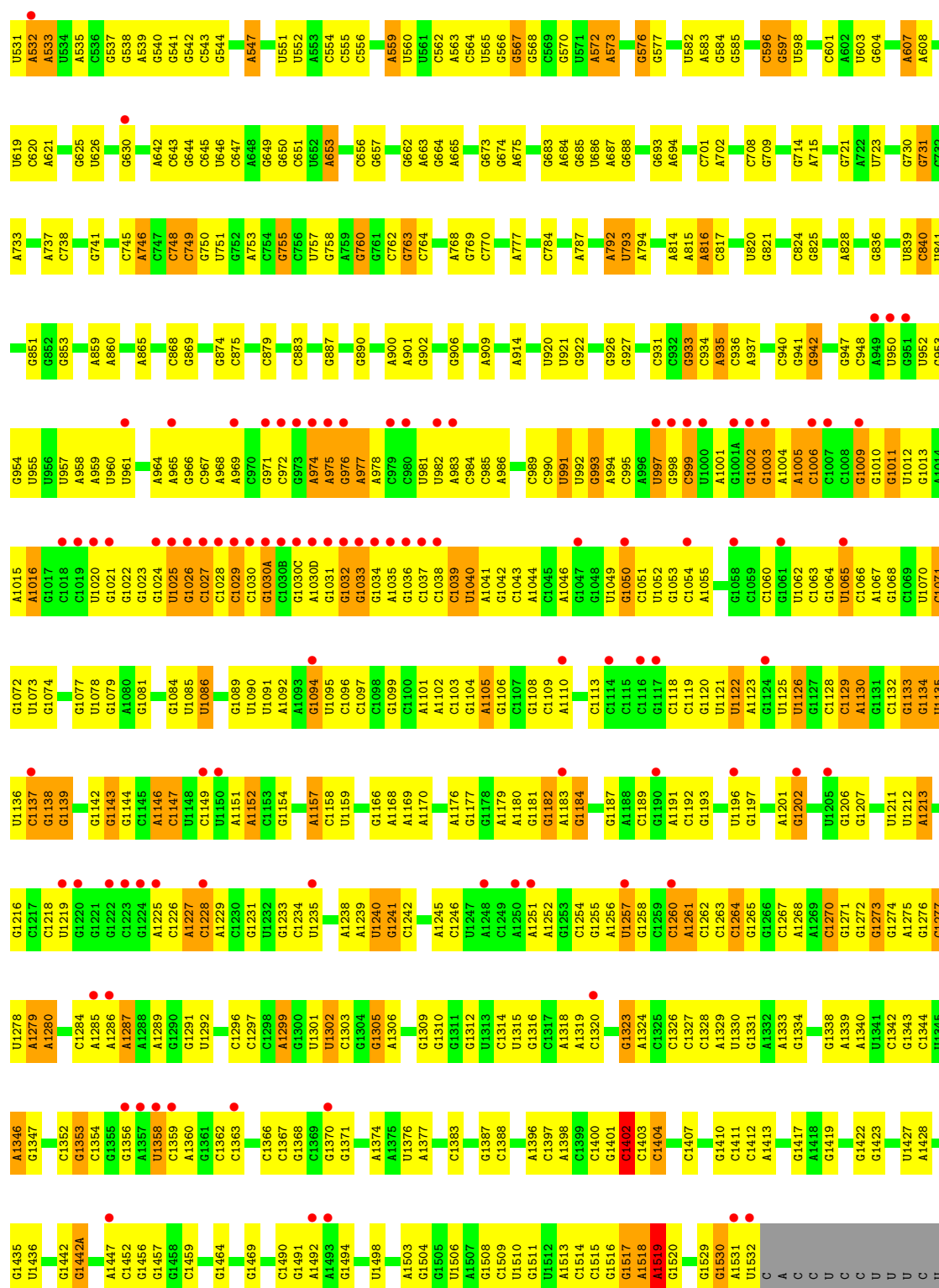
Chain 1a:  3% 61% 31% 6% .

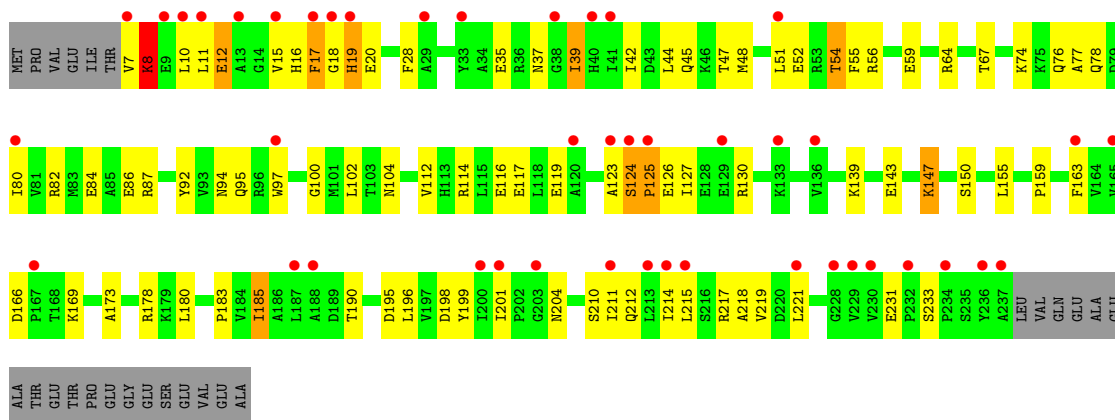




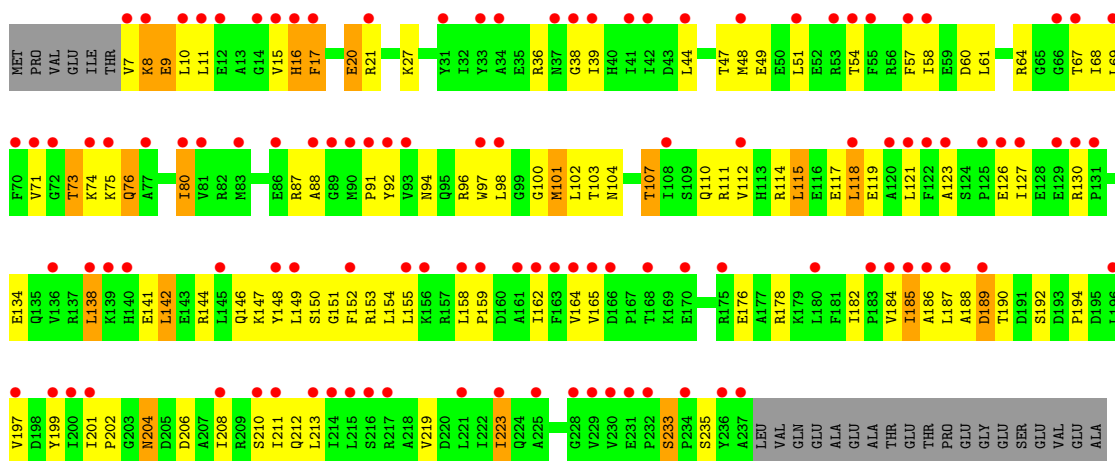
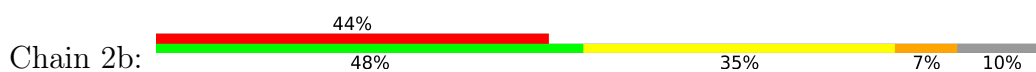
• Molecule 32: 16S Ribosomal RNA



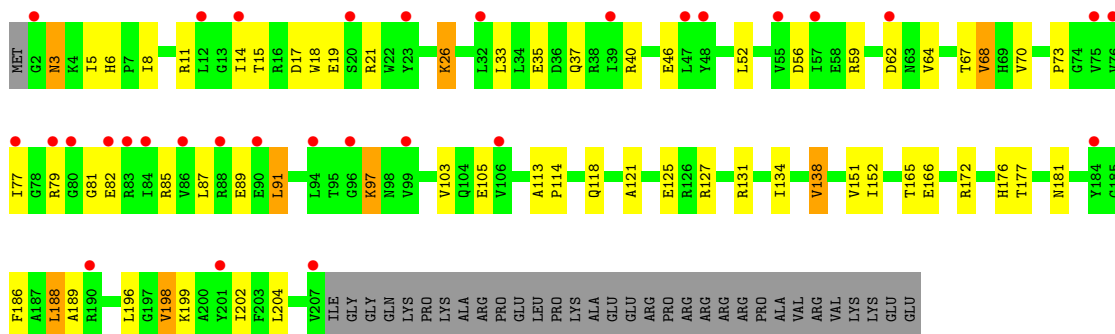




• Molecule 33: 30S ribosomal protein S2

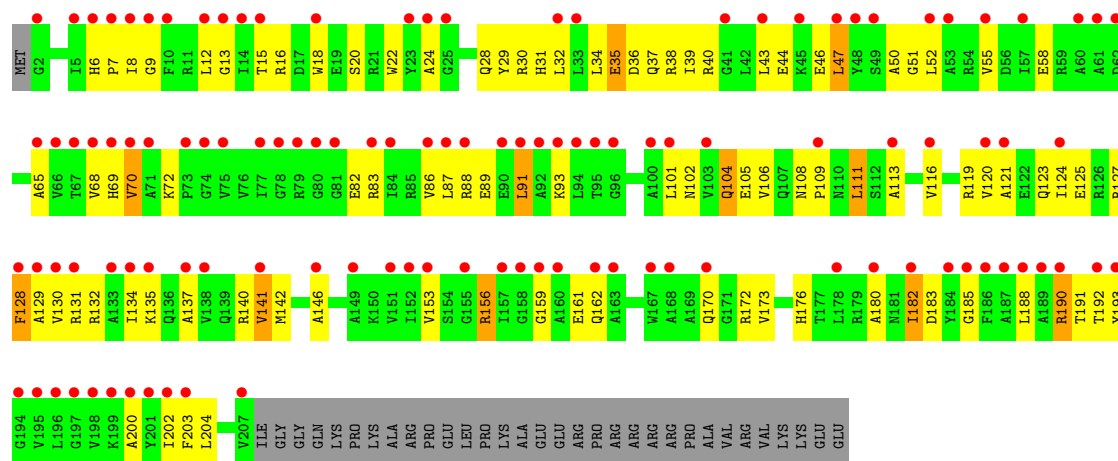


• Molecule 34: 30S ribosomal protein S3



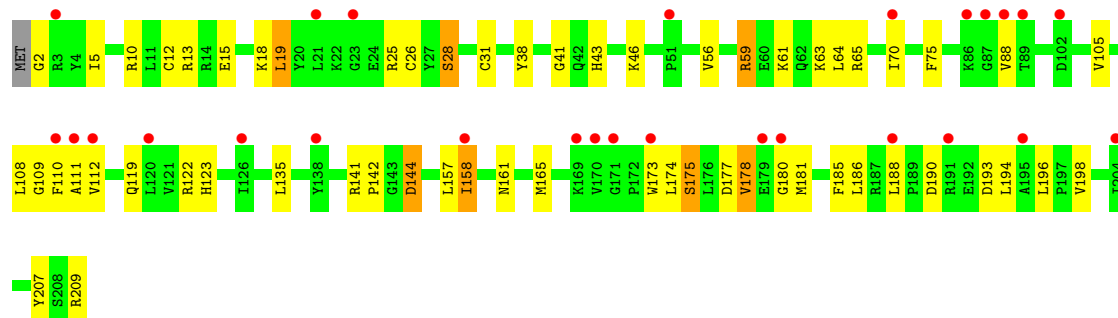
• Molecule 34: 30S ribosomal protein S3





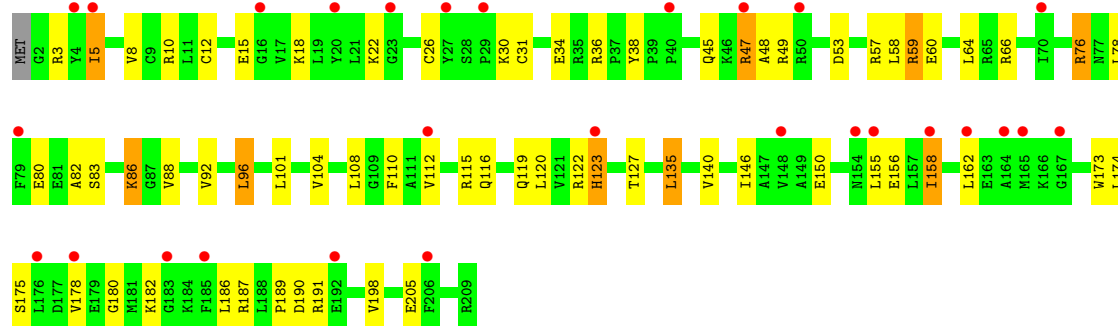
• Molecule 35: 30S ribosomal protein S4

Chain 1d: 13% 71% 25%



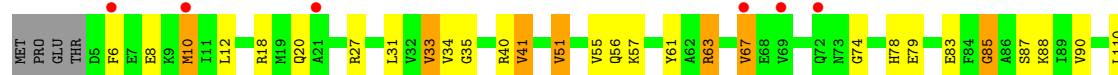
• Molecule 35: 30S ribosomal protein S4

Chain 2d: 13% 67% 28%



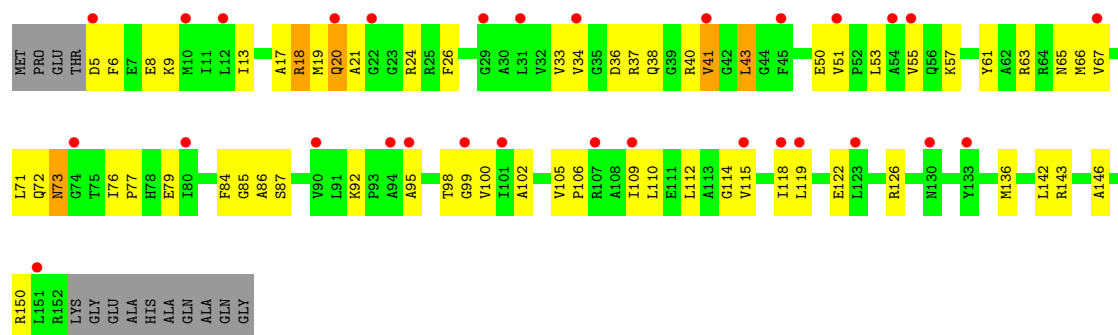
• Molecule 36: 30S ribosomal protein S5

Chain 1e: 4% 64% 22% 5% 9%

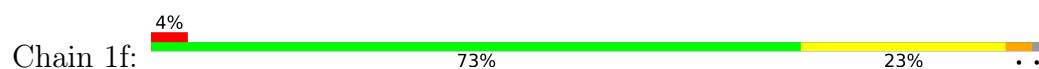




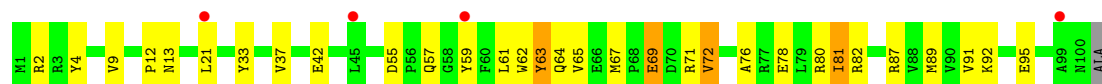
- Molecule 36: 30S ribosomal protein S5



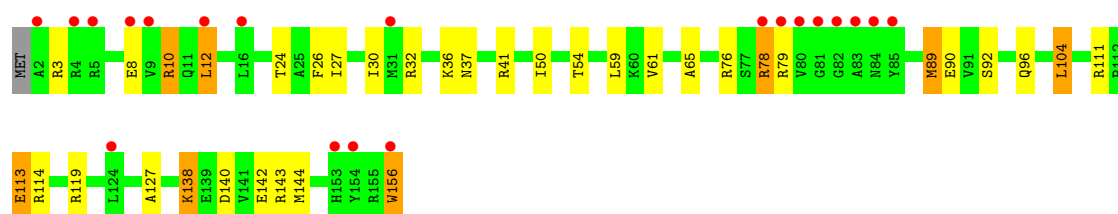
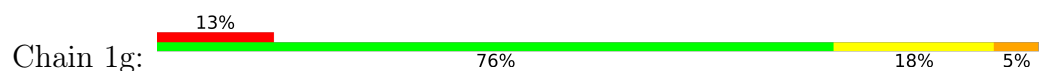
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

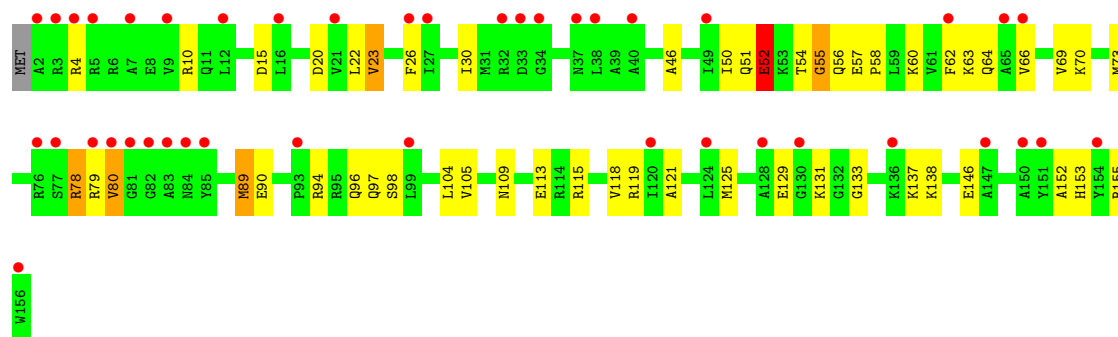


- Molecule 38: 30S ribosomal protein S7

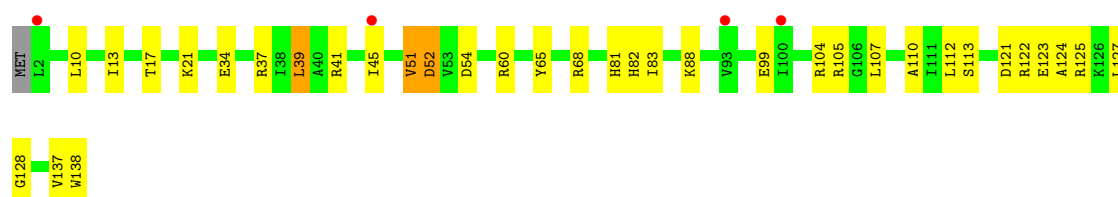
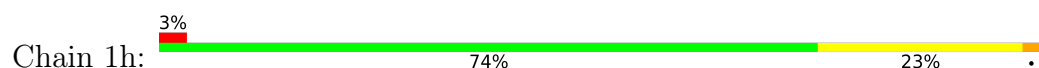


- Molecule 38: 30S ribosomal protein S7

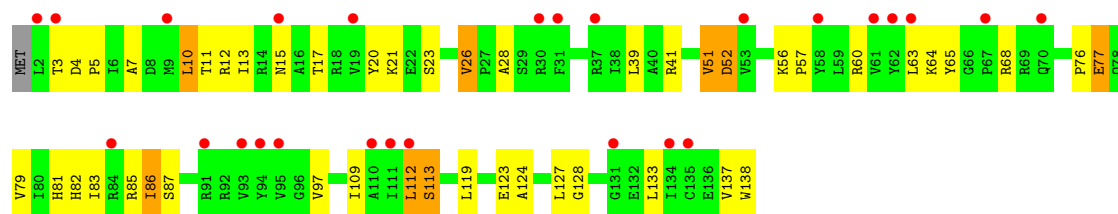




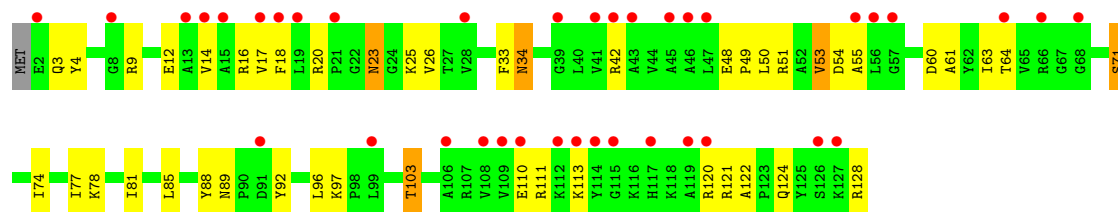
• Molecule 39: 30S ribosomal protein S8



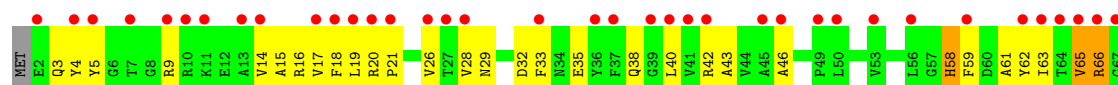
• Molecule 39: 30S ribosomal protein S8

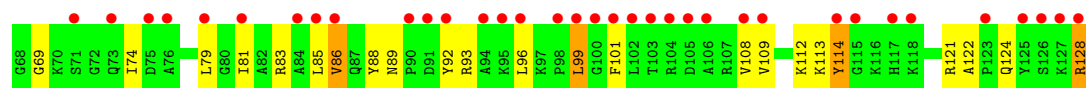


• Molecule 40: 30S ribosomal protein S9

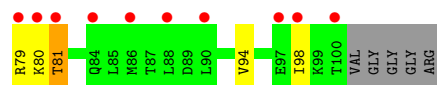
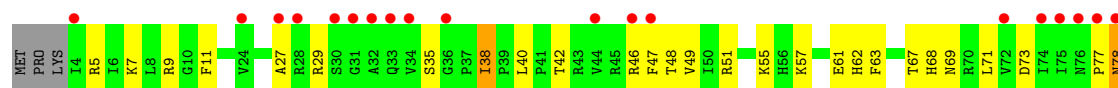


• Molecule 40: 30S ribosomal protein S9

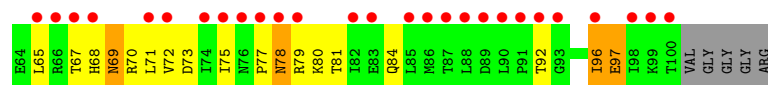
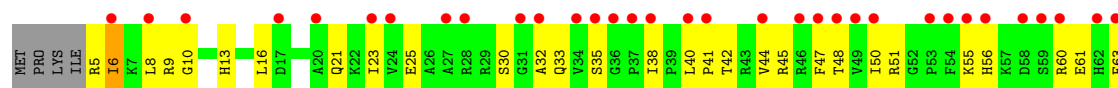




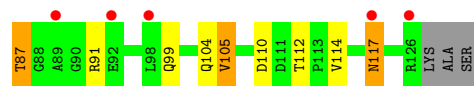
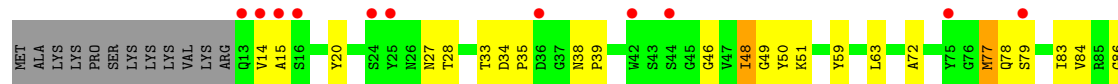
• Molecule 41: 30S ribosomal protein S10



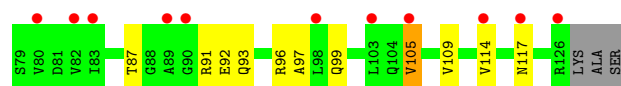
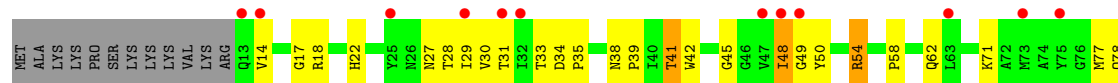
• Molecule 41: 30S ribosomal protein S10



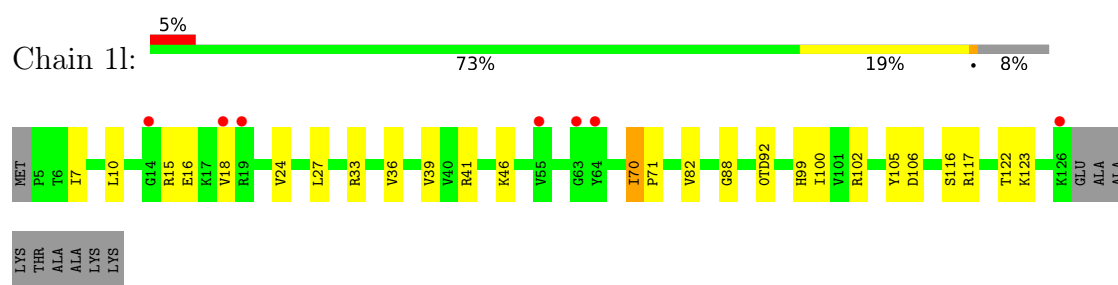
• Molecule 42: 30S ribosomal protein S11



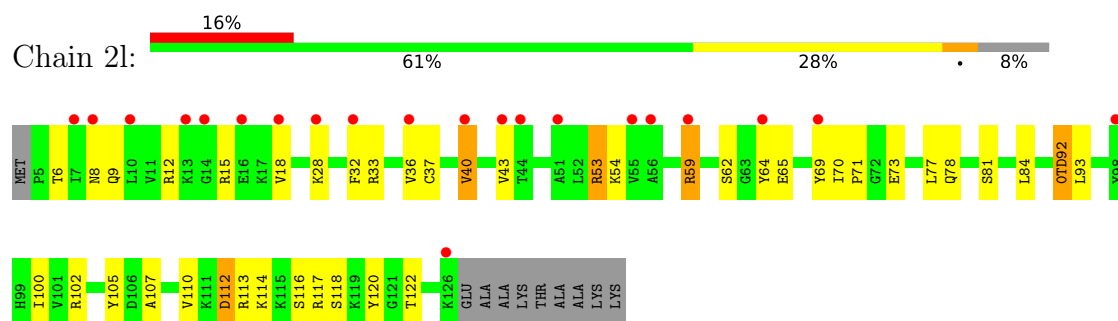
• Molecule 42: 30S ribosomal protein S11



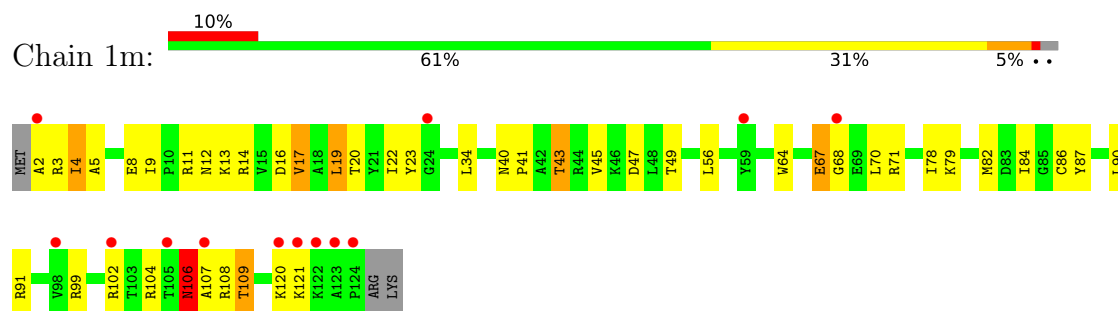
• Molecule 43: 30S ribosomal protein S12



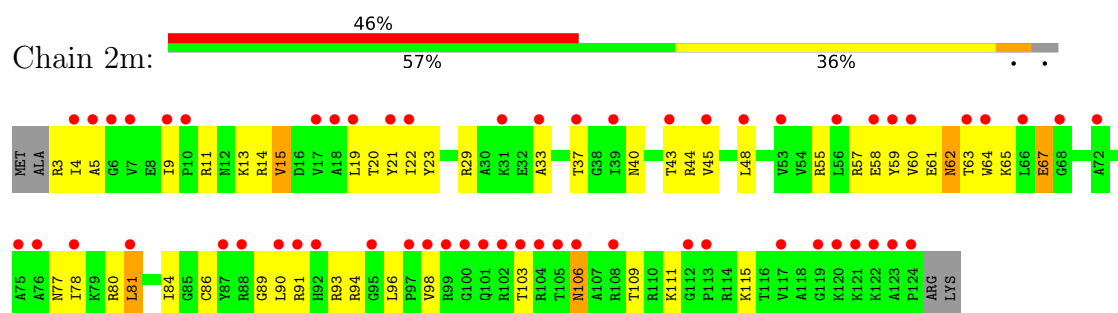
- Molecule 43: 30S ribosomal protein S12



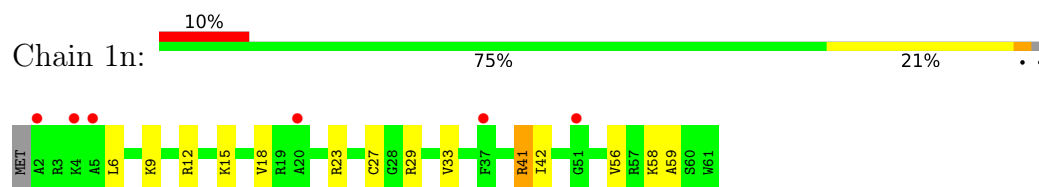
- Molecule 44: 30S ribosomal protein S13



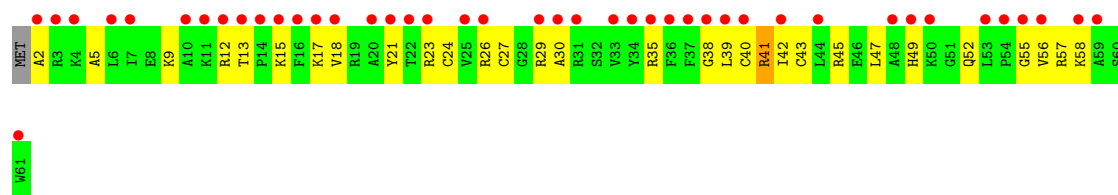
- Molecule 44: 30S ribosomal protein S13



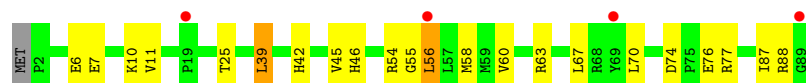
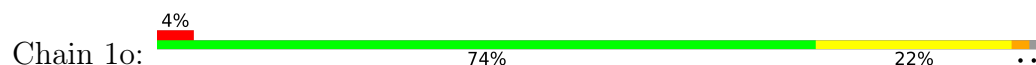
- Molecule 45: 30S ribosomal protein S14 type Z



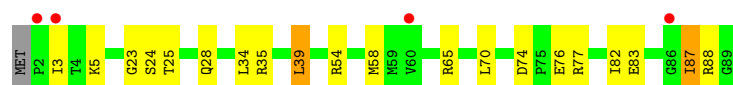
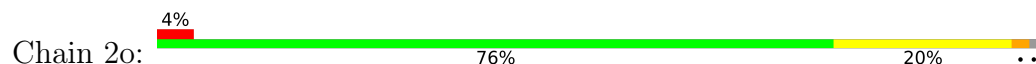
- Molecule 45: 30S ribosomal protein S14 type Z



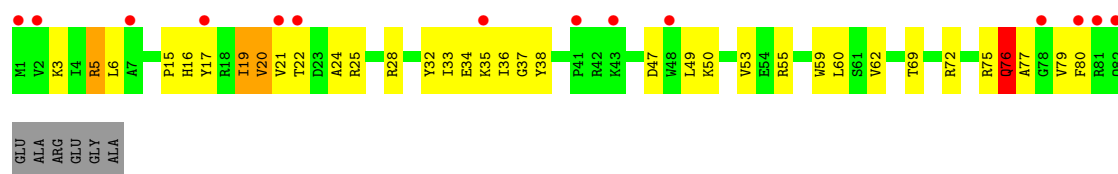
- Molecule 46: 30S ribosomal protein S15



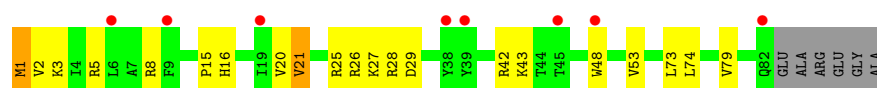
- Molecule 46: 30S ribosomal protein S15



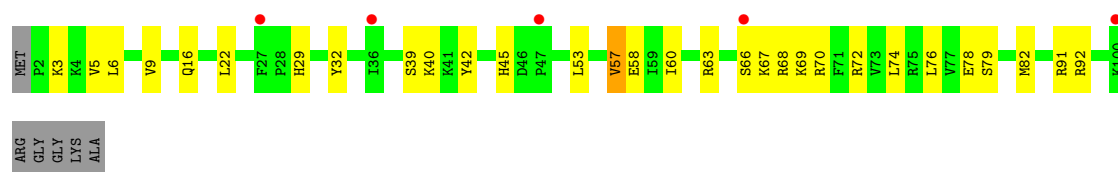
- Molecule 47: 30S ribosomal protein S16



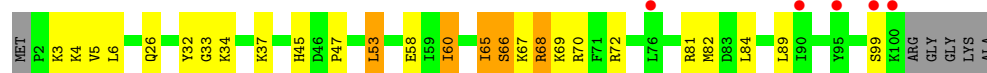
- Molecule 47: 30S ribosomal protein S16



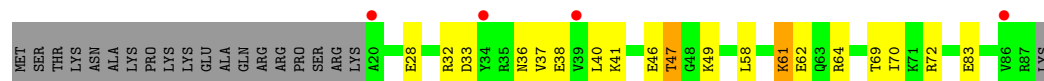
- Molecule 48: 30S ribosomal protein S17



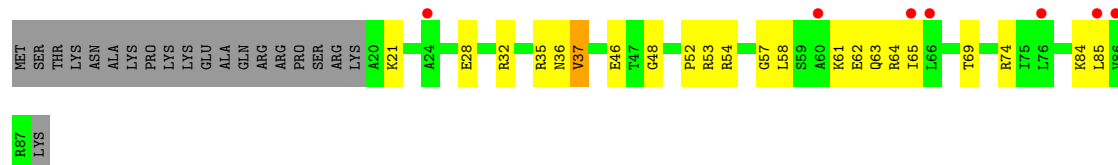
- Molecule 48: 30S ribosomal protein S17



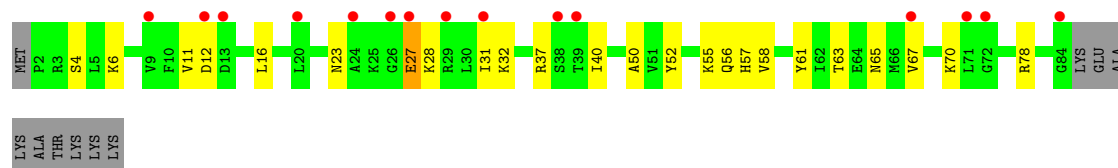
- Molecule 49: 30S ribosomal protein S18



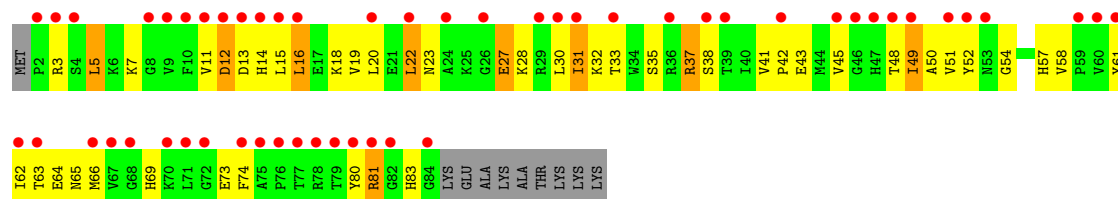
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19

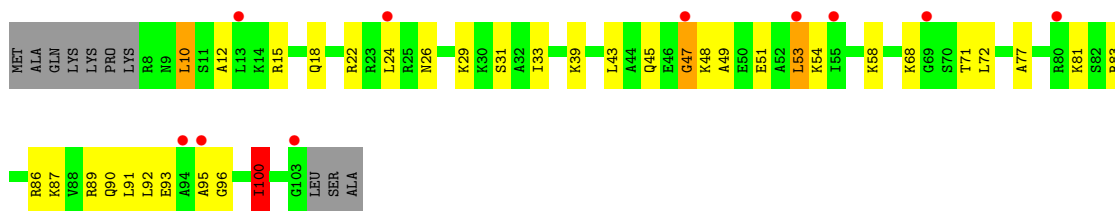


- Molecule 50: 30S ribosomal protein S19

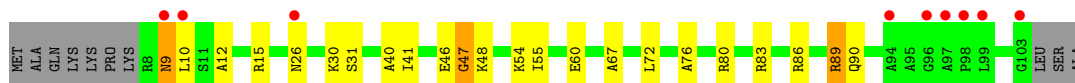


- Molecule 51: 30S ribosomal protein S20

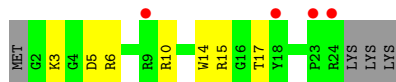




- Molecule 51: 30S ribosomal protein S20



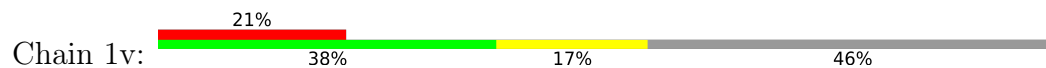
- Molecule 52: 30S ribosomal protein Thx



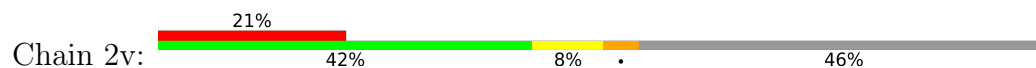
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: MG-mRNA



- Molecule 53: MG-mRNA

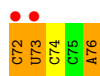
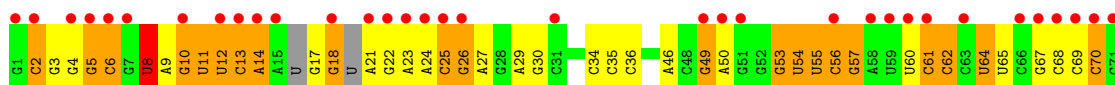


- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly

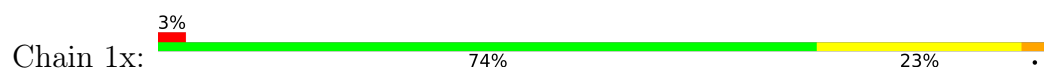




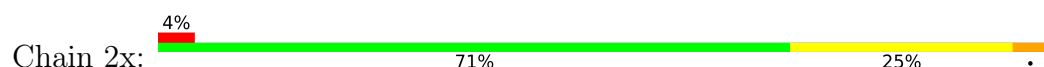
• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



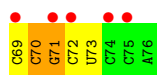
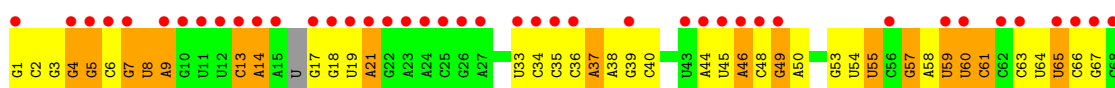
• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet



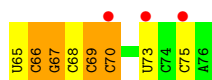
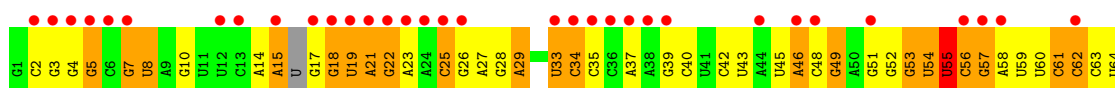
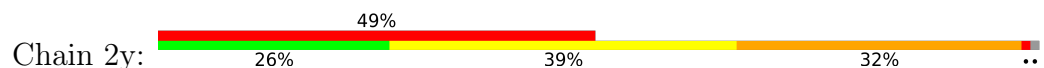
• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet



• Molecule 56: E-site Deacylated tRNAgly



• Molecule 56: E-site Deacylated tRNAgly



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.61Å 451.44Å 624.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.30 – 2.55 146.30 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (146.30-2.55) 99.4 (146.30-2.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.263 0.221 , 0.263	Depositor DCC
R_{free} test set	95245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299852	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: K, OMG, 31H, 5MC, G7M, MG, 4OC, ZN, L3X, 4SU, M2G, 0TD, OMU, 2MG, SF4, UR3, PSU, 5MU, 2MA, OMC, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.27	0/69011	0.47	3/107720 (0.0%)
1	2A	0.21	0/67295	0.41	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.19	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.49	0/2944
3	2D	0.21	0/2186	0.44	0/2944
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.26	0/1618	0.48	0/2191
5	2F	0.20	0/1614	0.45	2/2186 (0.1%)
6	1G	0.21	0/1448	0.45	0/1957
6	2G	0.20	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.38	0/1834
8	1I	0.19	0/1112	0.39	0/1514
8	2I	0.19	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.48	0/1543
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.25	0/943	0.45	0/1269
10	2O	0.19	0/943	0.41	0/1269
11	1P	0.25	0/1152	0.53	0/1533
11	2P	0.22	0/1152	0.50	0/1533
12	1Q	0.27	0/1143	0.46	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.48	0/1312
13	2R	0.20	0/982	0.46	0/1312
14	1S	0.21	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.25	0/1105	0.50	1/1477 (0.1%)
15	2T	0.19	0/1097	0.41	0/1468
16	1U	0.27	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.27	0/782	0.49	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.29	0/897	0.45	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.26	0/764	0.52	0/1025
19	2X	0.19	0/764	0.45	2/1025 (0.2%)
20	1Y	0.21	0/819	0.46	0/1095
20	2Y	0.19	0/819	0.45	0/1095
21	1Z	0.22	0/1267	0.45	0/1717
21	2Z	0.24	0/1299	0.42	0/1763
22	10	0.27	0/662	0.48	0/881
22	20	0.20	0/662	0.47	0/881
23	11	0.25	0/762	0.47	0/1014
23	21	0.22	0/762	0.40	0/1014
24	12	0.26	0/590	0.44	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.18	0/469	0.40	0/630
26	14	0.25	0/565	0.59	0/761
26	24	0.26	0/545	0.47	0/737
27	15	0.26	0/469	0.49	0/635
27	25	0.21	0/469	0.40	0/635
28	16	0.26	0/460	0.44	0/613
28	26	0.22	0/456	0.42	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.23	0/426	0.48	0/561
30	18	0.24	0/525	0.49	0/691
30	28	0.17	0/525	0.39	0/691
31	19	0.26	0/310	0.50	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.20	0/35795	0.40	1/55864 (0.0%)
32	2a	0.19	0/35886	0.37	0/56005
33	1b	0.21	0/1881	0.47	0/2542
33	2b	0.22	0/1860	0.48	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.22	0/1566	0.43	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.21	0/1145	0.45	0/1543
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.20	0/823	0.41	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	0.40	0/1679
38	2g	0.20	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.39	0/1494
39	2h	0.18	0/1108	0.38	0/1494
40	1i	0.19	0/1002	0.47	0/1346
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.20	0/722	0.46	0/982
41	2j	0.22	0/727	0.44	0/988
42	1k	0.19	0/844	0.42	0/1145
42	2k	0.18	0/848	0.37	0/1149
43	1l	0.20	0/937	0.41	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.21	0/969	0.47	0/1302
44	2m	0.20	0/961	0.47	0/1291
45	1n	0.18	0/501	0.40	0/664
45	2n	0.19	0/501	0.44	0/664
46	1o	0.20	0/739	0.37	0/985
46	2o	0.16	0/739	0.38	0/985
47	1p	0.20	0/697	0.48	0/939
47	2p	0.18	0/693	0.43	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.19	0/836	0.44	1/1117 (0.1%)
49	1r	0.18	0/560	0.42	0/746
49	2r	0.17	0/560	0.37	0/746
50	1s	0.19	0/667	0.47	0/900
50	2s	0.25	0/661	0.57	0/893
51	1t	0.19	0/730	0.47	0/965
51	2t	0.19	0/729	0.43	0/965
52	1u	0.18	0/203	0.46	0/266
52	2u	0.20	0/203	0.42	0/266
53	1v	0.21	0/322	0.30	0/501
53	2v	0.21	0/322	0.34	0/501
54	1w	0.28	1/1639 (0.1%)	0.42	0/2548
54	2w	0.29	1/1616 (0.1%)	0.42	0/2510
55	1x	0.26	0/1723	0.41	0/2684
55	2x	0.24	0/1723	0.38	0/2684
56	1y	0.29	0/1664	0.43	0/2587
56	2y	0.31	1/1664 (0.1%)	0.46	0/2587
All	All	0.23	3/316940 (0.0%)	0.43	11/474518 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	8	4SU	O3'-P	5.61	1.61	1.56
54	1w	8	4SU	O3'-P	5.38	1.61	1.56
54	2w	8	4SU	O3'-P	5.31	1.61	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.74	119.61	109.50
1	1A	2689	U	C4'-C3'-O3'	6.12	118.58	109.40
1	2A	1992	G	C2'-C3'-O3'	5.92	118.38	109.50
48	2q	65	ILE	N-CA-C	-5.77	107.19	112.96
1	1A	2689	U	P-O3'-C3'	5.57	128.56	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	508	0
1	2A	60322	0	30427	611	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	50	0
3	1D	2136	0	2218	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2D	2136	0	2218	39	0
4	1E	1559	0	1618	22	0
4	2E	1559	0	1618	26	0
5	1F	1583	0	1625	35	0
5	2F	1579	0	1619	45	0
6	1G	1423	0	1436	26	0
6	2G	1428	0	1438	55	0
7	1H	1330	0	1407	19	0
7	2H	1330	0	1407	25	0
8	1I	1097	0	1140	29	0
8	2I	1064	0	1082	42	0
9	1N	1117	0	1184	9	0
9	2N	1117	0	1184	12	0
10	1O	933	0	996	17	0
10	2O	933	0	996	9	0
11	1P	1135	0	1212	24	0
11	2P	1135	0	1212	29	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	8	0
13	2R	968	0	1033	18	0
14	1S	873	0	927	13	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	7	0
16	2U	959	0	1019	18	0
17	1V	771	0	830	7	0
17	2V	771	0	830	12	0
18	1W	886	0	940	7	0
18	2W	886	0	940	6	0
19	1X	750	0	814	20	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	42	0
22	10	653	0	674	13	0
22	20	653	0	674	14	0
23	11	755	0	826	10	0
23	21	755	0	826	15	0
24	12	588	0	643	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	22	588	0	643	10	0
25	13	469	0	518	5	0
25	23	464	0	514	8	0
26	14	552	0	533	28	0
26	24	532	0	503	33	0
27	15	455	0	465	0	0
27	25	455	0	465	2	0
28	16	453	0	473	8	0
28	26	449	0	469	12	0
29	17	418	0	467	6	0
29	27	418	0	467	7	0
30	18	517	0	582	12	0
30	28	517	0	582	10	0
31	19	307	0	335	2	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	344	0
32	2a	32327	0	16338	482	0
33	1b	1846	0	1867	47	0
33	2b	1825	0	1828	84	0
34	1c	1548	0	1535	37	0
34	2c	1542	0	1517	77	0
35	1d	1655	0	1672	35	0
35	2d	1674	0	1714	48	0
36	1e	1129	0	1185	28	0
36	2e	1133	0	1191	41	0
37	1f	810	0	804	16	0
37	2f	816	0	808	20	0
38	1g	1231	0	1238	20	0
38	2g	1235	0	1249	32	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	37	0
40	1i	983	0	986	26	0
40	2i	978	0	966	45	0
41	1j	709	0	650	21	0
41	2j	714	0	672	35	0
42	1k	829	0	825	19	0
42	2k	833	0	836	22	0
43	1l	932	0	980	13	0
43	2l	932	0	980	26	0
44	1m	958	0	1002	32	0
44	2m	950	0	988	49	0
45	1n	492	0	529	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	2n	492	0	529	27	0
46	1o	728	0	760	12	0
46	2o	728	0	760	11	0
47	1p	681	0	697	26	0
47	2p	677	0	686	12	0
48	1q	823	0	891	22	0
48	2q	823	0	891	16	0
49	1r	555	0	618	12	0
49	2r	555	0	618	13	0
50	1s	652	0	662	19	0
50	2s	646	0	644	35	0
51	1t	728	0	798	27	0
51	2t	727	0	796	16	0
52	1u	199	0	208	5	0
52	2u	199	0	208	10	0
53	1v	286	0	142	1	0
53	2v	286	0	142	3	0
54	1w	1556	0	779	42	0
54	2w	1536	0	770	44	0
55	1x	1656	0	849	10	0
55	2x	1656	0	849	11	0
56	1y	1552	0	791	24	0
56	2y	1552	0	791	41	0
57	10	9	0	0	0	0
57	11	2	0	0	0	0
57	12	1	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	7	0	0	0	0
57	16	3	0	0	0	0
57	17	5	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1096	0	0	0	0
57	1B	36	0	0	0	0
57	1D	12	0	0	0	0
57	1E	16	0	0	0	0
57	1F	15	0	0	0	0
57	1G	4	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1P	6	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	2	0	0	0	0
57	1U	9	0	0	0	0
57	1V	7	0	0	0	0
57	1W	7	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	224	0	0	0	0
57	1b	2	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	2	0	0	0	0
57	1n	2	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1w	9	0	0	0	0
57	1x	12	0	0	0	0
57	20	2	0	0	0	0
57	21	2	0	0	0	0
57	23	3	0	0	0	0
57	25	5	0	0	0	0
57	26	1	0	0	0	0
57	27	2	0	0	0	0
57	28	3	0	0	0	0
57	2A	861	0	0	0	0
57	2B	18	0	0	0	0
57	2D	7	0	0	0	0
57	2E	9	0	0	0	0
57	2F	6	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
57	2Q	4	0	0	0	0
57	2R	2	0	0	0	0
57	2T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2U	2	0	0	0	0
57	2V	3	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	2Z	1	0	0	0	0
57	2a	226	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	2	0	0	0	0
57	2k	1	0	0	0	0
57	2l	3	0	0	0	0
57	2q	2	0	0	0	0
57	2r	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	4	0	0	0	0
57	2x	6	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	1	0
60	2d	8	0	0	0	0
61	10	12	0	0	0	0
61	11	8	0	0	0	0
61	12	3	0	0	0	0
61	13	6	0	0	1	0
61	15	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	16	4	0	0	0	0
61	17	9	0	0	0	0
61	18	12	0	0	1	0
61	1A	1984	0	0	62	0
61	1B	63	0	0	5	0
61	1D	27	0	0	0	0
61	1E	27	0	0	1	0
61	1F	17	0	0	1	0
61	1G	4	0	0	1	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	4	0	0	0	0
61	1O	5	0	0	0	0
61	1P	17	0	0	0	0
61	1Q	8	0	0	0	0
61	1R	6	0	0	1	0
61	1S	2	0	0	0	0
61	1T	9	0	0	0	0
61	1U	10	0	0	0	0
61	1V	11	0	0	0	0
61	1W	9	0	0	1	0
61	1X	6	0	0	2	0
61	1Y	4	0	0	1	0
61	1a	278	0	0	18	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1e	1	0	0	0	0
61	1f	1	0	0	0	0
61	1i	1	0	0	0	0
61	1l	6	0	0	0	0
61	1m	1	0	0	0	0
61	1o	1	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	1	0
61	1v	4	0	0	0	0
61	1w	7	0	0	0	0
61	1x	12	0	0	0	0
61	1y	1	0	0	0	0
61	20	3	0	0	0	0
61	21	9	0	0	0	0
61	23	2	0	0	0	0
61	25	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	27	4	0	0	0	0
61	28	6	0	0	0	0
61	29	1	0	0	0	0
61	2A	1142	0	0	70	0
61	2B	21	0	0	1	0
61	2D	28	0	0	1	0
61	2E	12	0	0	0	0
61	2F	17	0	0	0	0
61	2I	1	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	8	0	0	0	0
61	2Q	1	0	0	0	0
61	2R	4	0	0	1	0
61	2T	5	0	0	0	0
61	2U	2	0	0	0	0
61	2W	2	0	0	0	0
61	2X	3	0	0	1	0
61	2Y	1	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	210	0	0	24	0
61	2d	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	3	0	0	1	0
61	2p	1	0	0	0	0
61	2q	2	0	0	0	0
61	2r	1	0	0	0	0
61	2t	3	0	0	0	0
61	2v	1	0	0	0	0
61	2w	1	0	0	0	0
61	2x	3	0	0	0	0
All	All	299852	0	196662	3800	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 3800 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:1054:A:N6	1:1A:1105:U:H3	1.39	1.20
1:1A:1082:U:H3	1:1A:1086:A:N6	1.42	1.17
1:1A:1055:G:H1	1:1A:1104:C:H42	1.07	1.00
32:2a:1025:U:H3	32:2a:1036:G:H1	1.10	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	2.00	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	34
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	34
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	24	34
5	2F	200/210 (95%)	188 (94%)	10 (5%)	2 (1%)	12	17
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11	15
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	7	8
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	29
7	2H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	21	29
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18	25
9	1N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	25
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	25
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	22
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	11
11	2P	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	9	11
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	20
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7	9
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%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	17
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	17
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	14	20
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5	5
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	7
20	2Y	105/110 (96%)	95 (90%)	7 (7%)	3 (3%)	3	3
21	1Z	148/206 (72%)	127 (86%)	19 (13%)	2 (1%)	9	11
21	2Z	156/206 (76%)	132 (85%)	22 (14%)	2 (1%)	9	12
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	15
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	15
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	7
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	30 (13%)	7 (3%)	3	2
33	2b	229/256 (90%)	181 (79%)	43 (19%)	5 (2%)	5	5
34	1c	204/239 (85%)	184 (90%)	20 (10%)	0	100	100
34	2c	204/239 (85%)	173 (85%)	29 (14%)	2 (1%)	12	17
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24	34
35	2d	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
36	1e	146/162 (90%)	132 (90%)	13 (9%)	1 (1%)	18	25
36	2e	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	18	25
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	17
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9	12
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	6
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
39	2h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	18	25
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	22
40	2i	125/128 (98%)	102 (82%)	23 (18%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2	1
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2	1
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	4	3
42	2k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	14	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	114 (96%)	4 (3%)	1 (1%)	16	22
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	22
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	7	8
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	4	4
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9	12
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	5	5
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	8	10
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10	13
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	4	4
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	2
51	2t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	11	15
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11368/12128 (94%)	10449 (92%)	813 (7%)	106 (1%)	14	20

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
26	14	47	GLN
26	14	49	PHE
26	14	62	ARG

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	17	26
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	33
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26	39
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	21
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	5
5	2F	159/166 (96%)	152 (96%)	7 (4%)	25	38
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10	14
6	2G	143/156 (92%)	123 (86%)	20 (14%)	3	3
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22	34
7	2H	144/148 (97%)	132 (92%)	12 (8%)	10	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	2
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	4
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	17
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	27
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	42
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	53
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	9
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	9
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	51	70
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	23
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11	16
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	27
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	8
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	5
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	32
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	19
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	39
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	39
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12	17
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	50
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	29
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	76
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	59
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	18	27
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13	19
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	15
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5	6
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	62 (95%)	3 (5%)	24	36
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	60
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	17
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	53
24	22	65/67 (97%)	63 (97%)	2 (3%)	35	53
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	9
25	23	50/52 (96%)	48 (96%)	2 (4%)	28	42
26	14	59/63 (94%)	50 (85%)	9 (15%)	3	2
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	1
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	42
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	26
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	43
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	9
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	18
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	4
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	45
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	45
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	12
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9	12
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	4
34	2c	140/188 (74%)	123 (88%)	17 (12%)	5	5
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5	5
35	2d	173/181 (96%)	150 (87%)	23 (13%)	4	4
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	12
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6	8
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13	19
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18	27
38	1g	119/127 (94%)	102 (86%)	17 (14%)	3	3
38	2g	120/127 (94%)	112 (93%)	8 (7%)	15	21
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17	25
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	16
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	4
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3	2
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	7
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	6
42	1k	82/99 (83%)	76 (93%)	6 (7%)	13	18
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	7
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	18
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	8
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	7
44	2m	92/101 (91%)	86 (94%)	6 (6%)	15	22
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	33
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	17
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	8
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	12
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	31
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	23
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14	20
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59	75
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	2
51	1t	70/82 (85%)	66 (94%)	4 (6%)	18	28
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	28
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	29
All	All	9303/10064 (92%)	8561 (92%)	742 (8%)	11	15

5 of 742 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	2S	85	VAL
33	2b	184	VAL
16	2U	77	SER
14	2S	75	GLU
23	21	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
36	2e	78	HIS
51	2t	45	GLN
37	2f	100	ASN
42	2k	93	GLN
40	1i	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	418 (14%)	32 (1%)
1	2A	2791/2915 (95%)	430 (15%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	23 (19%)	0
32	1a	1497/1521 (98%)	234 (15%)	0
32	2a	1501/1521 (98%)	283 (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%)	2 (16%)	0
54	1w	70/74 (94%)	27 (38%)	0
54	2w	68/74 (91%)	31 (45%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
56	1y	71/74 (95%)	29 (40%)	0
56	2y	71/74 (95%)	35 (49%)	0
All	All	9344/9612 (97%)	1535 (16%)	57 (0%)

5 of 1535 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	71	A

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2439	A
1	2A	2439	A
1	2A	271(K)	U
1	2A	2406	U
1	2A	1913	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.78	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
56	PSU	2y	55	56	18,21,22	1.42	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.08	9 (27%)
54	PSU	2w	55	57,54	18,21,22	1.38	2 (11%)	21,30,33	2.08	3 (14%)
1	OMU	1A	2552	1	19,22,23	1.24	3 (15%)	25,31,34	1.96	6 (24%)
32	2MG	2a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.13	6 (18%)
54	L3X	2w	76	1,54	24,28,29	1.44	3 (12%)	27,40,43	2.07	8 (29%)
56	5MU	1y	54	56	19,22,23	1.44	4 (21%)	27,32,35	2.04	6 (22%)
54	4SU	1w	8	54	18,21,22	1.84	5 (27%)	25,30,33	2.11	6 (24%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.05	7 (25%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.97	1 (4%)
1	PSU	1A	2605	1,57	18,21,22	1.46	3 (16%)	21,30,33	2.01	5 (23%)
55	5MU	1x	54	55,57	19,22,23	1.46	5 (26%)	27,32,35	1.95	5 (18%)
56	4SU	2y	8	56	18,21,22	1.69	4 (22%)	25,30,33	2.08	4 (16%)
32	2MG	1a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.26	9 (27%)
32	5MC	1a	967	32	19,22,23	1.58	3 (15%)	26,32,35	1.15	2 (7%)
1	OMU	2A	2552	1,57	19,22,23	1.23	2 (10%)	25,31,34	1.88	5 (20%)
32	G7M	2a	527	32,57	23,26,27	1.49	4 (17%)	34,39,42	1.71	5 (14%)
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	1A	1942	1	19,22,23	1.55	3 (15%)	26,32,35	1.23	2 (7%)
1	2MA	2A	2503	1,57	22,25,26	1.46	4 (18%)	32,37,40	2.30	9 (28%)
54	5MU	2w	54	54	19,22,23	1.39	4 (21%)	27,32,35	1.67	6 (22%)
54	4SU	2w	8	54	18,21,22	1.73	4 (22%)	25,30,33	2.79	5 (20%)
56	5MU	2y	54	56	19,22,23	1.50	4 (21%)	27,32,35	1.74	8 (29%)
43	0TD	1l	92	43	8,9,10	4.42	1 (12%)	6,11,13	7.30	2 (33%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
55	5MC	1x	32	55	19,22,23	1.58	3 (15%)	26,32,35	1.25	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.00	4 (19%)
43	0TD	2l	92	43	8,9,10	4.55	1 (12%)	6,11,13	3.19	3 (50%)
1	OMG	2A	2251	1,55	23,26,27	1.23	3 (13%)	32,38,41	1.94	6 (18%)
1	5MC	2A	1962	1,57	19,22,23	1.74	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.98	3 (14%)
32	G7M	1a	527	32,57	23,26,27	1.54	4 (17%)	34,39,42	1.72	5 (14%)
1	2MA	1A	2503	1,57	22,25,26	1.49	4 (18%)	32,37,40	2.36	8 (25%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.06	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	27,32,35	1.95	6 (22%)
32	5MC	2a	967	32	19,22,23	1.78	3 (15%)	26,32,35	1.10	3 (11%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.19	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.18	4 (15%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.05	4 (19%)
1	OMG	1A	2251	1,55,57	23,26,27	1.25	3 (13%)	32,38,41	1.95	7 (21%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.91	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.75	4 (15%)
54	L3X	1w	76	1,54	24,28,29	1.40	3 (12%)	27,40,43	2.10	9 (33%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.06	9 (27%)
55	4SU	1x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.68	6 (24%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.25	3 (11%)
55	31H	2x	76	55,57	31,34,35	1.15	3 (9%)	35,47,50	2.38	14 (40%)
32	PSU	1a	516	32	18,21,22	1.42	2 (11%)	21,30,33	1.92	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.85	3 (15%)	26,32,35	1.25	4 (15%)
1	5MU	2A	1939	1,57	19,22,23	1.38	5 (26%)	27,32,35	2.38	6 (22%)
54	5MU	1w	54	54	19,22,23	1.38	4 (21%)	27,32,35	1.79	6 (22%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.06	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.54	2 (10%)	26,32,35	1.16	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.07	5 (18%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.99	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.00	9 (27%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.89	5 (15%)
55	31H	1x	76	55,57	31,34,35	1.18	3 (9%)	35,47,50	2.05	13 (37%)
1	5MC	2A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.12	2 (7%)
1	5MC	1A	1962	1	19,22,23	1.85	3 (15%)	26,32,35	1.24	3 (11%)
56	4SU	1y	8	56	18,21,22	1.87	6 (33%)	25,30,33	1.66	5 (20%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	2.07	9 (27%)
55	4SU	2x	8	55	18,21,22	1.98	5 (27%)	25,30,33	1.32	4 (16%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.89	6 (18%)
54	PSU	1w	55	57,54	18,21,22	1.42	2 (11%)	21,30,33	2.00	3 (14%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	1.94	4 (19%)
1	5MU	1A	1939	1,57	19,22,23	1.47	4 (21%)	27,32,35	2.12	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.10	3 (11%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	1.07	3 (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
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	PSU	2w	55	57,54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
54	L3X	2w	76	1,54	-	2/13/31/32	0/3/3/3
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
32	G7M	2a	527	32,57	-	1/7/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	32,57	-	3/7/25/26	0/3/3/3
1	2MA	1A	2503	1,57	-	2/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	L3X	1w	76	1,54	-	0/13/31/32	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	5/22/40/41	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
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
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	31H	1x	76	55,57	-	6/22/40/41	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1w	55	57,54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.44	1.69	1.82
43	1l	92	0TD	CB-SB	-11.93	1.70	1.82
32	1a	1404	5MC	C5-C4	6.93	1.49	1.44
1	1A	1962	5MC	C5-C4	6.90	1.49	1.44
32	2a	967	5MC	C5-C4	6.66	1.49	1.44

The worst 5 of 356 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.50	70.91	102.36
54	2w	8	4SU	C4-N3-C2	-8.54	119.13	127.31
1	2A	2503	2MA	C5-C4-N3	-8.31	118.43	127.18
1	1A	2503	2MA	C5-C4-N3	-8.01	118.75	127.18
32	2a	1498	UR3	C4-N3-C2	-7.02	118.93	124.58

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	76	L3X	O4'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'

There are no ring outliers.

31 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2y	55	PSU	1	0
32	2a	1519	MA6	3	0
54	2w	55	PSU	1	0
54	2w	76	L3X	1	0
56	2y	8	4SU	4	0
32	2a	1404	5MC	1	0
1	2A	2503	2MA	1	0
54	2w	54	5MU	1	0
54	2w	8	4SU	3	0
56	2y	54	5MU	1	0
43	2l	92	0TD	1	0
1	2A	2251	OMG	2	0
32	1a	1400	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1917	PSU	1	0
1	1A	2251	OMG	1	0
32	1a	1402	4OC	2	0
54	1w	76	L3X	1	0
32	1a	1519	MA6	2	0
55	1x	8	4SU	2	0
55	2x	76	31H	2	0
1	2A	1939	5MU	1	0
54	1w	54	5MU	2	0
32	2a	1518	MA6	3	0
55	1x	76	31H	1	0
56	1y	8	4SU	2	0
32	1a	1518	MA6	2	0
55	2x	8	4SU	2	0
54	1w	55	PSU	4	0
1	1A	1939	5MU	1	0
56	1y	55	PSU	1	0
32	2a	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2762 ligands modelled in this entry, 2760 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	1d	501	35	0,12,12	-	-	-		
60	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
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	501	SF4	1	0

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%)	-0.51	143 (5%) 34 33	17, 34, 92, 102	0
1	2A	2789/2915 (95%)	0.03	141 (5%) 33 33	32, 55, 90, 102	0
2	1B	120/121 (99%)	-0.36	0 100 100	29, 49, 63, 84	0
2	2B	120/121 (99%)	0.93	4 (3%) 49 50	61, 77, 85, 93	0
3	1D	275/276 (99%)	-0.07	4 (1%) 72 73	18, 35, 48, 70	0
3	2D	275/276 (99%)	0.42	7 (2%) 58 59	30, 49, 61, 78	0
4	1E	204/206 (99%)	-0.10	1 (0%) 87 89	17, 37, 57, 72	0
4	2E	204/206 (99%)	0.49	6 (2%) 53 55	32, 55, 67, 79	0
5	1F	202/210 (96%)	-0.13	2 (0%) 79 80	17, 40, 63, 81	0
5	2F	202/210 (96%)	0.48	3 (1%) 72 73	33, 65, 75, 80	0
6	1G	181/182 (99%)	0.67	15 (8%) 17 17	38, 58, 70, 80	0
6	2G	181/182 (99%)	1.60	50 (27%) 1 1	67, 77, 82, 88	0
7	1H	174/180 (96%)	0.24	2 (1%) 78 79	34, 50, 61, 64	0
7	2H	174/180 (96%)	1.31	23 (13%) 7 6	66, 78, 85, 88	0
8	1I	146/148 (98%)	0.99	11 (7%) 20 19	45, 70, 78, 83	0
8	2I	146/148 (98%)	1.40	31 (21%) 2 2	54, 71, 79, 81	0
9	1N	140/140 (100%)	-0.08	1 (0%) 84 86	24, 36, 57, 70	0
9	2N	140/140 (100%)	1.11	13 (9%) 14 13	44, 63, 75, 81	0
10	1O	122/122 (100%)	-0.09	1 (0%) 82 84	28, 38, 55, 63	0
10	2O	122/122 (100%)	0.42	0 100 100	42, 54, 68, 72	0
11	1P	149/150 (99%)	0.17	3 (2%) 65 65	18, 43, 63, 70	0
11	2P	149/150 (99%)	0.90	15 (10%) 12 11	39, 64, 77, 87	0
12	1Q	141/141 (100%)	-0.02	1 (0%) 84 86	25, 39, 52, 70	0
12	2Q	141/141 (100%)	0.95	11 (7%) 19 18	45, 63, 72, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.27	0 100 100	23, 32, 46, 56	0
13	2R	118/118 (100%)	0.17	0 100 100	38, 49, 58, 65	0
14	1S	110/112 (98%)	0.10	0 100 100	36, 49, 58, 66	0
14	2S	110/112 (98%)	1.52	29 (26%) 1 1	61, 72, 79, 83	0
15	1T	131/146 (89%)	0.23	4 (3%) 51 52	32, 43, 67, 76	0
15	2T	131/146 (89%)	0.55	5 (3%) 44 45	46, 57, 72, 77	0
16	1U	116/118 (98%)	-0.41	0 100 100	19, 27, 44, 61	0
16	2U	116/118 (98%)	0.75	2 (1%) 69 69	43, 60, 72, 77	0
17	1V	101/101 (100%)	-0.33	0 100 100	20, 35, 50, 63	0
17	2V	101/101 (100%)	1.16	9 (8%) 15 14	42, 69, 76, 79	0
18	1W	112/113 (99%)	-0.22	1 (0%) 81 83	22, 30, 49, 71	0
18	2W	112/113 (99%)	0.29	1 (0%) 81 83	38, 47, 65, 78	0
19	1X	95/96 (98%)	0.01	2 (2%) 63 64	25, 37, 57, 75	0
19	2X	95/96 (98%)	0.84	8 (8%) 17 16	45, 57, 73, 82	0
20	1Y	107/110 (97%)	0.19	2 (1%) 66 66	34, 47, 64, 75	0
20	2Y	107/110 (97%)	1.20	11 (10%) 12 11	55, 67, 77, 86	0
21	1Z	154/206 (74%)	1.06	28 (18%) 3 3	39, 61, 83, 86	0
21	2Z	160/206 (77%)	1.64	41 (25%) 1 1	62, 78, 87, 91	0
22	10	83/85 (97%)	0.12	4 (4%) 35 35	27, 36, 51, 64	0
22	20	83/85 (97%)	1.25	15 (18%) 3 3	43, 63, 71, 77	0
23	11	97/98 (98%)	0.26	1 (1%) 79 80	25, 44, 65, 69	0
23	21	97/98 (98%)	0.72	3 (3%) 51 52	39, 54, 71, 76	0
24	12	70/72 (97%)	0.20	2 (2%) 53 55	33, 46, 57, 72	0
24	22	70/72 (97%)	0.95	6 (8%) 16 15	58, 67, 76, 79	0
25	13	59/60 (98%)	-0.20	0 100 100	26, 33, 55, 70	0
25	23	59/60 (98%)	0.95	6 (10%) 12 11	52, 64, 72, 78	0
26	14	69/71 (97%)	1.32	17 (24%) 2 1	51, 72, 85, 89	0
26	24	69/71 (97%)	1.92	29 (42%) 0 0	74, 83, 89, 93	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 69	18, 28, 49, 59	0
27	25	59/60 (98%)	0.19	0 100 100	33, 48, 62, 75	0
28	16	53/54 (98%)	-0.20	0 100 100	30, 40, 55, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.76	0 100 100	54, 60, 66, 71	0
29	17	48/49 (97%)	-0.29	2 (4%) 40 41	19, 26, 51, 58	0
29	27	48/49 (97%)	0.25	4 (8%) 17 17	32, 39, 65, 70	0
30	18	64/65 (98%)	-0.28	0 100 100	24, 31, 39, 53	0
30	28	64/65 (98%)	0.56	0 100 100	44, 56, 63, 65	0
31	19	37/37 (100%)	-0.06	0 100 100	29, 37, 53, 55	0
31	29	37/37 (100%)	0.98	1 (2%) 56 57	58, 63, 75, 76	0
32	1a	1488/1521 (97%)	0.31	39 (2%) 57 58	33, 66, 89, 100	0
32	2a	1491/1521 (98%)	0.66	99 (6%) 24 24	48, 75, 92, 102	0
33	1b	231/256 (90%)	1.31	44 (19%) 3 2	59, 74, 82, 88	0
33	2b	231/256 (90%)	2.14	112 (48%) 0 0	73, 82, 87, 92	0
34	1c	206/239 (86%)	1.19	31 (15%) 5 5	58, 70, 78, 85	0
34	2c	206/239 (86%)	2.22	114 (55%) 0 0	70, 82, 86, 89	0
35	1d	208/209 (99%)	1.23	27 (12%) 7 6	53, 68, 76, 82	0
35	2d	208/209 (99%)	1.28	28 (13%) 7 5	60, 70, 77, 81	0
36	1e	148/162 (91%)	0.77	7 (4%) 36 36	46, 62, 71, 76	0
36	2e	148/162 (91%)	1.50	30 (20%) 3 2	67, 74, 81, 83	0
37	1f	100/101 (99%)	1.02	4 (4%) 42 43	55, 65, 73, 76	0
37	2f	100/101 (99%)	0.95	4 (4%) 42 43	59, 67, 75, 78	0
38	1g	155/156 (99%)	1.16	20 (12%) 7 6	58, 69, 81, 85	0
38	2g	155/156 (99%)	1.62	42 (27%) 1 1	69, 77, 84, 88	0
39	1h	137/138 (99%)	0.76	4 (2%) 53 55	51, 63, 70, 74	0
39	2h	137/138 (99%)	1.48	26 (18%) 3 2	65, 74, 79, 82	0
40	1i	127/128 (99%)	1.57	38 (29%) 1 1	51, 73, 78, 82	0
40	2i	127/128 (99%)	2.20	72 (56%) 0 0	73, 82, 86, 88	0
41	1j	97/105 (92%)	1.58	29 (29%) 1 1	57, 74, 81, 87	0
41	2j	96/105 (91%)	2.36	60 (62%) 0 0	75, 83, 87, 89	0
42	1k	114/129 (88%)	1.22	16 (14%) 6 5	41, 64, 74, 80	0
42	2k	114/129 (88%)	1.47	23 (20%) 3 2	56, 72, 78, 81	0
43	1l	121/132 (91%)	0.73	7 (5%) 29 28	42, 55, 65, 77	0
43	2l	121/132 (91%)	1.26	21 (17%) 4 3	59, 70, 77, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.28	13 (10%) 11 11	57, 68, 76, 87	0
44	2m	122/126 (96%)	2.24	58 (47%) 0 0	71, 80, 84, 91	0
45	1n	60/61 (98%)	1.14	6 (10%) 12 12	61, 66, 72, 76	0
45	2n	60/61 (98%)	2.75	43 (71%) 0 0	77, 82, 85, 87	0
46	1o	88/89 (98%)	0.93	4 (4%) 38 38	46, 62, 72, 74	0
46	2o	88/89 (98%)	0.97	4 (4%) 38 38	59, 70, 78, 82	0
47	1p	82/88 (93%)	1.45	14 (17%) 4 3	55, 69, 75, 82	0
47	2p	82/88 (93%)	1.16	8 (9%) 13 12	57, 67, 74, 78	0
48	1q	99/105 (94%)	1.08	5 (5%) 33 33	51, 64, 71, 73	0
48	2q	99/105 (94%)	0.99	5 (5%) 33 33	58, 70, 77, 80	0
49	1r	68/88 (77%)	0.89	4 (5%) 28 27	54, 64, 72, 76	0
49	2r	68/88 (77%)	1.10	7 (10%) 12 11	63, 71, 78, 79	0
50	1s	83/93 (89%)	1.44	15 (18%) 3 3	63, 73, 78, 82	0
50	2s	83/93 (89%)	2.47	53 (63%) 0 0	76, 82, 86, 88	0
51	1t	96/106 (90%)	1.20	10 (10%) 11 11	60, 68, 75, 79	0
51	2t	96/106 (90%)	0.95	9 (9%) 14 13	56, 67, 76, 80	0
52	1u	23/27 (85%)	1.14	4 (17%) 4 3	62, 66, 72, 74	0
52	2u	23/27 (85%)	2.29	12 (52%) 0 0	74, 79, 81, 82	0
53	1v	13/24 (54%)	1.19	5 (38%) 1 0	49, 67, 89, 95	0
53	2v	13/24 (54%)	1.79	5 (38%) 1 0	71, 83, 96, 97	0
54	1w	69/74 (93%)	1.62	20 (28%) 1 1	49, 91, 97, 99	0
54	2w	68/74 (91%)	2.02	36 (52%) 0 0	62, 95, 98, 99	0
55	1x	72/77 (93%)	0.39	2 (2%) 55 56	29, 63, 78, 88	0
55	2x	72/77 (93%)	0.84	3 (4%) 40 41	49, 80, 88, 94	0
56	1y	70/74 (94%)	2.30	47 (67%) 0 0	54, 95, 99, 100	0
56	2y	70/74 (94%)	2.18	36 (51%) 0 0	66, 97, 100, 103	0
All	All	20885/21740 (96%)	0.52	2047 (9%) 13 12	17, 62, 87, 103	0

The worst 5 of 2047 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	12.6
44	2m	123	ALA	10.9

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Mol	Chain	Res	Type	RSRZ
44	1m	123	ALA	8.4
44	1m	124	PRO	7.3
1	2A	2111	C	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	4SU	2w	8	20/21	0.39	0.18	89,95,110,110	0
56	4SU	2y	8	20/21	0.40	0.18	90,98,104,115	0
56	PSU	2y	55	20/21	0.42	0.18	93,99,107,111	0
54	PSU	2w	55	20/21	0.52	0.17	87,94,102,114	0
56	5MU	2y	54	21/22	0.55	0.17	88,95,99,117	0
56	5MU	1y	54	21/22	0.55	0.16	86,90,94,107	0
56	4SU	1y	8	20/21	0.57	0.16	90,95,100,115	0
54	5MU	2w	54	21/22	0.59	0.16	83,91,97,101	0
56	PSU	1y	55	20/21	0.60	0.16	88,93,98,104	0
54	4SU	1w	8	20/21	0.68	0.15	87,93,103,113	0
54	PSU	1w	55	20/21	0.69	0.16	81,89,98,101	0
54	5MU	1w	54	21/22	0.78	0.14	67,82,88,91	0
32	2MG	2a	1207	24/25	0.79	0.15	81,85,92,101	0
1	5MU	2A	1915	21/22	0.80	0.16	74,78,82,92	0
55	4SU	2x	8	20/21	0.82	0.13	75,78,83,86	0
55	PSU	2x	55	20/21	0.82	0.12	73,78,87,92	0
55	5MU	2x	54	21/22	0.83	0.13	74,82,88,92	0
1	PSU	2A	1917	20/21	0.87	0.12	58,71,80,82	0
32	G7M	2a	527	24/25	0.88	0.12	67,70,74,82	0
32	PSU	2a	516	20/21	0.88	0.12	73,79,84,84	0
43	0TD	2l	92	10/11	0.88	0.14	67,71,78,82	0
32	M2G	2a	966	25/26	0.89	0.16	62,68,83,90	0
32	5MC	2a	1404	21/22	0.90	0.12	54,60,69,71	0
55	5MU	1x	54	21/22	0.90	0.11	60,68,70,74	0
32	2MG	1a	1207	24/25	0.90	0.12	68,72,77,77	0
43	0TD	1l	92	10/11	0.90	0.12	44,53,59,67	0
32	5MC	2a	1400	21/22	0.90	0.18	68,74,78,82	0
54	L3X	2w	76	26/27	0.91	0.13	45,57,62,63	0
32	5MC	2a	967	21/22	0.91	0.13	66,69,78,82	0
55	5MC	2x	32	21/22	0.91	0.12	66,73,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	2a	1402	22/23	0.91	0.13	52,66,68,73	0
55	PSU	1x	55	20/21	0.92	0.10	53,62,69,73	0
1	PSU	2A	1911	20/21	0.92	0.10	58,63,68,70	0
55	4SU	1x	8	20/21	0.92	0.11	51,61,66,67	0
1	5MU	1A	1915	21/22	0.92	0.11	49,61,65,74	0
55	5MC	1x	32	21/22	0.93	0.12	51,56,61,64	0
32	PSU	1a	516	20/21	0.93	0.09	60,63,66,72	0
32	M2G	1a	966	25/26	0.94	0.11	44,52,60,65	0
1	PSU	1A	1917	20/21	0.94	0.10	42,54,60,61	0
32	5MC	2a	1407	21/22	0.94	0.11	45,57,65,68	0
32	MA6	2a	1519	24/25	0.94	0.13	54,64,68,68	0
1	OMC	2A	1920	21/22	0.94	0.10	57,63,66,68	0
55	31H	2x	76	32/33	0.94	0.12	46,53,59,61	0
32	5MC	1a	1400	21/22	0.95	0.10	38,49,54,58	0
1	5MC	1A	1942	21/22	0.95	0.10	31,41,46,55	0
32	G7M	1a	527	24/25	0.95	0.10	43,48,54,58	0
32	MA6	2a	1518	24/25	0.95	0.11	47,62,70,71	0
55	31H	1x	76	32/33	0.95	0.10	21,31,39,51	10
54	L3X	1w	76	26/27	0.95	0.09	31,42,47,48	0
32	UR3	2a	1498	21/22	0.96	0.10	54,59,65,68	0
1	5MC	2A	1962	21/22	0.96	0.09	36,45,56,57	0
1	OMG	2A	2251	24/25	0.96	0.09	37,42,44,51	0
1	PSU	2A	2605	20/21	0.96	0.08	35,40,45,46	0
32	MA6	1a	1519	24/25	0.96	0.09	35,40,44,46	0
32	5MC	1a	967	21/22	0.96	0.10	49,54,59,60	0
32	5MC	1a	1404	21/22	0.96	0.09	30,37,41,43	0
1	2MA	2A	2503	23/24	0.97	0.09	30,36,40,43	0
1	OMU	2A	2552	21/22	0.97	0.07	32,39,42,47	0
1	PSU	1A	1911	20/21	0.97	0.09	39,47,52,52	0
32	4OC	1a	1402	22/23	0.97	0.07	37,46,50,58	0
1	5MU	2A	1939	21/22	0.97	0.08	30,35,40,47	0
1	5MC	2A	1942	21/22	0.97	0.08	43,53,57,61	0
1	OMC	1A	1920	21/22	0.97	0.09	34,45,48,50	0
32	5MC	1a	1407	21/22	0.97	0.08	36,41,44,48	0
1	PSU	1A	2605	20/21	0.98	0.06	23,26,32,32	0
1	5MU	1A	1939	21/22	0.98	0.06	24,27,30,32	0
32	UR3	1a	1498	21/22	0.98	0.07	32,39,43,46	0
32	MA6	1a	1518	24/25	0.98	0.09	34,38,46,50	0
1	5MC	1A	1962	21/22	0.98	0.06	23,32,37,41	0
1	OMU	1A	2552	21/22	0.98	0.07	22,28,31,33	0
1	2MA	1A	2503	23/24	0.99	0.05	17,22,25,28	0
1	OMG	1A	2251	24/25	0.99	0.05	22,25,26,27	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	4071	1/1	0.40	0.21	73,73,73,73	0
57	MG	2A	3089	1/1	0.49	0.17	86,86,86,86	0
57	MG	2A	3325	1/1	0.57	0.28	80,80,80,80	0
57	MG	2v	101	1/1	0.57	0.24	83,83,83,83	0
57	MG	2a	1806	1/1	0.60	0.20	79,79,79,79	0
57	MG	1E	313	1/1	0.60	0.24	68,68,68,68	0
57	MG	1B	229	1/1	0.62	0.25	84,84,84,84	0
57	MG	2a	1812	1/1	0.64	0.23	76,76,76,76	0
57	MG	1A	3101	1/1	0.65	0.27	74,74,74,74	0
57	MG	1B	230	1/1	0.66	0.19	71,71,71,71	0
57	MG	2j	202	1/1	0.67	0.13	85,85,85,85	0
57	MG	2B	216	1/1	0.67	0.20	77,77,77,77	0
57	MG	2a	1649	1/1	0.69	0.18	80,80,80,80	0
57	MG	1a	1633	1/1	0.69	0.18	69,69,69,69	0
57	MG	2A	3524	1/1	0.69	0.32	71,71,71,71	0
57	MG	2A	3678	1/1	0.69	0.20	68,68,68,68	0
57	MG	2A	3109	1/1	0.69	0.24	66,66,66,66	0
57	MG	2A	3609	1/1	0.70	0.22	62,62,62,62	0
57	MG	2A	3423	1/1	0.70	0.42	84,84,84,84	0
57	MG	2a	1817	1/1	0.71	0.15	77,77,77,77	0
57	MG	1x	110	1/1	0.72	0.23	70,70,70,70	0
57	MG	1A	3704	1/1	0.72	0.12	72,72,72,72	0
57	MG	2a	1743	1/1	0.72	0.46	84,84,84,84	0
57	MG	2A	3763	1/1	0.72	0.24	50,50,50,50	0
57	MG	2a	1805	1/1	0.73	0.16	82,82,82,82	0
57	MG	1A	3743	1/1	0.73	0.16	61,61,61,61	0
57	MG	2A	3342	1/1	0.73	0.24	62,62,62,62	0
57	MG	2A	3229	1/1	0.73	0.21	67,67,67,67	0
57	MG	2a	1742	1/1	0.73	0.31	79,79,79,79	0
57	MG	2A	3742	1/1	0.73	0.17	41,41,41,41	0
57	MG	2A	3561	1/1	0.74	0.15	40,40,40,40	0
57	MG	2A	3098	1/1	0.74	0.31	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3883	1/1	0.74	0.13	36,36,36,36	0
57	MG	1B	207	1/1	0.74	0.25	76,76,76,76	0
57	MG	2A	3298	1/1	0.74	0.32	67,67,67,67	0
57	MG	2a	1710	1/1	0.75	0.26	75,75,75,75	0
57	MG	2a	1714	1/1	0.75	0.30	77,77,77,77	0
57	MG	1w	101	1/1	0.75	0.16	84,84,84,84	0
57	MG	1x	103	1/1	0.75	0.28	76,76,76,76	0
57	MG	2A	3662	1/1	0.75	0.13	68,68,68,68	0
57	MG	1A	3644	1/1	0.75	0.19	58,58,58,58	0
57	MG	1A	4036	1/1	0.75	0.17	61,61,61,61	0
57	MG	1A	3818	1/1	0.75	0.12	53,53,53,53	0
57	MG	1A	3863	1/1	0.75	0.16	68,68,68,68	0
57	MG	2A	3531	1/1	0.75	0.24	77,77,77,77	0
57	MG	2a	1707	1/1	0.76	0.28	76,76,76,76	0
57	MG	1A	3477	1/1	0.76	0.16	70,70,70,70	0
57	MG	1B	234	1/1	0.76	0.29	75,75,75,75	0
57	MG	2a	1740	1/1	0.76	0.23	74,74,74,74	0
57	MG	2A	3318	1/1	0.76	0.29	62,62,62,62	0
57	MG	1A	3826	1/1	0.76	0.18	55,55,55,55	0
57	MG	2a	1768	1/1	0.76	0.12	82,82,82,82	0
57	MG	2A	3738	1/1	0.76	0.26	60,60,60,60	0
57	MG	1A	3480	1/1	0.76	0.15	68,68,68,68	0
57	MG	1A	3535	1/1	0.76	0.29	57,57,57,57	0
57	MG	2A	3793	1/1	0.76	0.13	56,56,56,56	0
57	MG	2A	3169	1/1	0.76	0.24	79,79,79,79	0
57	MG	2A	3194	1/1	0.76	0.22	64,64,64,64	0
57	MG	1a	1677	1/1	0.77	0.26	74,74,74,74	0
57	MG	2A	3622	1/1	0.77	0.18	61,61,61,61	0
57	MG	1A	3197	1/1	0.77	0.25	55,55,55,55	0
57	MG	2A	3361	1/1	0.77	0.17	75,75,75,75	0
57	MG	2A	3708	1/1	0.77	0.20	66,66,66,66	0
57	MG	1E	309	1/1	0.77	0.23	68,68,68,68	0
57	MG	1A	3366	1/1	0.77	0.20	76,76,76,76	0
57	MG	2A	3748	1/1	0.77	0.15	43,43,43,43	0
57	MG	2a	1802	1/1	0.77	0.15	74,74,74,74	0
57	MG	13	104	1/1	0.77	0.20	54,54,54,54	0
57	MG	2A	3792	1/1	0.77	0.21	86,86,86,86	0
57	MG	1A	4090	1/1	0.77	0.15	58,58,58,58	0
57	MG	2A	3862	1/1	0.77	0.15	73,73,73,73	0
57	MG	2A	3574	1/1	0.77	0.12	67,67,67,67	0
57	MG	2a	1615	1/1	0.77	0.21	73,73,73,73	0
57	MG	2A	3613	1/1	0.78	0.19	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	1r	101	1/1	0.78	0.26	72,72,72,72	0
57	MG	2A	3204	1/1	0.78	0.17	75,75,75,75	0
57	MG	2B	209	1/1	0.78	0.30	75,75,75,75	0
57	MG	1D	311	1/1	0.78	0.38	77,77,77,77	0
57	MG	2a	1603	1/1	0.78	0.16	72,72,72,72	0
57	MG	2A	3296	1/1	0.78	0.23	68,68,68,68	0
57	MG	1A	3855	1/1	0.78	0.15	51,51,51,51	0
57	MG	2A	3167	1/1	0.78	0.21	76,76,76,76	0
57	MG	1a	1721	1/1	0.78	0.29	63,63,63,63	0
57	MG	2A	3333	1/1	0.78	0.14	74,74,74,74	0
57	MG	26	101	1/1	0.79	0.16	64,64,64,64	0
57	MG	2A	3328	1/1	0.79	0.18	80,80,80,80	0
57	MG	2a	1614	1/1	0.79	0.26	78,78,78,78	0
57	MG	1A	3026	1/1	0.79	0.28	66,66,66,66	0
57	MG	2a	1617	1/1	0.79	0.35	77,77,77,77	0
57	MG	1A	3266	1/1	0.79	0.22	70,70,70,70	0
57	MG	2a	1702	1/1	0.79	0.27	80,80,80,80	0
57	MG	2A	3188	1/1	0.79	0.16	59,59,59,59	0
57	MG	2A	3732	1/1	0.79	0.23	70,70,70,70	0
57	MG	2A	3734	1/1	0.79	0.16	72,72,72,72	0
57	MG	2a	1725	1/1	0.79	0.45	78,78,78,78	0
57	MG	2a	1729	1/1	0.79	0.23	87,87,87,87	0
57	MG	2A	3362	1/1	0.79	0.20	70,70,70,70	0
57	MG	1A	3567	1/1	0.79	0.17	71,71,71,71	0
57	MG	1w	105	1/1	0.79	0.17	77,77,77,77	0
57	MG	2A	3526	1/1	0.79	0.18	69,69,69,69	0
57	MG	2A	3779	1/1	0.79	0.19	81,81,81,81	0
57	MG	1A	3619	1/1	0.79	0.16	50,50,50,50	0
57	MG	1S	203	1/1	0.79	0.13	75,75,75,75	0
57	MG	2A	3812	1/1	0.79	0.14	48,48,48,48	0
57	MG	1B	228	1/1	0.79	0.20	81,81,81,81	0
57	MG	1A	3895	1/1	0.79	0.23	61,61,61,61	0
57	MG	1A	3984	1/1	0.79	0.19	67,67,67,67	0
57	MG	1A	3899	1/1	0.80	0.20	30,30,30,30	0
57	MG	2N	201	1/1	0.80	0.21	71,71,71,71	0
57	MG	1a	1789	1/1	0.80	0.14	70,70,70,70	0
57	MG	2A	3249	1/1	0.80	0.32	65,65,65,65	0
57	MG	2A	3286	1/1	0.80	0.14	63,63,63,63	0
57	MG	1A	3907	1/1	0.80	0.17	45,45,45,45	0
57	MG	2A	3629	1/1	0.80	0.20	52,52,52,52	0
57	MG	2a	1621	1/1	0.80	0.35	75,75,75,75	0
57	MG	2a	1627	1/1	0.80	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1637	1/1	0.80	0.38	83,83,83,83	0
57	MG	1A	3518	1/1	0.80	0.17	66,66,66,66	0
57	MG	2A	3666	1/1	0.80	0.20	68,68,68,68	0
57	MG	1A	4033	1/1	0.80	0.26	69,69,69,69	0
57	MG	2A	3680	1/1	0.80	0.23	76,76,76,76	0
57	MG	2a	1713	1/1	0.80	0.16	79,79,79,79	0
57	MG	1A	3360	1/1	0.80	0.14	61,61,61,61	0
57	MG	2A	3730	1/1	0.80	0.18	65,65,65,65	0
57	MG	1A	4059	1/1	0.80	0.17	63,63,63,63	0
57	MG	1A	3248	1/1	0.80	0.28	66,66,66,66	0
57	MG	1A	3732	1/1	0.80	0.18	62,62,62,62	0
57	MG	1A	3618	1/1	0.80	0.19	65,65,65,65	0
57	MG	1a	1668	1/1	0.80	0.26	65,65,65,65	0
57	MG	2A	3379	1/1	0.80	0.21	64,64,64,64	0
57	MG	1A	3765	1/1	0.80	0.17	61,61,61,61	0
57	MG	2A	3483	1/1	0.80	0.24	64,64,64,64	0
57	MG	2A	3505	1/1	0.80	0.29	72,72,72,72	0
57	MG	2A	3186	1/1	0.80	0.26	72,72,72,72	0
57	MG	1a	1678	1/1	0.80	0.22	66,66,66,66	0
57	MG	1a	1687	1/1	0.80	0.13	72,72,72,72	0
57	MG	2w	103	1/1	0.80	0.22	79,79,79,79	0
57	MG	1a	1692	1/1	0.81	0.18	70,70,70,70	0
57	MG	2A	3513	1/1	0.81	0.13	71,71,71,71	0
57	MG	1a	1707	1/1	0.81	0.17	63,63,63,63	0
57	MG	1a	1712	1/1	0.81	0.16	61,61,61,61	0
57	MG	1A	3666	1/1	0.81	0.13	63,63,63,63	0
57	MG	2Q	203	1/1	0.81	0.16	72,72,72,72	0
57	MG	1A	3088	1/1	0.81	0.12	46,46,46,46	0
57	MG	28	103	1/1	0.81	0.11	88,88,88,88	0
57	MG	2A	3565	1/1	0.81	0.24	77,77,77,77	0
57	MG	2A	3255	1/1	0.81	0.15	62,62,62,62	0
57	MG	2A	3601	1/1	0.81	0.25	64,64,64,64	0
57	MG	1A	3898	1/1	0.81	0.20	59,59,59,59	0
57	MG	1A	4082	1/1	0.81	0.16	34,34,34,34	0
57	MG	1A	3264	1/1	0.81	0.23	69,69,69,69	0
57	MG	2A	3309	1/1	0.81	0.19	62,62,62,62	0
57	MG	1a	1607	1/1	0.81	0.36	74,74,74,74	0
57	MG	2a	1701	1/1	0.81	0.32	75,75,75,75	0
57	MG	1A	3854	1/1	0.81	0.22	67,67,67,67	0
57	MG	2A	3672	1/1	0.81	0.15	55,55,55,55	0
57	MG	2A	3674	1/1	0.81	0.15	65,65,65,65	0
57	MG	2A	3677	1/1	0.81	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1645	1/1	0.81	0.18	75,75,75,75	0
57	MG	2A	3332	1/1	0.81	0.15	74,74,74,74	0
57	MG	2A	3694	1/1	0.81	0.17	69,69,69,69	0
57	MG	2A	3094	1/1	0.81	0.13	72,72,72,72	0
57	MG	1a	1665	1/1	0.81	0.15	71,71,71,71	0
57	MG	1A	3610	1/1	0.81	0.34	61,61,61,61	0
57	MG	2A	3111	1/1	0.81	0.29	71,71,71,71	0
57	MG	2a	1785	1/1	0.81	0.17	66,66,66,66	0
57	MG	1A	4001	1/1	0.81	0.13	31,31,31,31	0
57	MG	2A	3417	1/1	0.81	0.33	59,59,59,59	0
57	MG	1A	4007	1/1	0.81	0.12	82,82,82,82	0
57	MG	2A	3426	1/1	0.81	0.28	59,59,59,59	0
57	MG	1A	3751	1/1	0.81	0.17	60,60,60,60	0
57	MG	2A	3791	1/1	0.81	0.15	66,66,66,66	0
57	MG	2A	3487	1/1	0.81	0.15	61,61,61,61	0
57	MG	2A	3504	1/1	0.81	0.26	64,64,64,64	0
57	MG	2R	201	1/1	0.82	0.25	68,68,68,68	0
57	MG	20	102	1/1	0.82	0.18	71,71,71,71	0
57	MG	1a	1639	1/1	0.82	0.19	65,65,65,65	0
57	MG	2A	3649	1/1	0.82	0.12	73,73,73,73	0
57	MG	2a	1601	1/1	0.82	0.11	61,61,61,61	0
57	MG	1A	3595	1/1	0.82	0.15	57,57,57,57	0
57	MG	2A	3334	1/1	0.82	0.15	73,73,73,73	0
57	MG	2A	3341	1/1	0.82	0.27	64,64,64,64	0
57	MG	1A	3460	1/1	0.82	0.29	73,73,73,73	0
57	MG	2a	1620	1/1	0.82	0.25	74,74,74,74	0
57	MG	2A	3106	1/1	0.82	0.18	76,76,76,76	0
57	MG	1A	3530	1/1	0.82	0.20	73,73,73,73	0
57	MG	1a	1676	1/1	0.82	0.17	69,69,69,69	0
57	MG	1A	3320	1/1	0.82	0.14	44,44,44,44	0
57	MG	1A	3996	1/1	0.82	0.11	31,31,31,31	0
57	MG	1a	1682	1/1	0.82	0.13	75,75,75,75	0
57	MG	1A	3620	1/1	0.82	0.17	47,47,47,47	0
57	MG	1A	3870	1/1	0.82	0.16	62,62,62,62	0
57	MG	1A	4022	1/1	0.82	0.11	68,68,68,68	0
57	MG	1A	3879	1/1	0.82	0.15	51,51,51,51	0
57	MG	1A	3882	1/1	0.82	0.15	47,47,47,47	0
57	MG	2A	3759	1/1	0.82	0.16	57,57,57,57	0
57	MG	1R	205	1/1	0.82	0.20	43,43,43,43	0
57	MG	1a	1809	1/1	0.82	0.12	71,71,71,71	0
57	MG	2A	3788	1/1	0.82	0.18	53,53,53,53	0
57	MG	1a	1822	1/1	0.82	0.15	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	1A	4043	1/1	0.82	0.12	56,56,56,56	0
57	MG	2a	1786	1/1	0.82	0.21	72,72,72,72	0
57	MG	1A	4045	1/1	0.82	0.16	58,58,58,58	0
57	MG	2A	3568	1/1	0.82	0.13	45,45,45,45	0
57	MG	1A	3382	1/1	0.82	0.21	57,57,57,57	0
57	MG	2B	201	1/1	0.82	0.40	79,79,79,79	0
57	MG	2a	1814	1/1	0.82	0.14	78,78,78,78	0
57	MG	2a	1816	1/1	0.82	0.18	66,66,66,66	0
57	MG	2A	3323	1/1	0.82	0.15	74,74,74,74	0
57	MG	2g	201	1/1	0.82	0.18	81,81,81,81	0
57	MG	1a	1628	1/1	0.82	0.26	61,61,61,61	0
57	MG	2r	102	1/1	0.82	0.16	76,76,76,76	0
57	MG	1A	3776	1/1	0.82	0.09	15,15,15,15	0
57	MG	2A	3331	1/1	0.82	0.31	75,75,75,75	0
57	MG	2A	3438	1/1	0.83	0.21	74,74,74,74	0
57	MG	10	108	1/1	0.83	0.18	60,60,60,60	0
57	MG	2A	3268	1/1	0.83	0.40	75,75,75,75	0
57	MG	1B	221	1/1	0.83	0.21	62,62,62,62	0
57	MG	1A	3399	1/1	0.83	0.13	51,51,51,51	0
57	MG	2A	3062	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3063	1/1	0.83	0.18	74,74,74,74	0
57	MG	2a	1644	1/1	0.83	0.19	70,70,70,70	0
57	MG	2A	3739	1/1	0.83	0.19	75,75,75,75	0
57	MG	2a	1698	1/1	0.83	0.17	64,64,64,64	0
57	MG	2A	3071	1/1	0.83	0.14	50,50,50,50	0
57	MG	1A	3972	1/1	0.83	0.09	29,29,29,29	0
57	MG	1A	3061	1/1	0.83	0.23	65,65,65,65	0
57	MG	1A	3829	1/1	0.83	0.13	46,46,46,46	0
57	MG	1A	3849	1/1	0.83	0.15	59,59,59,59	0
57	MG	2A	3783	1/1	0.83	0.12	53,53,53,53	0
57	MG	2A	3786	1/1	0.83	0.15	58,58,58,58	0
57	MG	1a	1782	1/1	0.83	0.22	75,75,75,75	0
57	MG	1a	1783	1/1	0.83	0.11	75,75,75,75	0
57	MG	2a	1741	1/1	0.83	0.21	70,70,70,70	0
57	MG	2A	3165	1/1	0.83	0.17	68,68,68,68	0
57	MG	1A	4080	1/1	0.83	0.11	52,52,52,52	0
57	MG	2A	3614	1/1	0.83	0.21	65,65,65,65	0
57	MG	2A	3619	1/1	0.83	0.20	72,72,72,72	0
57	MG	1a	1666	1/1	0.83	0.09	66,66,66,66	0
57	MG	2B	203	1/1	0.83	0.13	71,71,71,71	0
57	MG	2A	3357	1/1	0.83	0.25	54,54,54,54	0
57	MG	1a	1813	1/1	0.83	0.13	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	2B	217	1/1	0.83	0.14	63,63,63,63	0
57	MG	2A	3654	1/1	0.83	0.22	67,67,67,67	0
57	MG	1a	1814	1/1	0.83	0.31	76,76,76,76	0
57	MG	2A	3665	1/1	0.83	0.14	52,52,52,52	0
57	MG	2a	1819	1/1	0.83	0.21	82,82,82,82	0
57	MG	1a	1817	1/1	0.83	0.31	64,64,64,64	0
57	MG	2j	201	1/1	0.83	0.18	73,73,73,73	0
57	MG	2A	3411	1/1	0.83	0.20	61,61,61,61	0
57	MG	1A	3724	1/1	0.83	0.14	26,26,26,26	0
57	MG	1A	3470	1/1	0.83	0.23	63,63,63,63	0
57	MG	1A	3788	1/1	0.83	0.10	15,15,15,15	0
57	MG	2A	3090	1/1	0.84	0.22	67,67,67,67	0
57	MG	1A	3424	1/1	0.84	0.11	55,55,55,55	0
57	MG	1A	3902	1/1	0.84	0.14	32,32,32,32	0
57	MG	2A	3102	1/1	0.84	0.23	77,77,77,77	0
57	MG	2a	1604	1/1	0.84	0.31	71,71,71,71	0
57	MG	1a	1748	1/1	0.84	0.19	66,66,66,66	0
57	MG	1a	1763	1/1	0.84	0.19	65,65,65,65	0
57	MG	1a	1774	1/1	0.84	0.15	70,70,70,70	0
57	MG	2a	1619	1/1	0.84	0.24	78,78,78,78	0
57	MG	2A	3371	1/1	0.84	0.28	71,71,71,71	0
57	MG	2A	3373	1/1	0.84	0.15	70,70,70,70	0
57	MG	2a	1624	1/1	0.84	0.11	66,66,66,66	0
57	MG	2A	3148	1/1	0.84	0.18	73,73,73,73	0
57	MG	14	101	1/1	0.84	0.28	74,74,74,74	0
57	MG	2a	1640	1/1	0.84	0.13	74,74,74,74	0
57	MG	1A	3722	1/1	0.84	0.17	52,52,52,52	0
57	MG	1a	1627	1/1	0.84	0.25	64,64,64,64	0
57	MG	2a	1671	1/1	0.84	0.23	62,62,62,62	0
57	MG	2a	1695	1/1	0.84	0.21	80,80,80,80	0
57	MG	1A	3922	1/1	0.84	0.11	47,47,47,47	0
57	MG	1A	4087	1/1	0.84	0.15	64,64,64,64	0
57	MG	2A	3446	1/1	0.84	0.11	65,65,65,65	0
57	MG	2A	3193	1/1	0.84	0.21	63,63,63,63	0
57	MG	2A	3743	1/1	0.84	0.14	60,60,60,60	0
57	MG	1A	3926	1/1	0.84	0.19	60,60,60,60	0
57	MG	2A	3755	1/1	0.84	0.11	65,65,65,65	0
57	MG	2a	1716	1/1	0.84	0.32	77,77,77,77	0
57	MG	2a	1721	1/1	0.84	0.12	68,68,68,68	0
57	MG	2A	3198	1/1	0.84	0.16	69,69,69,69	0
57	MG	1A	3517	1/1	0.84	0.20	57,57,57,57	0
57	MG	1A	3458	1/1	0.84	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3238	1/1	0.84	0.11	63,63,63,63	0
57	MG	1A	3024	1/1	0.84	0.25	60,60,60,60	0
57	MG	1A	3354	1/1	0.84	0.17	54,54,54,54	0
57	MG	1w	103	1/1	0.84	0.20	74,74,74,74	0
57	MG	2a	1769	1/1	0.84	0.12	76,76,76,76	0
57	MG	2A	3283	1/1	0.84	0.35	68,68,68,68	0
57	MG	1A	3627	1/1	0.84	0.14	52,52,52,52	0
57	MG	1w	109	1/1	0.84	0.29	71,71,71,71	0
57	MG	2A	3855	1/1	0.84	0.22	63,63,63,63	0
57	MG	2A	3598	1/1	0.84	0.19	58,58,58,58	0
57	MG	1A	3774	1/1	0.84	0.18	52,52,52,52	0
57	MG	1A	4024	1/1	0.84	0.13	67,67,67,67	0
57	MG	2A	3043	1/1	0.84	0.15	68,68,68,68	0
57	MG	1A	3552	1/1	0.84	0.14	59,59,59,59	0
57	MG	1A	3651	1/1	0.84	0.09	22,22,22,22	0
57	MG	1A	3816	1/1	0.84	0.10	36,36,36,36	0
57	MG	2A	3087	1/1	0.84	0.30	75,75,75,75	0
57	MG	2A	3636	1/1	0.84	0.14	36,36,36,36	0
57	MG	2l	203	1/1	0.84	0.13	73,73,73,73	0
57	MG	2Z	301	1/1	0.84	0.15	74,74,74,74	0
57	MG	1A	3157	1/1	0.84	0.12	29,29,29,29	0
57	MG	2l	102	1/1	0.84	0.41	52,52,52,52	0
57	MG	2x	105	1/1	0.84	0.14	75,75,75,75	0
57	MG	2a	1605	1/1	0.85	0.18	73,73,73,73	0
57	MG	1B	212	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3686	1/1	0.85	0.12	70,70,70,70	0
57	MG	1a	1719	1/1	0.85	0.16	62,62,62,62	0
57	MG	2A	3211	1/1	0.85	0.29	70,70,70,70	0
57	MG	2A	3712	1/1	0.85	0.10	56,56,56,56	0
57	MG	2A	3212	1/1	0.85	0.19	66,66,66,66	0
57	MG	2A	3031	1/1	0.85	0.12	56,56,56,56	0
57	MG	2A	3042	1/1	0.85	0.21	59,59,59,59	0
57	MG	2a	1629	1/1	0.85	0.21	76,76,76,76	0
57	MG	2a	1633	1/1	0.85	0.29	69,69,69,69	0
57	MG	1A	3333	1/1	0.85	0.26	58,58,58,58	0
57	MG	2A	3054	1/1	0.85	0.16	70,70,70,70	0
57	MG	2A	3265	1/1	0.85	0.14	67,67,67,67	0
57	MG	2a	1648	1/1	0.85	0.20	73,73,73,73	0
57	MG	2A	3266	1/1	0.85	0.13	69,69,69,69	0
57	MG	2a	1657	1/1	0.85	0.17	87,87,87,87	0
57	MG	2A	3746	1/1	0.85	0.19	66,66,66,66	0
57	MG	2a	1680	1/1	0.85	0.20	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	1a	1738	1/1	0.85	0.14	76,76,76,76	0
57	MG	2a	1697	1/1	0.85	0.20	70,70,70,70	0
57	MG	1A	3942	1/1	0.85	0.11	27,27,27,27	0
57	MG	2A	3529	1/1	0.85	0.17	46,46,46,46	0
57	MG	1a	1629	1/1	0.85	0.13	57,57,57,57	0
57	MG	2A	3540	1/1	0.85	0.14	52,52,52,52	0
57	MG	2A	3288	1/1	0.85	0.22	65,65,65,65	0
57	MG	1A	3697	1/1	0.85	0.17	55,55,55,55	0
57	MG	1A	3834	1/1	0.85	0.18	59,59,59,59	0
57	MG	2A	3789	1/1	0.85	0.10	90,90,90,90	0
57	MG	1A	4060	1/1	0.85	0.08	15,15,15,15	0
57	MG	1A	4069	1/1	0.85	0.17	51,51,51,51	0
57	MG	1a	1793	1/1	0.85	0.15	70,70,70,70	0
57	MG	2A	3604	1/1	0.85	0.16	57,57,57,57	0
57	MG	2A	3827	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3842	1/1	0.85	0.13	56,56,56,56	0
57	MG	2A	3101	1/1	0.85	0.33	72,72,72,72	0
57	MG	2a	1750	1/1	0.85	0.21	82,82,82,82	0
57	MG	1A	3444	1/1	0.85	0.23	61,61,61,61	0
57	MG	1a	1811	1/1	0.85	0.19	70,70,70,70	0
57	MG	2a	1778	1/1	0.85	0.10	80,80,80,80	0
57	MG	1A	4074	1/1	0.85	0.20	39,39,39,39	0
57	MG	2B	204	1/1	0.85	0.21	70,70,70,70	0
57	MG	2B	208	1/1	0.85	0.12	70,70,70,70	0
57	MG	1A	3451	1/1	0.85	0.21	46,46,46,46	0
57	MG	2A	3118	1/1	0.85	0.15	60,60,60,60	0
57	MG	1A	3510	1/1	0.85	0.14	69,69,69,69	0
57	MG	2A	3154	1/1	0.85	0.23	66,66,66,66	0
57	MG	2Q	202	1/1	0.85	0.26	58,58,58,58	0
57	MG	1T	201	1/1	0.85	0.19	56,56,56,56	0
57	MG	2A	3661	1/1	0.85	0.20	64,64,64,64	0
57	MG	2a	1820	1/1	0.85	0.20	67,67,67,67	0
57	MG	2a	1822	1/1	0.85	0.23	62,62,62,62	0
57	MG	1n	102	1/1	0.85	0.14	62,62,62,62	0
57	MG	10	106	1/1	0.85	0.11	51,51,51,51	0
57	MG	1a	1683	1/1	0.85	0.13	55,55,55,55	0
57	MG	2A	3671	1/1	0.85	0.14	64,64,64,64	0
57	MG	1A	3861	1/1	0.85	0.18	56,56,56,56	0
57	MG	1A	3079	1/1	0.85	0.17	53,53,53,53	0
57	MG	2A	3381	1/1	0.85	0.28	65,65,65,65	0
57	MG	2w	104	1/1	0.85	0.25	72,72,72,72	0
57	MG	1A	3415	1/1	0.85	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1625	1/1	0.86	0.27	55,55,55,55	0
57	MG	2A	3174	1/1	0.86	0.15	52,52,52,52	0
57	MG	1A	3946	1/1	0.86	0.10	42,42,42,42	0
57	MG	2E	303	1/1	0.86	0.27	62,62,62,62	0
57	MG	1A	3949	1/1	0.86	0.13	56,56,56,56	0
57	MG	1A	3958	1/1	0.86	0.13	31,31,31,31	0
57	MG	1a	1816	1/1	0.86	0.13	64,64,64,64	0
57	MG	2A	3196	1/1	0.86	0.11	54,54,54,54	0
57	MG	1a	1632	1/1	0.86	0.31	60,60,60,60	0
57	MG	2A	3548	1/1	0.86	0.13	71,71,71,71	0
57	MG	1A	3736	1/1	0.86	0.15	50,50,50,50	0
57	MG	1A	3974	1/1	0.86	0.09	22,22,22,22	0
57	MG	1A	3980	1/1	0.86	0.11	47,47,47,47	0
57	MG	1A	3165	1/1	0.86	0.13	36,36,36,36	0
57	MG	2A	3575	1/1	0.86	0.15	69,69,69,69	0
57	MG	2A	3233	1/1	0.86	0.27	57,57,57,57	0
57	MG	2A	3599	1/1	0.86	0.14	62,62,62,62	0
57	MG	2a	1613	1/1	0.86	0.17	57,57,57,57	0
57	MG	1A	3417	1/1	0.86	0.36	66,66,66,66	0
57	MG	2A	3240	1/1	0.86	0.29	69,69,69,69	0
57	MG	1B	225	1/1	0.86	0.13	63,63,63,63	0
57	MG	2a	1618	1/1	0.86	0.15	70,70,70,70	0
57	MG	1a	1672	1/1	0.86	0.20	60,60,60,60	0
57	MG	1x	101	1/1	0.86	0.19	70,70,70,70	0
57	MG	1B	226	1/1	0.86	0.14	65,65,65,65	0
57	MG	1x	104	1/1	0.86	0.21	68,68,68,68	0
57	MG	2a	1625	1/1	0.86	0.22	67,67,67,67	0
57	MG	2A	3269	1/1	0.86	0.13	72,72,72,72	0
57	MG	2A	3270	1/1	0.86	0.13	63,63,63,63	0
57	MG	2A	3278	1/1	0.86	0.23	67,67,67,67	0
57	MG	2A	3281	1/1	0.86	0.27	67,67,67,67	0
57	MG	2A	3655	1/1	0.86	0.15	68,68,68,68	0
57	MG	2A	3659	1/1	0.86	0.14	51,51,51,51	0
57	MG	2a	1646	1/1	0.86	0.23	73,73,73,73	0
57	MG	2a	1647	1/1	0.86	0.21	69,69,69,69	0
57	MG	1x	106	1/1	0.86	0.18	62,62,62,62	0
57	MG	1A	3628	1/1	0.86	0.13	32,32,32,32	0
57	MG	2A	3008	1/1	0.86	0.15	61,61,61,61	0
57	MG	2a	1660	1/1	0.86	0.14	64,64,64,64	0
57	MG	2A	3291	1/1	0.86	0.19	81,81,81,81	0
57	MG	2A	3295	1/1	0.86	0.20	59,59,59,59	0
57	MG	2a	1689	1/1	0.86	0.24	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3024	1/1	0.86	0.11	52,52,52,52	0
57	MG	1A	3554	1/1	0.86	0.19	57,57,57,57	0
57	MG	2A	3301	1/1	0.86	0.16	67,67,67,67	0
57	MG	1A	3302	1/1	0.86	0.34	71,71,71,71	0
57	MG	2A	3312	1/1	0.86	0.14	60,60,60,60	0
57	MG	2a	1703	1/1	0.86	0.11	79,79,79,79	0
57	MG	1A	3652	1/1	0.86	0.15	63,63,63,63	0
57	MG	2A	3053	1/1	0.86	0.20	71,71,71,71	0
57	MG	1A	4027	1/1	0.86	0.16	52,52,52,52	0
57	MG	2A	3055	1/1	0.86	0.20	58,58,58,58	0
57	MG	2A	3715	1/1	0.86	0.12	72,72,72,72	0
57	MG	2A	3330	1/1	0.86	0.19	59,59,59,59	0
57	MG	1A	3808	1/1	0.86	0.19	80,80,80,80	0
57	MG	1a	1702	1/1	0.86	0.24	61,61,61,61	0
57	MG	1A	3256	1/1	0.86	0.12	61,61,61,61	0
57	MG	2A	3081	1/1	0.86	0.17	58,58,58,58	0
57	MG	1A	3601	1/1	0.86	0.38	67,67,67,67	0
57	MG	1A	3702	1/1	0.86	0.10	40,40,40,40	0
57	MG	1A	4051	1/1	0.86	0.12	31,31,31,31	0
57	MG	1U	203	1/1	0.86	0.15	56,56,56,56	0
57	MG	2A	3751	1/1	0.86	0.21	58,58,58,58	0
57	MG	1A	3368	1/1	0.86	0.17	57,57,57,57	0
57	MG	2A	3364	1/1	0.86	0.16	64,64,64,64	0
57	MG	1a	1759	1/1	0.86	0.24	76,76,76,76	0
57	MG	2a	1787	1/1	0.86	0.16	82,82,82,82	0
57	MG	2a	1799	1/1	0.86	0.17	56,56,56,56	0
57	MG	2A	3764	1/1	0.86	0.15	79,79,79,79	0
57	MG	1A	3611	1/1	0.86	0.15	50,50,50,50	0
57	MG	2A	3378	1/1	0.86	0.30	75,75,75,75	0
57	MG	1A	4065	1/1	0.86	0.16	40,40,40,40	0
57	MG	1A	3027	1/1	0.86	0.27	70,70,70,70	0
57	MG	2A	3389	1/1	0.86	0.11	65,65,65,65	0
57	MG	1a	1601	1/1	0.86	0.22	68,68,68,68	0
57	MG	1a	1605	1/1	0.86	0.10	68,68,68,68	0
57	MG	2A	3130	1/1	0.86	0.12	48,48,48,48	0
57	MG	1a	1791	1/1	0.86	0.16	52,52,52,52	0
57	MG	2A	3432	1/1	0.86	0.14	66,66,66,66	0
57	MG	2A	3839	1/1	0.86	0.14	69,69,69,69	0
57	MG	1A	3344	1/1	0.86	0.35	69,69,69,69	0
57	MG	1a	1794	1/1	0.86	0.16	50,50,50,50	0
57	MG	2A	3453	1/1	0.86	0.22	71,71,71,71	0
57	MG	2A	3166	1/1	0.86	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2w	101	1/1	0.86	0.16	70,70,70,70	0
57	MG	1a	1795	1/1	0.86	0.13	62,62,62,62	0
57	MG	2A	3499	1/1	0.86	0.13	52,52,52,52	0
57	MG	2A	3502	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3832	1/1	0.87	0.18	63,63,63,63	0
57	MG	2A	3583	1/1	0.87	0.11	69,69,69,69	0
57	MG	2A	3590	1/1	0.87	0.16	68,68,68,68	0
57	MG	1A	4097	1/1	0.87	0.12	58,58,58,58	0
57	MG	20	101	1/1	0.87	0.21	64,64,64,64	0
57	MG	1A	3343	1/1	0.87	0.14	60,60,60,60	0
57	MG	2A	3304	1/1	0.87	0.10	62,62,62,62	0
57	MG	2A	3602	1/1	0.87	0.10	60,60,60,60	0
57	MG	1A	3457	1/1	0.87	0.11	54,54,54,54	0
57	MG	1A	3981	1/1	0.87	0.26	49,49,49,49	0
57	MG	2A	3611	1/1	0.87	0.18	42,42,42,42	0
57	MG	2A	3316	1/1	0.87	0.12	68,68,68,68	0
57	MG	1A	3418	1/1	0.87	0.10	48,48,48,48	0
57	MG	2a	1609	1/1	0.87	0.34	75,75,75,75	0
57	MG	2a	1610	1/1	0.87	0.30	67,67,67,67	0
57	MG	2A	3319	1/1	0.87	0.17	59,59,59,59	0
57	MG	1a	1812	1/1	0.87	0.29	67,67,67,67	0
57	MG	1A	3727	1/1	0.87	0.14	41,41,41,41	0
57	MG	2A	3327	1/1	0.87	0.12	51,51,51,51	0
57	MG	2A	3127	1/1	0.87	0.11	69,69,69,69	0
57	MG	2A	3651	1/1	0.87	0.12	55,55,55,55	0
57	MG	1A	3207	1/1	0.87	0.20	60,60,60,60	0
57	MG	1A	3431	1/1	0.87	0.15	56,56,56,56	0
57	MG	1A	3742	1/1	0.87	0.12	43,43,43,43	0
57	MG	1a	1820	1/1	0.87	0.27	61,61,61,61	0
57	MG	1A	3546	1/1	0.87	0.28	61,61,61,61	0
57	MG	2A	3336	1/1	0.87	0.14	67,67,67,67	0
57	MG	1A	3550	1/1	0.87	0.16	59,59,59,59	0
57	MG	1A	3630	1/1	0.87	0.11	35,35,35,35	0
57	MG	1A	3438	1/1	0.87	0.15	60,60,60,60	0
57	MG	1R	204	1/1	0.87	0.15	37,37,37,37	0
57	MG	2a	1645	1/1	0.87	0.10	65,65,65,65	0
57	MG	2A	3676	1/1	0.87	0.16	61,61,61,61	0
57	MG	1A	3478	1/1	0.87	0.18	56,56,56,56	0
57	MG	2A	3192	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3370	1/1	0.87	0.37	65,65,65,65	0
57	MG	1A	3783	1/1	0.87	0.10	24,24,24,24	0
57	MG	2A	3692	1/1	0.87	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1662	1/1	0.87	0.13	67,67,67,67	0
57	MG	2a	1667	1/1	0.87	0.15	64,64,64,64	0
57	MG	1a	1696	1/1	0.87	0.08	59,59,59,59	0
57	MG	2A	3195	1/1	0.87	0.23	63,63,63,63	0
57	MG	2a	1686	1/1	0.87	0.12	80,80,80,80	0
57	MG	2a	1688	1/1	0.87	0.29	65,65,65,65	0
57	MG	1a	1700	1/1	0.87	0.25	59,59,59,59	0
57	MG	2A	3380	1/1	0.87	0.23	51,51,51,51	0
57	MG	2A	3720	1/1	0.87	0.11	60,60,60,60	0
57	MG	1A	3338	1/1	0.87	0.12	42,42,42,42	0
57	MG	1a	1705	1/1	0.87	0.27	71,71,71,71	0
57	MG	2A	3404	1/1	0.87	0.25	40,40,40,40	0
57	MG	1a	1706	1/1	0.87	0.31	64,64,64,64	0
57	MG	2a	1705	1/1	0.87	0.16	77,77,77,77	0
57	MG	1A	3500	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3216	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3023	1/1	0.87	0.28	67,67,67,67	0
57	MG	2A	3230	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3673	1/1	0.87	0.12	38,38,38,38	0
57	MG	2A	3235	1/1	0.87	0.14	63,63,63,63	0
57	MG	2a	1724	1/1	0.87	0.24	67,67,67,67	0
57	MG	1A	3599	1/1	0.87	0.26	64,64,64,64	0
57	MG	2A	3462	1/1	0.87	0.16	65,65,65,65	0
57	MG	2a	1731	1/1	0.87	0.12	80,80,80,80	0
57	MG	2A	3464	1/1	0.87	0.11	56,56,56,56	0
57	MG	2A	3478	1/1	0.87	0.09	64,64,64,64	0
57	MG	1A	3820	1/1	0.87	0.15	51,51,51,51	0
57	MG	2A	3782	1/1	0.87	0.13	61,61,61,61	0
57	MG	2A	3244	1/1	0.87	0.22	69,69,69,69	0
57	MG	2A	3488	1/1	0.87	0.27	58,58,58,58	0
57	MG	2A	3491	1/1	0.87	0.24	71,71,71,71	0
57	MG	2a	1771	1/1	0.87	0.11	75,75,75,75	0
57	MG	2A	3493	1/1	0.87	0.35	57,57,57,57	0
57	MG	1a	1736	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3050	1/1	0.87	0.23	61,61,61,61	0
57	MG	1A	3943	1/1	0.87	0.10	45,45,45,45	0
57	MG	2a	1797	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3811	1/1	0.87	0.14	56,56,56,56	0
57	MG	16	103	1/1	0.87	0.26	52,52,52,52	0
57	MG	1a	1757	1/1	0.87	0.14	56,56,56,56	0
57	MG	1A	3700	1/1	0.87	0.15	54,54,54,54	0
57	MG	1a	1603	1/1	0.87	0.20	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	2A	3852	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3527	1/1	0.87	0.25	65,65,65,65	0
57	MG	2A	3858	1/1	0.87	0.16	64,64,64,64	0
57	MG	2A	3066	1/1	0.87	0.33	68,68,68,68	0
57	MG	1a	1767	1/1	0.87	0.12	60,60,60,60	0
57	MG	2A	3282	1/1	0.87	0.14	65,65,65,65	0
57	MG	2a	1823	1/1	0.87	0.16	78,78,78,78	0
57	MG	2d	302	1/1	0.87	0.09	68,68,68,68	0
57	MG	2e	201	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3072	1/1	0.87	0.10	51,51,51,51	0
57	MG	2i	201	1/1	0.87	0.15	65,65,65,65	0
57	MG	2A	3551	1/1	0.87	0.19	44,44,44,44	0
57	MG	2A	3554	1/1	0.87	0.15	44,44,44,44	0
57	MG	2B	211	1/1	0.87	0.17	61,61,61,61	0
57	MG	2B	215	1/1	0.87	0.27	73,73,73,73	0
57	MG	1A	4079	1/1	0.87	0.16	49,49,49,49	0
57	MG	1A	3827	1/1	0.87	0.15	48,48,48,48	0
57	MG	1A	3509	1/1	0.87	0.25	71,71,71,71	0
57	MG	1A	3968	1/1	0.87	0.17	53,53,53,53	0
57	MG	2x	103	1/1	0.87	0.15	74,74,74,74	0
57	MG	2x	104	1/1	0.87	0.24	64,64,64,64	0
57	MG	2P	201	1/1	0.87	0.23	68,68,68,68	0
57	MG	1A	3350	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	4064	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3016	1/1	0.88	0.16	68,68,68,68	0
57	MG	2A	3223	1/1	0.88	0.15	50,50,50,50	0
57	MG	2A	3224	1/1	0.88	0.16	57,57,57,57	0
57	MG	1a	1709	1/1	0.88	0.20	62,62,62,62	0
57	MG	1l	102	1/1	0.88	0.11	75,75,75,75	0
57	MG	2A	3695	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3700	1/1	0.88	0.16	71,71,71,71	0
57	MG	1A	3845	1/1	0.88	0.15	46,46,46,46	0
57	MG	2A	3710	1/1	0.88	0.11	64,64,64,64	0
57	MG	1A	3049	1/1	0.88	0.10	33,33,33,33	0
57	MG	2a	1628	1/1	0.88	0.07	78,78,78,78	0
57	MG	1A	3534	1/1	0.88	0.20	52,52,52,52	0
57	MG	2a	1632	1/1	0.88	0.30	62,62,62,62	0
57	MG	2A	3717	1/1	0.88	0.14	51,51,51,51	0
57	MG	2a	1634	1/1	0.88	0.22	64,64,64,64	0
57	MG	2A	3044	1/1	0.88	0.15	55,55,55,55	0
57	MG	2A	3727	1/1	0.88	0.14	59,59,59,59	0
57	MG	1A	3960	1/1	0.88	0.15	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	3605	1/1	0.88	0.32	64,64,64,64	0
57	MG	2A	3252	1/1	0.88	0.13	54,54,54,54	0
57	MG	1A	3767	1/1	0.88	0.11	40,40,40,40	0
57	MG	1a	1758	1/1	0.88	0.11	57,57,57,57	0
57	MG	1A	3606	1/1	0.88	0.15	66,66,66,66	0
57	MG	2a	1651	1/1	0.88	0.14	63,63,63,63	0
57	MG	1A	3869	1/1	0.88	0.14	66,66,66,66	0
57	MG	2A	3745	1/1	0.88	0.09	34,34,34,34	0
57	MG	1A	3684	1/1	0.88	0.11	27,27,27,27	0
57	MG	1A	4093	1/1	0.88	0.19	64,64,64,64	0
57	MG	2A	3750	1/1	0.88	0.10	74,74,74,74	0
57	MG	2a	1675	1/1	0.88	0.11	62,62,62,62	0
57	MG	2A	3503	1/1	0.88	0.15	34,34,34,34	0
57	MG	2a	1681	1/1	0.88	0.13	62,62,62,62	0
57	MG	1A	3874	1/1	0.88	0.25	34,34,34,34	0
57	MG	2A	3756	1/1	0.88	0.19	69,69,69,69	0
57	MG	2A	3758	1/1	0.88	0.22	66,66,66,66	0
57	MG	2a	1693	1/1	0.88	0.17	62,62,62,62	0
57	MG	1A	3985	1/1	0.88	0.12	48,48,48,48	0
57	MG	1A	3169	1/1	0.88	0.25	65,65,65,65	0
57	MG	1a	1636	1/1	0.88	0.21	72,72,72,72	0
57	MG	2A	3766	1/1	0.88	0.15	73,73,73,73	0
57	MG	1A	3998	1/1	0.88	0.14	43,43,43,43	0
57	MG	2A	3287	1/1	0.88	0.24	67,67,67,67	0
57	MG	1B	223	1/1	0.88	0.13	55,55,55,55	0
57	MG	1a	1664	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3536	1/1	0.88	0.13	35,35,35,35	0
57	MG	2A	3099	1/1	0.88	0.22	65,65,65,65	0
57	MG	1a	1799	1/1	0.88	0.14	79,79,79,79	0
57	MG	1a	1806	1/1	0.88	0.11	64,64,64,64	0
57	MG	2a	1720	1/1	0.88	0.20	67,67,67,67	0
57	MG	1A	3880	1/1	0.88	0.14	66,66,66,66	0
57	MG	2A	3800	1/1	0.88	0.08	44,44,44,44	0
57	MG	2A	3804	1/1	0.88	0.09	69,69,69,69	0
57	MG	1A	3539	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	4009	1/1	0.88	0.09	60,60,60,60	0
57	MG	2a	1736	1/1	0.88	0.28	66,66,66,66	0
57	MG	2a	1737	1/1	0.88	0.17	70,70,70,70	0
57	MG	2a	1739	1/1	0.88	0.41	75,75,75,75	0
57	MG	2A	3117	1/1	0.88	0.19	70,70,70,70	0
57	MG	1a	1670	1/1	0.88	0.11	49,49,49,49	0
57	MG	2A	3124	1/1	0.88	0.19	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	3847	1/1	0.88	0.14	51,51,51,51	0
57	MG	2A	3579	1/1	0.88	0.15	69,69,69,69	0
57	MG	1a	1671	1/1	0.88	0.17	62,62,62,62	0
57	MG	1A	3806	1/1	0.88	0.09	39,39,39,39	0
57	MG	2A	3861	1/1	0.88	0.34	73,73,73,73	0
57	MG	2a	1777	1/1	0.88	0.12	66,66,66,66	0
57	MG	1A	3295	1/1	0.88	0.09	39,39,39,39	0
57	MG	1A	3507	1/1	0.88	0.10	56,56,56,56	0
57	MG	1A	3421	1/1	0.88	0.17	62,62,62,62	0
57	MG	2A	3329	1/1	0.88	0.14	75,75,75,75	0
57	MG	2a	1788	1/1	0.88	0.13	69,69,69,69	0
57	MG	2a	1792	1/1	0.88	0.20	74,74,74,74	0
57	MG	2a	1794	1/1	0.88	0.17	61,61,61,61	0
57	MG	2B	206	1/1	0.88	0.15	60,60,60,60	0
57	MG	2B	207	1/1	0.88	0.27	67,67,67,67	0
57	MG	1n	101	1/1	0.88	0.33	67,67,67,67	0
57	MG	2A	3605	1/1	0.88	0.19	68,68,68,68	0
57	MG	1a	1680	1/1	0.88	0.23	77,77,77,77	0
57	MG	2B	214	1/1	0.88	0.28	68,68,68,68	0
57	MG	1A	3623	1/1	0.88	0.13	51,51,51,51	0
57	MG	2A	3170	1/1	0.88	0.23	64,64,64,64	0
57	MG	1A	3164	1/1	0.88	0.28	59,59,59,59	0
57	MG	2A	3175	1/1	0.88	0.26	68,68,68,68	0
57	MG	2F	302	1/1	0.88	0.12	64,64,64,64	0
57	MG	1w	102	1/1	0.88	0.09	57,57,57,57	0
57	MG	1F	315	1/1	0.88	0.21	55,55,55,55	0
57	MG	2a	1826	1/1	0.88	0.29	60,60,60,60	0
57	MG	2A	3343	1/1	0.88	0.14	70,70,70,70	0
57	MG	2A	3640	1/1	0.88	0.14	57,57,57,57	0
57	MG	2A	3189	1/1	0.88	0.33	64,64,64,64	0
57	MG	1A	3559	1/1	0.88	0.13	60,60,60,60	0
57	MG	1w	108	1/1	0.88	0.12	64,64,64,64	0
57	MG	1a	1694	1/1	0.88	0.18	59,59,59,59	0
57	MG	1A	4046	1/1	0.88	0.10	50,50,50,50	0
57	MG	1A	4048	1/1	0.88	0.19	49,49,49,49	0
57	MG	1A	3314	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3201	1/1	0.88	0.17	66,66,66,66	0
57	MG	1A	3737	1/1	0.88	0.21	54,54,54,54	0
57	MG	2A	3207	1/1	0.88	0.25	70,70,70,70	0
57	MG	2A	3210	1/1	0.88	0.13	60,60,60,60	0
57	MG	2a	1606	1/1	0.88	0.36	77,77,77,77	0
57	MG	2A	3388	1/1	0.88	0.14	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	1a	1739	1/1	0.89	0.27	58,58,58,58	0
57	MG	2G	201	1/1	0.89	0.22	75,75,75,75	0
57	MG	1a	1740	1/1	0.89	0.25	66,66,66,66	0
57	MG	1A	3916	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3083	1/1	0.89	0.12	55,55,55,55	0
57	MG	2A	3084	1/1	0.89	0.11	52,52,52,52	0
57	MG	2A	3293	1/1	0.89	0.13	66,66,66,66	0
57	MG	1A	3920	1/1	0.89	0.14	36,36,36,36	0
57	MG	1A	3087	1/1	0.89	0.13	29,29,29,29	0
57	MG	1A	4062	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3688	1/1	0.89	0.09	38,38,38,38	0
57	MG	1A	3935	1/1	0.89	0.11	38,38,38,38	0
57	MG	2A	3307	1/1	0.89	0.29	75,75,75,75	0
57	MG	1A	3209	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3615	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3310	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1778	1/1	0.89	0.11	68,68,68,68	0
57	MG	1a	1779	1/1	0.89	0.12	49,49,49,49	0
57	MG	1a	1612	1/1	0.89	0.11	65,65,65,65	0
57	MG	2A	3637	1/1	0.89	0.12	49,49,49,49	0
57	MG	1a	1615	1/1	0.89	0.10	67,67,67,67	0
57	MG	1A	3341	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3271	1/1	0.89	0.12	44,44,44,44	0
57	MG	1A	3469	1/1	0.89	0.16	65,65,65,65	0
57	MG	1A	3831	1/1	0.89	0.12	57,57,57,57	0
57	MG	1A	3959	1/1	0.89	0.11	26,26,26,26	0
57	MG	1A	3709	1/1	0.89	0.10	23,23,23,23	0
57	MG	2A	3147	1/1	0.89	0.23	63,63,63,63	0
57	MG	1A	4089	1/1	0.89	0.10	47,47,47,47	0
57	MG	2A	3151	1/1	0.89	0.14	57,57,57,57	0
57	MG	2a	1626	1/1	0.89	0.17	60,60,60,60	0
57	MG	2A	3669	1/1	0.89	0.10	52,52,52,52	0
57	MG	1a	1637	1/1	0.89	0.33	78,78,78,78	0
57	MG	2A	3335	1/1	0.89	0.07	69,69,69,69	0
57	MG	2A	3155	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3612	1/1	0.89	0.18	63,63,63,63	0
57	MG	1A	3210	1/1	0.89	0.09	65,65,65,65	0
57	MG	2a	1635	1/1	0.89	0.21	66,66,66,66	0
57	MG	2a	1636	1/1	0.89	0.22	65,65,65,65	0
57	MG	1a	1646	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3679	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3351	1/1	0.89	0.17	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	2A	3683	1/1	0.89	0.12	51,51,51,51	0
57	MG	2A	3684	1/1	0.89	0.14	59,59,59,59	0
57	MG	2A	3355	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3356	1/1	0.89	0.21	53,53,53,53	0
57	MG	2A	3168	1/1	0.89	0.17	63,63,63,63	0
57	MG	1a	1647	1/1	0.89	0.14	60,60,60,60	0
57	MG	2a	1654	1/1	0.89	0.14	85,85,85,85	0
57	MG	1a	1657	1/1	0.89	0.09	43,43,43,43	0
57	MG	1a	1660	1/1	0.89	0.14	73,73,73,73	0
57	MG	1a	1661	1/1	0.89	0.13	65,65,65,65	0
57	MG	2A	3176	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3372	1/1	0.89	0.21	69,69,69,69	0
57	MG	1a	1821	1/1	0.89	0.21	65,65,65,65	0
57	MG	1A	3297	1/1	0.89	0.18	60,60,60,60	0
57	MG	2A	3724	1/1	0.89	0.11	57,57,57,57	0
57	MG	1b	302	1/1	0.89	0.16	77,77,77,77	0
57	MG	2A	3729	1/1	0.89	0.11	69,69,69,69	0
57	MG	2A	3190	1/1	0.89	0.14	72,72,72,72	0
57	MG	1A	3851	1/1	0.89	0.08	34,34,34,34	0
57	MG	2A	3387	1/1	0.89	0.13	69,69,69,69	0
57	MG	2a	1696	1/1	0.89	0.21	61,61,61,61	0
57	MG	1A	3090	1/1	0.89	0.09	40,40,40,40	0
57	MG	1A	3734	1/1	0.89	0.13	57,57,57,57	0
57	MG	2A	3740	1/1	0.89	0.12	65,65,65,65	0
57	MG	2A	3390	1/1	0.89	0.15	76,76,76,76	0
57	MG	2A	3398	1/1	0.89	0.19	64,64,64,64	0
57	MG	1t	201	1/1	0.89	0.16	57,57,57,57	0
57	MG	1A	3093	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3416	1/1	0.89	0.26	64,64,64,64	0
57	MG	2a	1712	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3994	1/1	0.89	0.12	22,22,22,22	0
57	MG	2A	3421	1/1	0.89	0.25	60,60,60,60	0
57	MG	1A	3488	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3203	1/1	0.89	0.14	64,64,64,64	0
57	MG	1A	3489	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3556	1/1	0.89	0.12	68,68,68,68	0
57	MG	1A	3558	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3499	1/1	0.89	0.15	41,41,41,41	0
57	MG	2A	3456	1/1	0.89	0.12	68,68,68,68	0
57	MG	1A	4013	1/1	0.89	0.12	37,37,37,37	0
57	MG	2A	3213	1/1	0.89	0.34	63,63,63,63	0
57	MG	2A	3472	1/1	0.89	0.16	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	1E	301	1/1	0.89	0.13	30,30,30,30	0
57	MG	2A	3221	1/1	0.89	0.21	57,57,57,57	0
57	MG	1E	306	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	4019	1/1	0.89	0.09	48,48,48,48	0
57	MG	1x	112	1/1	0.89	0.21	68,68,68,68	0
57	MG	2a	1764	1/1	0.89	0.09	68,68,68,68	0
57	MG	1a	1693	1/1	0.89	0.20	68,68,68,68	0
57	MG	2A	3799	1/1	0.89	0.14	49,49,49,49	0
57	MG	2A	3231	1/1	0.89	0.14	70,70,70,70	0
57	MG	1E	311	1/1	0.89	0.10	26,26,26,26	0
57	MG	1a	1695	1/1	0.89	0.26	70,70,70,70	0
57	MG	2a	1781	1/1	0.89	0.17	75,75,75,75	0
57	MG	2A	3236	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3822	1/1	0.89	0.17	66,66,66,66	0
57	MG	2A	3823	1/1	0.89	0.13	36,36,36,36	0
57	MG	2A	3824	1/1	0.89	0.13	50,50,50,50	0
57	MG	1A	4021	1/1	0.89	0.18	63,63,63,63	0
57	MG	2a	1793	1/1	0.89	0.23	66,66,66,66	0
57	MG	2A	3830	1/1	0.89	0.08	60,60,60,60	0
57	MG	2A	3833	1/1	0.89	0.11	61,61,61,61	0
57	MG	2A	3838	1/1	0.89	0.12	59,59,59,59	0
57	MG	2A	3507	1/1	0.89	0.15	57,57,57,57	0
57	MG	2A	3239	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3029	1/1	0.89	0.20	55,55,55,55	0
57	MG	1E	315	1/1	0.89	0.20	55,55,55,55	0
57	MG	2a	1813	1/1	0.89	0.13	83,83,83,83	0
57	MG	1A	3434	1/1	0.89	0.13	42,42,42,42	0
57	MG	2A	3857	1/1	0.89	0.12	73,73,73,73	0
57	MG	1A	3881	1/1	0.89	0.08	22,22,22,22	0
57	MG	2a	1818	1/1	0.89	0.19	61,61,61,61	0
57	MG	2A	3530	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3656	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3258	1/1	0.89	0.15	56,56,56,56	0
57	MG	2B	202	1/1	0.89	0.35	76,76,76,76	0
57	MG	2A	3047	1/1	0.89	0.25	71,71,71,71	0
57	MG	1A	3660	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3263	1/1	0.89	0.26	66,66,66,66	0
57	MG	1A	3330	1/1	0.89	0.11	47,47,47,47	0
57	MG	2A	3556	1/1	0.89	0.11	59,59,59,59	0
57	MG	1V	205	1/1	0.89	0.14	51,51,51,51	0
57	MG	1A	3681	1/1	0.89	0.09	52,52,52,52	0
57	MG	2A	3279	1/1	0.89	0.09	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	2q	202	1/1	0.89	0.14	76,76,76,76	0
57	MG	2A	3572	1/1	0.89	0.18	52,52,52,52	0
57	MG	1A	3682	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3809	1/1	0.89	0.13	51,51,51,51	0
57	MG	2D	303	1/1	0.89	0.33	68,68,68,68	0
57	MG	2D	307	1/1	0.89	0.13	62,62,62,62	0
57	MG	2E	301	1/1	0.89	0.12	57,57,57,57	0
57	MG	2A	3577	1/1	0.89	0.16	64,64,64,64	0
57	MG	2E	307	1/1	0.89	0.15	55,55,55,55	0
57	MG	2A	3033	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3272	1/1	0.90	0.30	70,70,70,70	0
57	MG	2A	3275	1/1	0.90	0.11	66,66,66,66	0
57	MG	2A	3277	1/1	0.90	0.12	59,59,59,59	0
57	MG	2E	305	1/1	0.90	0.12	56,56,56,56	0
57	MG	2E	306	1/1	0.90	0.11	31,31,31,31	0
57	MG	1A	3094	1/1	0.90	0.16	51,51,51,51	0
57	MG	2E	309	1/1	0.90	0.20	58,58,58,58	0
57	MG	2A	3578	1/1	0.90	0.18	62,62,62,62	0
57	MG	1A	3370	1/1	0.90	0.12	51,51,51,51	0
57	MG	2A	3581	1/1	0.90	0.20	59,59,59,59	0
57	MG	1A	3379	1/1	0.90	0.19	47,47,47,47	0
57	MG	2A	3585	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3045	1/1	0.90	0.17	70,70,70,70	0
57	MG	2Q	204	1/1	0.90	0.15	56,56,56,56	0
57	MG	1B	203	1/1	0.90	0.07	34,34,34,34	0
57	MG	2R	202	1/1	0.90	0.09	54,54,54,54	0
57	MG	2X	101	1/1	0.90	0.19	65,65,65,65	0
57	MG	2A	3285	1/1	0.90	0.30	57,57,57,57	0
57	MG	1A	3381	1/1	0.90	0.34	61,61,61,61	0
57	MG	1B	210	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3945	1/1	0.90	0.07	49,49,49,49	0
57	MG	23	102	1/1	0.90	0.13	60,60,60,60	0
57	MG	2A	3289	1/1	0.90	0.10	65,65,65,65	0
57	MG	2A	3606	1/1	0.90	0.17	65,65,65,65	0
57	MG	2A	3607	1/1	0.90	0.09	31,31,31,31	0
57	MG	1a	1691	1/1	0.90	0.27	74,74,74,74	0
57	MG	2A	3058	1/1	0.90	0.20	65,65,65,65	0
57	MG	1B	215	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3492	1/1	0.90	0.15	44,44,44,44	0
57	MG	1A	3784	1/1	0.90	0.15	30,30,30,30	0
57	MG	1B	224	1/1	0.90	0.09	55,55,55,55	0
57	MG	1A	3315	1/1	0.90	0.13	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	1A	3384	1/1	0.90	0.28	43,43,43,43	0
57	MG	1A	3392	1/1	0.90	0.12	50,50,50,50	0
57	MG	1A	3961	1/1	0.90	0.12	62,62,62,62	0
57	MG	2A	3311	1/1	0.90	0.10	51,51,51,51	0
57	MG	2A	3642	1/1	0.90	0.18	73,73,73,73	0
57	MG	2A	3648	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3966	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	3316	1/1	0.90	0.25	54,54,54,54	0
57	MG	1A	3814	1/1	0.90	0.10	27,27,27,27	0
57	MG	1a	1710	1/1	0.90	0.27	60,60,60,60	0
57	MG	2A	3657	1/1	0.90	0.17	68,68,68,68	0
57	MG	1A	3411	1/1	0.90	0.11	41,41,41,41	0
57	MG	2A	3660	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3324	1/1	0.90	0.28	62,62,62,62	0
57	MG	1a	1716	1/1	0.90	0.26	68,68,68,68	0
57	MG	1a	1717	1/1	0.90	0.20	53,53,53,53	0
57	MG	1A	3414	1/1	0.90	0.15	39,39,39,39	0
57	MG	1A	3319	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3416	1/1	0.90	0.27	69,69,69,69	0
57	MG	1A	3659	1/1	0.90	0.16	57,57,57,57	0
57	MG	2A	3673	1/1	0.90	0.11	72,72,72,72	0
57	MG	1E	314	1/1	0.90	0.20	45,45,45,45	0
57	MG	1A	3986	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3989	1/1	0.90	0.15	65,65,65,65	0
57	MG	1Q	204	1/1	0.90	0.15	61,61,61,61	0
57	MG	1A	3992	1/1	0.90	0.09	30,30,30,30	0
57	MG	2a	1650	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3134	1/1	0.90	0.20	62,62,62,62	0
57	MG	2a	1653	1/1	0.90	0.31	62,62,62,62	0
57	MG	2A	3145	1/1	0.90	0.14	55,55,55,55	0
57	MG	2a	1656	1/1	0.90	0.21	76,76,76,76	0
57	MG	1A	3068	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3344	1/1	0.90	0.16	66,66,66,66	0
57	MG	2A	3691	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3350	1/1	0.90	0.17	70,70,70,70	0
57	MG	2a	1669	1/1	0.90	0.26	66,66,66,66	0
57	MG	1A	3329	1/1	0.90	0.17	55,55,55,55	0
57	MG	2a	1674	1/1	0.90	0.18	65,65,65,65	0
57	MG	2A	3354	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3697	1/1	0.90	0.11	60,60,60,60	0
57	MG	2A	3150	1/1	0.90	0.16	66,66,66,66	0
57	MG	2a	1682	1/1	0.90	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3058	1/1	0.90	0.09	42,42,42,42	0
57	MG	1A	3678	1/1	0.90	0.08	24,24,24,24	0
57	MG	2A	3359	1/1	0.90	0.08	69,69,69,69	0
57	MG	2A	3360	1/1	0.90	0.17	48,48,48,48	0
57	MG	1A	3542	1/1	0.90	0.27	53,53,53,53	0
57	MG	2A	3159	1/1	0.90	0.23	58,58,58,58	0
57	MG	2A	3721	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3363	1/1	0.90	0.30	62,62,62,62	0
57	MG	2a	1700	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3725	1/1	0.90	0.10	65,65,65,65	0
57	MG	1A	3265	1/1	0.90	0.11	41,41,41,41	0
57	MG	1a	1781	1/1	0.90	0.17	65,65,65,65	0
57	MG	1A	3425	1/1	0.90	0.19	63,63,63,63	0
57	MG	2A	3731	1/1	0.90	0.16	52,52,52,52	0
57	MG	2a	1708	1/1	0.90	0.23	71,71,71,71	0
57	MG	10	109	1/1	0.90	0.09	43,43,43,43	0
57	MG	1a	1787	1/1	0.90	0.07	77,77,77,77	0
57	MG	2A	3737	1/1	0.90	0.08	59,59,59,59	0
57	MG	1A	3853	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3551	1/1	0.90	0.11	55,55,55,55	0
57	MG	2a	1717	1/1	0.90	0.17	66,66,66,66	0
57	MG	2a	1719	1/1	0.90	0.10	64,64,64,64	0
57	MG	13	105	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3336	1/1	0.90	0.33	67,67,67,67	0
57	MG	2a	1722	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3385	1/1	0.90	0.10	67,67,67,67	0
57	MG	2A	3178	1/1	0.90	0.15	51,51,51,51	0
57	MG	2A	3184	1/1	0.90	0.11	57,57,57,57	0
57	MG	15	107	1/1	0.90	0.11	54,54,54,54	0
57	MG	2a	1734	1/1	0.90	0.31	60,60,60,60	0
57	MG	1A	3181	1/1	0.90	0.30	56,56,56,56	0
57	MG	1A	3437	1/1	0.90	0.33	73,73,73,73	0
57	MG	2A	3403	1/1	0.90	0.27	50,50,50,50	0
57	MG	1A	4029	1/1	0.90	0.08	58,58,58,58	0
57	MG	1A	4032	1/1	0.90	0.17	52,52,52,52	0
57	MG	1A	3864	1/1	0.90	0.19	52,52,52,52	0
57	MG	1A	3270	1/1	0.90	0.16	47,47,47,47	0
57	MG	2a	1744	1/1	0.90	0.18	78,78,78,78	0
57	MG	2a	1749	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3707	1/1	0.90	0.11	39,39,39,39	0
57	MG	2a	1751	1/1	0.90	0.17	73,73,73,73	0
57	MG	2a	1761	1/1	0.90	0.10	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	1a	1624	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3234	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3427	1/1	0.90	0.10	69,69,69,69	0
57	MG	1A	3243	1/1	0.90	0.24	42,42,42,42	0
57	MG	2a	1775	1/1	0.90	0.19	58,58,58,58	0
57	MG	2A	3435	1/1	0.90	0.33	65,65,65,65	0
57	MG	1A	4047	1/1	0.90	0.07	25,25,25,25	0
57	MG	2a	1779	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3439	1/1	0.90	0.39	59,59,59,59	0
57	MG	1A	3579	1/1	0.90	0.30	39,39,39,39	0
57	MG	1A	3592	1/1	0.90	0.09	37,37,37,37	0
57	MG	1l	202	1/1	0.90	0.10	78,78,78,78	0
57	MG	1A	4052	1/1	0.90	0.12	33,33,33,33	0
57	MG	2a	1789	1/1	0.90	0.24	65,65,65,65	0
57	MG	2a	1791	1/1	0.90	0.11	64,64,64,64	0
57	MG	1A	4053	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	4054	1/1	0.90	0.09	62,62,62,62	0
57	MG	2A	3809	1/1	0.90	0.08	40,40,40,40	0
57	MG	1A	3730	1/1	0.90	0.10	44,44,44,44	0
57	MG	1a	1641	1/1	0.90	0.16	52,52,52,52	0
57	MG	2A	3814	1/1	0.90	0.08	45,45,45,45	0
57	MG	2A	3486	1/1	0.90	0.23	53,53,53,53	0
57	MG	1a	1642	1/1	0.90	0.32	71,71,71,71	0
57	MG	2a	1810	1/1	0.90	0.12	73,73,73,73	0
57	MG	1A	3188	1/1	0.90	0.15	41,41,41,41	0
57	MG	1A	4061	1/1	0.90	0.14	63,63,63,63	0
57	MG	1w	106	1/1	0.90	0.17	71,71,71,71	0
57	MG	2a	1815	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3887	1/1	0.90	0.07	26,26,26,26	0
57	MG	1a	1651	1/1	0.90	0.12	67,67,67,67	0
57	MG	1a	1652	1/1	0.90	0.21	66,66,66,66	0
57	MG	1A	3892	1/1	0.90	0.17	51,51,51,51	0
57	MG	1A	3299	1/1	0.90	0.15	51,51,51,51	0
57	MG	1A	3357	1/1	0.90	0.16	57,57,57,57	0
57	MG	2A	3512	1/1	0.90	0.13	65,65,65,65	0
57	MG	2a	1825	1/1	0.90	0.24	64,64,64,64	0
57	MG	1x	107	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3520	1/1	0.90	0.10	36,36,36,36	0
57	MG	1x	108	1/1	0.90	0.11	35,35,35,35	0
57	MG	1A	3604	1/1	0.90	0.23	64,64,64,64	0
57	MG	1A	3250	1/1	0.90	0.22	58,58,58,58	0
57	MG	1A	3365	1/1	0.90	0.12	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	3256	1/1	0.90	0.22	61,61,61,61	0
57	MG	1A	3913	1/1	0.90	0.17	30,30,30,30	0
57	MG	2A	3262	1/1	0.90	0.11	65,65,65,65	0
57	MG	2A	3263	1/1	0.90	0.12	61,61,61,61	0
57	MG	2A	3264	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3549	1/1	0.90	0.09	47,47,47,47	0
57	MG	1A	3307	1/1	0.90	0.09	31,31,31,31	0
57	MG	1A	3753	1/1	0.90	0.09	49,49,49,49	0
57	MG	2A	3267	1/1	0.90	0.11	59,59,59,59	0
57	MG	1A	3754	1/1	0.90	0.19	57,57,57,57	0
57	MG	1a	1674	1/1	0.90	0.21	70,70,70,70	0
57	MG	1A	3246	1/1	0.91	0.28	60,60,60,60	0
57	MG	2A	3626	1/1	0.91	0.08	49,49,49,49	0
57	MG	1A	3450	1/1	0.91	0.14	47,47,47,47	0
57	MG	2A	3634	1/1	0.91	0.12	52,52,52,52	0
57	MG	2A	3182	1/1	0.91	0.10	59,59,59,59	0
57	MG	25	104	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3347	1/1	0.91	0.14	62,62,62,62	0
57	MG	27	102	1/1	0.91	0.11	47,47,47,47	0
57	MG	28	102	1/1	0.91	0.13	48,48,48,48	0
57	MG	2A	3348	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3755	1/1	0.91	0.07	51,51,51,51	0
57	MG	2a	1602	1/1	0.91	0.28	60,60,60,60	0
57	MG	1A	3275	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3352	1/1	0.91	0.17	67,67,67,67	0
57	MG	2A	3353	1/1	0.91	0.13	68,68,68,68	0
57	MG	2A	3187	1/1	0.91	0.18	70,70,70,70	0
57	MG	2a	1607	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3331	1/1	0.91	0.30	58,58,58,58	0
57	MG	1A	3247	1/1	0.91	0.12	60,60,60,60	0
57	MG	2a	1611	1/1	0.91	0.21	69,69,69,69	0
57	MG	1A	3296	1/1	0.91	0.23	50,50,50,50	0
57	MG	2A	3358	1/1	0.91	0.09	61,61,61,61	0
57	MG	1A	3657	1/1	0.91	0.07	21,21,21,21	0
57	MG	1a	1686	1/1	0.91	0.15	48,48,48,48	0
57	MG	1F	303	1/1	0.91	0.32	32,32,32,32	0
57	MG	1a	1689	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3658	1/1	0.91	0.07	16,16,16,16	0
57	MG	2A	3197	1/1	0.91	0.15	66,66,66,66	0
57	MG	1N	201	1/1	0.91	0.14	56,56,56,56	0
57	MG	1A	3785	1/1	0.91	0.13	31,31,31,31	0
57	MG	1x	105	1/1	0.91	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3911	1/1	0.91	0.17	75,75,75,75	0
57	MG	2A	3374	1/1	0.91	0.13	67,67,67,67	0
57	MG	2A	3206	1/1	0.91	0.17	67,67,67,67	0
57	MG	1A	3463	1/1	0.91	0.09	51,51,51,51	0
57	MG	2A	3208	1/1	0.91	0.19	44,44,44,44	0
57	MG	1A	3801	1/1	0.91	0.08	74,74,74,74	0
57	MG	2A	3382	1/1	0.91	0.08	69,69,69,69	0
57	MG	2A	3685	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3384	1/1	0.91	0.16	61,61,61,61	0
57	MG	2A	3690	1/1	0.91	0.15	62,62,62,62	0
57	MG	2a	1641	1/1	0.91	0.19	67,67,67,67	0
57	MG	2a	1643	1/1	0.91	0.09	74,74,74,74	0
57	MG	1x	109	1/1	0.91	0.10	61,61,61,61	0
57	MG	1a	1699	1/1	0.91	0.27	47,47,47,47	0
57	MG	1A	3468	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3001	1/1	0.91	0.33	59,59,59,59	0
57	MG	2A	3218	1/1	0.91	0.32	41,41,41,41	0
57	MG	2A	3393	1/1	0.91	0.24	63,63,63,63	0
57	MG	1A	3089	1/1	0.91	0.08	34,34,34,34	0
57	MG	1A	3200	1/1	0.91	0.12	47,47,47,47	0
57	MG	1A	3931	1/1	0.91	0.10	20,20,20,20	0
57	MG	2A	3408	1/1	0.91	0.34	68,68,68,68	0
57	MG	2A	3409	1/1	0.91	0.18	39,39,39,39	0
57	MG	2A	3718	1/1	0.91	0.09	60,60,60,60	0
57	MG	1A	3933	1/1	0.91	0.16	35,35,35,35	0
57	MG	2A	3415	1/1	0.91	0.27	63,63,63,63	0
57	MG	2A	3723	1/1	0.91	0.11	64,64,64,64	0
57	MG	1A	3934	1/1	0.91	0.19	56,56,56,56	0
57	MG	1A	3472	1/1	0.91	0.24	67,67,67,67	0
57	MG	2a	1672	1/1	0.91	0.28	72,72,72,72	0
57	MG	2a	1673	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3420	1/1	0.91	0.36	61,61,61,61	0
57	MG	2A	3728	1/1	0.91	0.16	49,49,49,49	0
57	MG	2a	1679	1/1	0.91	0.19	70,70,70,70	0
57	MG	1a	1711	1/1	0.91	0.18	67,67,67,67	0
57	MG	1A	3052	1/1	0.91	0.08	40,40,40,40	0
57	MG	1a	1715	1/1	0.91	0.11	63,63,63,63	0
57	MG	2a	1683	1/1	0.91	0.14	64,64,64,64	0
57	MG	1A	3257	1/1	0.91	0.13	72,72,72,72	0
57	MG	1A	3568	1/1	0.91	0.11	48,48,48,48	0
57	MG	2A	3433	1/1	0.91	0.23	51,51,51,51	0
57	MG	1A	4063	1/1	0.91	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1694	1/1	0.91	0.15	68,68,68,68	0
57	MG	2A	3436	1/1	0.91	0.36	65,65,65,65	0
57	MG	2A	3243	1/1	0.91	0.39	60,60,60,60	0
57	MG	1A	3123	1/1	0.91	0.09	40,40,40,40	0
57	MG	2A	3441	1/1	0.91	0.13	52,52,52,52	0
57	MG	2A	3051	1/1	0.91	0.14	54,54,54,54	0
57	MG	1a	1724	1/1	0.91	0.11	53,53,53,53	0
57	MG	2A	3254	1/1	0.91	0.31	64,64,64,64	0
57	MG	2A	3457	1/1	0.91	0.17	66,66,66,66	0
57	MG	2A	3461	1/1	0.91	0.10	69,69,69,69	0
57	MG	2A	3754	1/1	0.91	0.13	64,64,64,64	0
57	MG	1a	1727	1/1	0.91	0.24	61,61,61,61	0
57	MG	1a	1728	1/1	0.91	0.20	50,50,50,50	0
57	MG	2A	3056	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3057	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3591	1/1	0.91	0.08	33,33,33,33	0
57	MG	1A	3952	1/1	0.91	0.06	26,26,26,26	0
57	MG	2A	3765	1/1	0.91	0.25	68,68,68,68	0
57	MG	1A	3351	1/1	0.91	0.21	39,39,39,39	0
57	MG	1A	3171	1/1	0.91	0.35	41,41,41,41	0
57	MG	2A	3489	1/1	0.91	0.33	63,63,63,63	0
57	MG	1a	1744	1/1	0.91	0.28	56,56,56,56	0
57	MG	2a	1723	1/1	0.91	0.37	71,71,71,71	0
57	MG	2A	3785	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1747	1/1	0.91	0.19	60,60,60,60	0
57	MG	2a	1726	1/1	0.91	0.32	63,63,63,63	0
57	MG	2A	3495	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3078	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3500	1/1	0.91	0.11	74,74,74,74	0
57	MG	2A	3501	1/1	0.91	0.10	64,64,64,64	0
57	MG	1a	1610	1/1	0.91	0.07	66,66,66,66	0
57	MG	1a	1756	1/1	0.91	0.22	64,64,64,64	0
57	MG	1A	3226	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3833	1/1	0.91	0.10	31,31,31,31	0
57	MG	2A	3807	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	4081	1/1	0.91	0.10	21,21,21,21	0
57	MG	2A	3509	1/1	0.91	0.14	46,46,46,46	0
57	MG	2a	1747	1/1	0.91	0.20	77,77,77,77	0
57	MG	2a	1748	1/1	0.91	0.07	68,68,68,68	0
57	MG	1A	3497	1/1	0.91	0.13	44,44,44,44	0
57	MG	1A	3603	1/1	0.91	0.26	44,44,44,44	0
57	MG	2A	3515	1/1	0.91	0.14	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	3097	1/1	0.91	0.19	64,64,64,64	0
57	MG	2a	1763	1/1	0.91	0.11	69,69,69,69	0
57	MG	1A	3848	1/1	0.91	0.24	53,53,53,53	0
57	MG	2a	1765	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3714	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3358	1/1	0.91	0.10	42,42,42,42	0
57	MG	1A	3130	1/1	0.91	0.08	64,64,64,64	0
57	MG	2a	1772	1/1	0.91	0.18	69,69,69,69	0
57	MG	2A	3835	1/1	0.91	0.10	70,70,70,70	0
57	MG	1B	202	1/1	0.91	0.24	54,54,54,54	0
57	MG	1A	3982	1/1	0.91	0.17	53,53,53,53	0
57	MG	1a	1786	1/1	0.91	0.15	63,63,63,63	0
57	MG	1A	3361	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3851	1/1	0.91	0.13	64,64,64,64	0
57	MG	1a	1788	1/1	0.91	0.17	65,65,65,65	0
57	MG	1a	1640	1/1	0.91	0.17	56,56,56,56	0
57	MG	1B	208	1/1	0.91	0.26	65,65,65,65	0
57	MG	2A	3300	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3364	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1643	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3563	1/1	0.91	0.09	39,39,39,39	0
57	MG	2A	3306	1/1	0.91	0.11	74,74,74,74	0
57	MG	2a	1796	1/1	0.91	0.11	72,72,72,72	0
57	MG	2A	3136	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3433	1/1	0.91	0.09	41,41,41,41	0
57	MG	2B	205	1/1	0.91	0.18	70,70,70,70	0
57	MG	2a	1803	1/1	0.91	0.11	61,61,61,61	0
57	MG	2a	1804	1/1	0.91	0.21	56,56,56,56	0
57	MG	2A	3573	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3146	1/1	0.91	0.11	48,48,48,48	0
57	MG	1A	3511	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3576	1/1	0.91	0.10	28,28,28,28	0
57	MG	2B	210	1/1	0.91	0.24	68,68,68,68	0
57	MG	1B	219	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3315	1/1	0.91	0.13	53,53,53,53	0
57	MG	1A	3065	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3317	1/1	0.91	0.37	54,54,54,54	0
57	MG	1A	3866	1/1	0.91	0.18	36,36,36,36	0
57	MG	1A	3325	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3586	1/1	0.91	0.07	54,54,54,54	0
57	MG	1a	1659	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3527	1/1	0.91	0.24	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	3161	1/1	0.91	0.23	62,62,62,62	0
57	MG	2A	3162	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3163	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3529	1/1	0.91	0.24	70,70,70,70	0
57	MG	1A	4003	1/1	0.91	0.19	32,32,32,32	0
57	MG	1A	4006	1/1	0.91	0.11	68,68,68,68	0
57	MG	1A	3745	1/1	0.91	0.14	66,66,66,66	0
57	MG	2A	3608	1/1	0.91	0.10	29,29,29,29	0
57	MG	1B	232	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3328	1/1	0.91	0.19	61,61,61,61	0
57	MG	2A	3171	1/1	0.91	0.08	56,56,56,56	0
57	MG	1h	201	1/1	0.91	0.09	60,60,60,60	0
57	MG	2v	102	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3337	1/1	0.91	0.18	61,61,61,61	0
57	MG	2w	102	1/1	0.91	0.12	62,62,62,62	0
57	MG	2U	201	1/1	0.91	0.29	59,59,59,59	0
57	MG	2U	202	1/1	0.91	0.15	51,51,51,51	0
57	MG	2x	101	1/1	0.91	0.23	49,49,49,49	0
57	MG	2V	203	1/1	0.91	0.28	67,67,67,67	0
57	MG	2W	201	1/1	0.91	0.10	64,64,64,64	0
57	MG	1D	309	1/1	0.91	0.12	47,47,47,47	0
57	MG	2x	106	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3305	1/1	0.92	0.17	49,49,49,49	0
57	MG	1A	3225	1/1	0.92	0.14	46,46,46,46	0
57	MG	2A	3137	1/1	0.92	0.18	49,49,49,49	0
57	MG	2A	3139	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3479	1/1	0.92	0.29	65,65,65,65	0
57	MG	1A	3932	1/1	0.92	0.09	33,33,33,33	0
57	MG	1A	4049	1/1	0.92	0.07	49,49,49,49	0
57	MG	2A	3294	1/1	0.92	0.25	53,53,53,53	0
57	MG	1a	1681	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3733	1/1	0.92	0.12	43,43,43,43	0
57	MG	1e	201	1/1	0.92	0.11	70,70,70,70	0
57	MG	2a	1638	1/1	0.92	0.14	52,52,52,52	0
57	MG	2a	1639	1/1	0.92	0.15	62,62,62,62	0
57	MG	1f	201	1/1	0.92	0.17	53,53,53,53	0
57	MG	2A	3299	1/1	0.92	0.12	67,67,67,67	0
57	MG	2a	1642	1/1	0.92	0.09	62,62,62,62	0
57	MG	1N	202	1/1	0.92	0.28	43,43,43,43	0
57	MG	2A	3497	1/1	0.92	0.19	58,58,58,58	0
57	MG	1O	205	1/1	0.92	0.10	67,67,67,67	0
57	MG	2A	3302	1/1	0.92	0.22	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	1P	206	1/1	0.92	0.22	49,49,49,49	0
57	MG	1A	3277	1/1	0.92	0.13	49,49,49,49	0
57	MG	2A	3747	1/1	0.92	0.20	43,43,43,43	0
57	MG	1A	3828	1/1	0.92	0.08	26,26,26,26	0
57	MG	1A	3719	1/1	0.92	0.11	30,30,30,30	0
57	MG	1A	3291	1/1	0.92	0.08	45,45,45,45	0
57	MG	2A	3752	1/1	0.92	0.10	62,62,62,62	0
57	MG	2a	1655	1/1	0.92	0.08	60,60,60,60	0
57	MG	1A	3617	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3342	1/1	0.92	0.08	58,58,58,58	0
57	MG	2a	1658	1/1	0.92	0.21	63,63,63,63	0
57	MG	2A	3314	1/1	0.92	0.27	71,71,71,71	0
57	MG	2A	3757	1/1	0.92	0.17	63,63,63,63	0
57	MG	2a	1664	1/1	0.92	0.13	68,68,68,68	0
57	MG	1A	3420	1/1	0.92	0.10	35,35,35,35	0
57	MG	1A	3292	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3760	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3847	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3523	1/1	0.92	0.20	67,67,67,67	0
57	MG	1A	3622	1/1	0.92	0.09	31,31,31,31	0
57	MG	1A	3543	1/1	0.92	0.15	36,36,36,36	0
57	MG	2A	3770	1/1	0.92	0.18	68,68,68,68	0
57	MG	2A	3776	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3321	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3322	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	4066	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3784	1/1	0.92	0.15	73,73,73,73	0
57	MG	2a	1687	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3422	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3534	1/1	0.92	0.11	60,60,60,60	0
57	MG	1A	3293	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3539	1/1	0.92	0.11	49,49,49,49	0
57	MG	1A	3964	1/1	0.92	0.08	61,61,61,61	0
57	MG	16	101	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3204	1/1	0.92	0.09	43,43,43,43	0
57	MG	2A	3185	1/1	0.92	0.09	74,74,74,74	0
57	MG	17	105	1/1	0.92	0.15	51,51,51,51	0
57	MG	1a	1713	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3806	1/1	0.92	0.08	41,41,41,41	0
57	MG	1x	111	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3639	1/1	0.92	0.11	27,27,27,27	0
57	MG	1A	3971	1/1	0.92	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3566	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3859	1/1	0.92	0.08	63,63,63,63	0
57	MG	2a	1711	1/1	0.92	0.11	67,67,67,67	0
57	MG	1A	3082	1/1	0.92	0.16	40,40,40,40	0
57	MG	1A	3975	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3172	1/1	0.92	0.13	51,51,51,51	0
57	MG	1a	1613	1/1	0.92	0.15	67,67,67,67	0
57	MG	1a	1614	1/1	0.92	0.27	60,60,60,60	0
57	MG	2A	3831	1/1	0.92	0.09	57,57,57,57	0
57	MG	2A	3345	1/1	0.92	0.19	68,68,68,68	0
57	MG	1a	1732	1/1	0.92	0.24	63,63,63,63	0
57	MG	2A	3836	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3199	1/1	0.92	0.14	62,62,62,62	0
57	MG	2A	3349	1/1	0.92	0.16	70,70,70,70	0
57	MG	2A	3200	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3584	1/1	0.92	0.13	61,61,61,61	0
57	MG	2A	3848	1/1	0.92	0.09	52,52,52,52	0
57	MG	2a	1730	1/1	0.92	0.26	70,70,70,70	0
57	MG	2A	3036	1/1	0.92	0.10	57,57,57,57	0
57	MG	2a	1732	1/1	0.92	0.31	64,64,64,64	0
57	MG	1A	3385	1/1	0.92	0.09	44,44,44,44	0
57	MG	2a	1735	1/1	0.92	0.17	70,70,70,70	0
57	MG	1a	1620	1/1	0.92	0.09	47,47,47,47	0
57	MG	1a	1622	1/1	0.92	0.31	73,73,73,73	0
57	MG	1A	3490	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3600	1/1	0.92	0.21	65,65,65,65	0
57	MG	1a	1742	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3209	1/1	0.92	0.24	57,57,57,57	0
57	MG	1A	3435	1/1	0.92	0.17	44,44,44,44	0
57	MG	1a	1745	1/1	0.92	0.08	69,69,69,69	0
57	MG	2A	3052	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3120	1/1	0.92	0.08	36,36,36,36	0
57	MG	1A	3773	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	3875	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3258	1/1	0.92	0.11	22,22,22,22	0
57	MG	2a	1752	1/1	0.92	0.17	66,66,66,66	0
57	MG	2a	1757	1/1	0.92	0.08	61,61,61,61	0
57	MG	2A	3366	1/1	0.92	0.26	63,63,63,63	0
57	MG	2a	1762	1/1	0.92	0.12	70,70,70,70	0
57	MG	1B	211	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3440	1/1	0.92	0.09	44,44,44,44	0
57	MG	2B	213	1/1	0.92	0.15	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	2A	3616	1/1	0.92	0.19	65,65,65,65	0
57	MG	2A	3226	1/1	0.92	0.21	44,44,44,44	0
57	MG	2A	3620	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3228	1/1	0.92	0.14	65,65,65,65	0
57	MG	2A	3059	1/1	0.92	0.15	54,54,54,54	0
57	MG	1B	214	1/1	0.92	0.20	62,62,62,62	0
57	MG	1a	1764	1/1	0.92	0.11	61,61,61,61	0
57	MG	1a	1638	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3070	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3779	1/1	0.92	0.11	20,20,20,20	0
57	MG	1A	3997	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3073	1/1	0.92	0.21	69,69,69,69	0
57	MG	1A	3580	1/1	0.92	0.11	34,34,34,34	0
57	MG	2F	303	1/1	0.92	0.09	50,50,50,50	0
57	MG	2a	1790	1/1	0.92	0.17	64,64,64,64	0
57	MG	2F	304	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3581	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3583	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3245	1/1	0.92	0.16	63,63,63,63	0
57	MG	2A	3391	1/1	0.92	0.16	61,61,61,61	0
57	MG	2A	3246	1/1	0.92	0.06	60,60,60,60	0
57	MG	1A	3888	1/1	0.92	0.17	32,32,32,32	0
57	MG	2A	3251	1/1	0.92	0.12	64,64,64,64	0
57	MG	1A	3443	1/1	0.92	0.15	44,44,44,44	0
57	MG	2A	3405	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3407	1/1	0.92	0.35	59,59,59,59	0
57	MG	1A	3893	1/1	0.92	0.12	33,33,33,33	0
57	MG	2a	1807	1/1	0.92	0.22	56,56,56,56	0
57	MG	2a	1809	1/1	0.92	0.18	68,68,68,68	0
57	MG	1A	3791	1/1	0.92	0.07	21,21,21,21	0
57	MG	2A	3092	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3413	1/1	0.92	0.27	67,67,67,67	0
57	MG	2A	3414	1/1	0.92	0.26	64,64,64,64	0
57	MG	1A	3797	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3096	1/1	0.92	0.08	45,45,45,45	0
57	MG	1B	231	1/1	0.92	0.09	59,59,59,59	0
57	MG	25	102	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3401	1/1	0.92	0.30	42,42,42,42	0
57	MG	1A	3445	1/1	0.92	0.13	41,41,41,41	0
57	MG	1D	305	1/1	0.92	0.09	41,41,41,41	0
57	MG	28	101	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3447	1/1	0.92	0.10	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	3909	1/1	0.92	0.07	29,29,29,29	0
57	MG	2A	3428	1/1	0.92	0.19	56,56,56,56	0
57	MG	2A	3430	1/1	0.92	0.13	41,41,41,41	0
57	MG	2A	3431	1/1	0.92	0.27	49,49,49,49	0
57	MG	1a	1808	1/1	0.92	0.09	46,46,46,46	0
57	MG	2A	3110	1/1	0.92	0.22	61,61,61,61	0
57	MG	1A	3910	1/1	0.92	0.10	21,21,21,21	0
57	MG	2A	3113	1/1	0.92	0.10	45,45,45,45	0
57	MG	2q	201	1/1	0.92	0.10	65,65,65,65	0
57	MG	2a	1608	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3114	1/1	0.92	0.10	66,66,66,66	0
57	MG	2A	3702	1/1	0.92	0.10	70,70,70,70	0
57	MG	2A	3705	1/1	0.92	0.13	33,33,33,33	0
57	MG	1A	3513	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3440	1/1	0.92	0.29	59,59,59,59	0
57	MG	1A	3303	1/1	0.92	0.26	33,33,33,33	0
57	MG	2A	3713	1/1	0.92	0.08	51,51,51,51	0
57	MG	2A	3121	1/1	0.92	0.07	57,57,57,57	0
57	MG	2x	102	1/1	0.92	0.17	75,75,75,75	0
57	MG	1A	3815	1/1	0.92	0.13	21,21,21,21	0
57	MG	1A	3412	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3284	1/1	0.92	0.17	61,61,61,61	0
57	MG	1A	3526	1/1	0.92	0.20	47,47,47,47	0
59	ZN	24	501	1/1	0.92	0.15	138,138,138,138	0
57	MG	2A	3140	1/1	0.93	0.34	73,73,73,73	0
57	MG	2l	101	1/1	0.93	0.19	63,63,63,63	0
57	MG	2A	3623	1/1	0.93	0.16	34,34,34,34	0
57	MG	2A	3624	1/1	0.93	0.15	57,57,57,57	0
57	MG	25	101	1/1	0.93	0.16	56,56,56,56	0
57	MG	2A	3141	1/1	0.93	0.15	58,58,58,58	0
57	MG	1O	204	1/1	0.93	0.09	56,56,56,56	0
57	MG	25	105	1/1	0.93	0.11	58,58,58,58	0
57	MG	1a	1755	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3635	1/1	0.93	0.12	64,64,64,64	0
57	MG	1A	3976	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3798	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3380	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3312	1/1	0.93	0.21	53,53,53,53	0
57	MG	2A	3643	1/1	0.93	0.11	39,39,39,39	0
57	MG	2A	3646	1/1	0.93	0.26	64,64,64,64	0
57	MG	2A	3647	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3983	1/1	0.93	0.13	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	3471	1/1	0.93	0.11	31,31,31,31	0
57	MG	2A	3650	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3081	1/1	0.93	0.12	36,36,36,36	0
57	MG	1a	1772	1/1	0.93	0.09	54,54,54,54	0
57	MG	1T	202	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3095	1/1	0.93	0.14	39,39,39,39	0
57	MG	2a	1612	1/1	0.93	0.14	58,58,58,58	0
57	MG	1U	204	1/1	0.93	0.12	26,26,26,26	0
57	MG	1a	1780	1/1	0.93	0.08	56,56,56,56	0
57	MG	1U	208	1/1	0.93	0.21	39,39,39,39	0
57	MG	1A	3098	1/1	0.93	0.08	41,41,41,41	0
57	MG	1W	202	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	3388	1/1	0.93	0.15	58,58,58,58	0
57	MG	1A	3993	1/1	0.93	0.13	39,39,39,39	0
57	MG	2A	3172	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3817	1/1	0.93	0.05	38,38,38,38	0
57	MG	1A	3482	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3389	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3367	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3369	1/1	0.93	0.24	49,49,49,49	0
57	MG	1A	3391	1/1	0.93	0.19	43,43,43,43	0
57	MG	2a	1631	1/1	0.93	0.18	59,59,59,59	0
57	MG	1A	3099	1/1	0.93	0.21	65,65,65,65	0
57	MG	2A	3183	1/1	0.93	0.22	55,55,55,55	0
57	MG	2A	3682	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3182	1/1	0.93	0.17	38,38,38,38	0
57	MG	1A	3635	1/1	0.93	0.14	10,10,10,10	0
57	MG	2A	3377	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3638	1/1	0.93	0.08	56,56,56,56	0
57	MG	1A	3321	1/1	0.93	0.17	52,52,52,52	0
57	MG	18	105	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3642	1/1	0.93	0.13	42,42,42,42	0
57	MG	2A	3693	1/1	0.93	0.08	77,77,77,77	0
57	MG	1A	4017	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3404	1/1	0.93	0.29	37,37,37,37	0
57	MG	2A	3696	1/1	0.93	0.07	58,58,58,58	0
57	MG	1a	1606	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3699	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3840	1/1	0.93	0.10	27,27,27,27	0
57	MG	1A	3407	1/1	0.93	0.14	43,43,43,43	0
57	MG	1A	3501	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3706	1/1	0.93	0.09	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	1A	3409	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3709	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3184	1/1	0.93	0.14	66,66,66,66	0
57	MG	1A	3045	1/1	0.93	0.10	34,34,34,34	0
57	MG	2A	3396	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3852	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3402	1/1	0.93	0.24	62,62,62,62	0
57	MG	1e	202	1/1	0.93	0.20	52,52,52,52	0
57	MG	1A	3413	1/1	0.93	0.12	35,35,35,35	0
57	MG	2a	1666	1/1	0.93	0.15	62,62,62,62	0
57	MG	1a	1623	1/1	0.93	0.16	70,70,70,70	0
57	MG	2A	3722	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3115	1/1	0.93	0.22	39,39,39,39	0
57	MG	1m	3002	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3047	1/1	0.93	0.09	32,32,32,32	0
57	MG	2A	3726	1/1	0.93	0.17	74,74,74,74	0
57	MG	1A	3667	1/1	0.93	0.09	44,44,44,44	0
57	MG	2a	1677	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3062	1/1	0.93	0.18	51,51,51,51	0
57	MG	1A	3675	1/1	0.93	0.17	55,55,55,55	0
57	MG	1a	1630	1/1	0.93	0.34	68,68,68,68	0
57	MG	1a	1631	1/1	0.93	0.19	70,70,70,70	0
57	MG	2A	3215	1/1	0.93	0.23	66,66,66,66	0
57	MG	2a	1684	1/1	0.93	0.20	55,55,55,55	0
57	MG	1A	3521	1/1	0.93	0.32	35,35,35,35	0
57	MG	2A	3217	1/1	0.93	0.16	60,60,60,60	0
57	MG	1A	4050	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3425	1/1	0.93	0.39	63,63,63,63	0
57	MG	2A	3219	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3865	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3679	1/1	0.93	0.07	20,20,20,20	0
57	MG	2A	3429	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3744	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3680	1/1	0.93	0.07	16,16,16,16	0
57	MG	1A	3332	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	4056	1/1	0.93	0.08	42,42,42,42	0
57	MG	1A	3020	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3434	1/1	0.93	0.28	53,53,53,53	0
57	MG	2a	1704	1/1	0.93	0.10	71,71,71,71	0
57	MG	1A	3143	1/1	0.93	0.11	58,58,58,58	0
57	MG	1A	3144	1/1	0.93	0.09	42,42,42,42	0
57	MG	1a	1644	1/1	0.93	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	2A	3234	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3532	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3533	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3445	1/1	0.93	0.26	66,66,66,66	0
57	MG	1A	3214	1/1	0.93	0.16	49,49,49,49	0
57	MG	2A	3449	1/1	0.93	0.12	62,62,62,62	0
57	MG	1a	1648	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3423	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3242	1/1	0.93	0.37	62,62,62,62	0
57	MG	1A	3884	1/1	0.93	0.18	41,41,41,41	0
57	MG	2A	3767	1/1	0.93	0.16	67,67,67,67	0
57	MG	2A	3003	1/1	0.93	0.19	45,45,45,45	0
57	MG	1A	3288	1/1	0.93	0.13	50,50,50,50	0
57	MG	2A	3467	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3010	1/1	0.93	0.09	58,58,58,58	0
57	MG	2A	3476	1/1	0.93	0.19	70,70,70,70	0
57	MG	2A	3247	1/1	0.93	0.06	80,80,80,80	0
57	MG	2A	3248	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3289	1/1	0.93	0.20	49,49,49,49	0
57	MG	2A	3484	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3250	1/1	0.93	0.11	50,50,50,50	0
57	MG	2A	3018	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	3889	1/1	0.93	0.13	35,35,35,35	0
57	MG	1A	3712	1/1	0.93	0.11	26,26,26,26	0
57	MG	2A	3798	1/1	0.93	0.07	58,58,58,58	0
57	MG	1a	1663	1/1	0.93	0.07	66,66,66,66	0
57	MG	1A	3429	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3257	1/1	0.93	0.14	54,54,54,54	0
57	MG	1A	3715	1/1	0.93	0.10	28,28,28,28	0
57	MG	2A	3261	1/1	0.93	0.08	72,72,72,72	0
57	MG	1A	3222	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	4086	1/1	0.93	0.23	63,63,63,63	0
57	MG	1A	3720	1/1	0.93	0.05	20,20,20,20	0
57	MG	1A	3548	1/1	0.93	0.08	25,25,25,25	0
57	MG	2A	3816	1/1	0.93	0.13	34,34,34,34	0
57	MG	2a	1756	1/1	0.93	0.06	82,82,82,82	0
57	MG	1A	3348	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	4092	1/1	0.93	0.08	47,47,47,47	0
57	MG	1A	3726	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	4094	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	4096	1/1	0.93	0.12	61,61,61,61	0
57	MG	1a	1679	1/1	0.93	0.21	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	1A	3148	1/1	0.93	0.40	37,37,37,37	0
57	MG	1A	3152	1/1	0.93	0.19	39,39,39,39	0
57	MG	1A	3228	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3914	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3233	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3840	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3917	1/1	0.93	0.18	53,53,53,53	0
57	MG	2A	3844	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3060	1/1	0.93	0.21	58,58,58,58	0
57	MG	1A	3557	1/1	0.93	0.07	57,57,57,57	0
57	MG	1A	3439	1/1	0.93	0.07	47,47,47,47	0
57	MG	1A	3924	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	3050	1/1	0.93	0.14	27,27,27,27	0
57	MG	1A	3927	1/1	0.93	0.17	39,39,39,39	0
57	MG	1A	3298	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3860	1/1	0.93	0.18	57,57,57,57	0
57	MG	2A	3541	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3239	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3750	1/1	0.93	0.10	59,59,59,59	0
57	MG	2A	3079	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3571	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3091	1/1	0.93	0.20	55,55,55,55	0
57	MG	2a	1800	1/1	0.93	0.24	77,77,77,77	0
57	MG	1A	3446	1/1	0.93	0.09	54,54,54,54	0
57	MG	1A	3244	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3759	1/1	0.93	0.10	19,19,19,19	0
57	MG	1A	3448	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3585	1/1	0.93	0.22	56,56,56,56	0
57	MG	2A	3303	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3093	1/1	0.93	0.09	40,40,40,40	0
57	MG	1B	233	1/1	0.93	0.12	58,58,58,58	0
57	MG	2a	1811	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3304	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3308	1/1	0.93	0.10	68,68,68,68	0
57	MG	1B	235	1/1	0.93	0.07	44,44,44,44	0
57	MG	1A	3367	1/1	0.93	0.11	44,44,44,44	0
57	MG	2D	302	1/1	0.93	0.15	56,56,56,56	0
57	MG	1A	3245	1/1	0.93	0.09	46,46,46,46	0
57	MG	2D	306	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	3777	1/1	0.93	0.12	42,42,42,42	0
57	MG	2A	3313	1/1	0.93	0.09	46,46,46,46	0
57	MG	2a	1821	1/1	0.93	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1718	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3040	1/1	0.93	0.18	51,51,51,51	0
57	MG	1A	3371	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3375	1/1	0.93	0.32	42,42,42,42	0
57	MG	2d	301	1/1	0.93	0.26	62,62,62,62	0
57	MG	2E	308	1/1	0.93	0.11	32,32,32,32	0
57	MG	2A	3596	1/1	0.93	0.21	66,66,66,66	0
57	MG	1a	1726	1/1	0.93	0.26	43,43,43,43	0
57	MG	1E	310	1/1	0.93	0.23	38,38,38,38	0
57	MG	2A	3320	1/1	0.93	0.14	56,56,56,56	0
57	MG	2F	306	1/1	0.93	0.26	51,51,51,51	0
57	MG	1A	3967	1/1	0.93	0.08	52,52,52,52	0
57	MG	2A	3116	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3464	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3970	1/1	0.93	0.14	54,54,54,54	0
57	MG	2t	201	1/1	0.93	0.14	48,48,48,48	0
57	MG	1A	3786	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3122	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	3467	1/1	0.93	0.22	44,44,44,44	0
57	MG	1F	310	1/1	0.93	0.07	47,47,47,47	0
57	MG	2T	3502	1/1	0.93	0.28	59,59,59,59	0
57	MG	2A	3128	1/1	0.93	0.07	47,47,47,47	0
57	MG	1a	1741	1/1	0.93	0.22	58,58,58,58	0
57	MG	2A	3131	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3973	1/1	0.93	0.08	55,55,55,55	0
57	MG	2W	202	1/1	0.93	0.18	48,48,48,48	0
57	MG	1A	3308	1/1	0.93	0.16	51,51,51,51	0
57	MG	1A	3607	1/1	0.93	0.24	51,51,51,51	0
58	K	2A	3450	1/1	0.93	0.10	65,65,65,65	0
57	MG	1O	202	1/1	0.93	0.18	51,51,51,51	0
57	MG	1W	207	1/1	0.94	0.13	27,27,27,27	0
57	MG	1X	105	1/1	0.94	0.10	48,48,48,48	0
57	MG	1a	1751	1/1	0.94	0.07	66,66,66,66	0
57	MG	1Y	201	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3338	1/1	0.94	0.33	52,52,52,52	0
57	MG	2A	3340	1/1	0.94	0.14	53,53,53,53	0
57	MG	1Y	202	1/1	0.94	0.31	46,46,46,46	0
57	MG	1Z	302	1/1	0.94	0.18	51,51,51,51	0
57	MG	25	103	1/1	0.94	0.22	44,44,44,44	0
57	MG	1A	4034	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3613	1/1	0.94	0.19	46,46,46,46	0
57	MG	2A	3638	1/1	0.94	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3142	1/1	0.94	0.17	52,52,52,52	0
57	MG	2A	3641	1/1	0.94	0.07	51,51,51,51	0
57	MG	2A	3143	1/1	0.94	0.23	40,40,40,40	0
57	MG	1A	3885	1/1	0.94	0.06	35,35,35,35	0
57	MG	2A	3644	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3645	1/1	0.94	0.16	63,63,63,63	0
57	MG	11	101	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	4044	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3886	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3615	1/1	0.94	0.15	60,60,60,60	0
57	MG	1A	3073	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3272	1/1	0.94	0.12	39,39,39,39	0
57	MG	2A	3652	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	3309	1/1	0.94	0.24	53,53,53,53	0
57	MG	2A	3158	1/1	0.94	0.22	62,62,62,62	0
57	MG	1A	3386	1/1	0.94	0.22	42,42,42,42	0
57	MG	1A	3757	1/1	0.94	0.07	55,55,55,55	0
57	MG	18	101	1/1	0.94	0.25	52,52,52,52	0
57	MG	18	104	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1616	1/1	0.94	0.07	71,71,71,71	0
57	MG	2A	3164	1/1	0.94	0.14	55,55,55,55	0
57	MG	1A	3896	1/1	0.94	0.11	35,35,35,35	0
57	MG	18	106	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3667	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3537	1/1	0.94	0.24	30,30,30,30	0
57	MG	2a	1622	1/1	0.94	0.10	58,58,58,58	0
57	MG	2a	1623	1/1	0.94	0.09	65,65,65,65	0
57	MG	1A	3761	1/1	0.94	0.07	33,33,33,33	0
57	MG	1A	3762	1/1	0.94	0.05	14,14,14,14	0
57	MG	1A	3764	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	3538	1/1	0.94	0.24	47,47,47,47	0
57	MG	1a	1796	1/1	0.94	0.09	66,66,66,66	0
57	MG	1A	3427	1/1	0.94	0.14	55,55,55,55	0
57	MG	2a	1630	1/1	0.94	0.13	54,54,54,54	0
57	MG	1a	1803	1/1	0.94	0.08	66,66,66,66	0
57	MG	1a	1805	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3375	1/1	0.94	0.18	70,70,70,70	0
57	MG	2A	3681	1/1	0.94	0.18	67,67,67,67	0
57	MG	1A	3768	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3181	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3912	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3428	1/1	0.94	0.14	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	1a	1810	1/1	0.94	0.10	67,67,67,67	0
57	MG	1A	3078	1/1	0.94	0.10	25,25,25,25	0
57	MG	1a	1616	1/1	0.94	0.13	58,58,58,58	0
57	MG	1a	1617	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3386	1/1	0.94	0.11	61,61,61,61	0
57	MG	1A	3915	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3632	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3544	1/1	0.94	0.23	47,47,47,47	0
57	MG	2A	3191	1/1	0.94	0.29	63,63,63,63	0
57	MG	1a	1818	1/1	0.94	0.18	53,53,53,53	0
57	MG	2A	3392	1/1	0.94	0.16	53,53,53,53	0
57	MG	1a	1819	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3918	1/1	0.94	0.13	43,43,43,43	0
57	MG	2a	1652	1/1	0.94	0.09	62,62,62,62	0
57	MG	1A	4075	1/1	0.94	0.08	22,22,22,22	0
57	MG	2A	3707	1/1	0.94	0.19	64,64,64,64	0
57	MG	2A	3400	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3545	1/1	0.94	0.19	44,44,44,44	0
57	MG	1a	1823	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3313	1/1	0.94	0.24	49,49,49,49	0
57	MG	1A	3479	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3714	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3549	1/1	0.94	0.23	44,44,44,44	0
57	MG	1A	4085	1/1	0.94	0.12	72,72,72,72	0
57	MG	1A	3648	1/1	0.94	0.06	35,35,35,35	0
57	MG	1A	3928	1/1	0.94	0.13	32,32,32,32	0
57	MG	1m	3001	1/1	0.94	0.10	58,58,58,58	0
57	MG	1a	1635	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3787	1/1	0.94	0.08	28,28,28,28	0
57	MG	1A	3649	1/1	0.94	0.06	15,15,15,15	0
57	MG	1A	4091	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3789	1/1	0.94	0.07	65,65,65,65	0
57	MG	1A	3216	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3335	1/1	0.94	0.06	50,50,50,50	0
57	MG	2A	3424	1/1	0.94	0.21	55,55,55,55	0
57	MG	2A	3214	1/1	0.94	0.27	59,59,59,59	0
57	MG	1A	3654	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3483	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3553	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3394	1/1	0.94	0.28	60,60,60,60	0
57	MG	1A	3947	1/1	0.94	0.05	51,51,51,51	0
57	MG	1A	3555	1/1	0.94	0.12	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	1B	209	1/1	0.94	0.11	41,41,41,41	0
57	MG	1a	1649	1/1	0.94	0.10	49,49,49,49	0
57	MG	1a	1650	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3810	1/1	0.94	0.06	44,44,44,44	0
57	MG	1A	3362	1/1	0.94	0.07	49,49,49,49	0
57	MG	1a	1653	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3400	1/1	0.94	0.49	46,46,46,46	0
57	MG	2A	3232	1/1	0.94	0.12	57,57,57,57	0
57	MG	1a	1658	1/1	0.94	0.17	59,59,59,59	0
57	MG	2A	3749	1/1	0.94	0.19	67,67,67,67	0
57	MG	1A	3218	1/1	0.94	0.15	39,39,39,39	0
57	MG	1A	3493	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3566	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3965	1/1	0.94	0.09	52,52,52,52	0
57	MG	2a	1709	1/1	0.94	0.12	67,67,67,67	0
57	MG	2A	3454	1/1	0.94	0.05	48,48,48,48	0
57	MG	2A	3455	1/1	0.94	0.18	58,58,58,58	0
57	MG	2A	3005	1/1	0.94	0.24	62,62,62,62	0
57	MG	2A	3006	1/1	0.94	0.18	58,58,58,58	0
57	MG	1B	222	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	1715	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3494	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3402	1/1	0.94	0.20	55,55,55,55	0
57	MG	2A	3465	1/1	0.94	0.17	55,55,55,55	0
57	MG	1a	1667	1/1	0.94	0.14	68,68,68,68	0
57	MG	2A	3471	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3569	1/1	0.94	0.35	54,54,54,54	0
57	MG	2A	3769	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3473	1/1	0.94	0.12	62,62,62,62	0
57	MG	2A	3474	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3777	1/1	0.94	0.07	37,37,37,37	0
57	MG	1A	3441	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3301	1/1	0.94	0.23	51,51,51,51	0
57	MG	1A	3339	1/1	0.94	0.29	58,58,58,58	0
57	MG	2A	3482	1/1	0.94	0.14	61,61,61,61	0
57	MG	2a	1733	1/1	0.94	0.32	65,65,65,65	0
57	MG	2A	3032	1/1	0.94	0.08	44,44,44,44	0
57	MG	1a	1673	1/1	0.94	0.06	59,59,59,59	0
57	MG	2A	3485	1/1	0.94	0.37	73,73,73,73	0
57	MG	1A	3060	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3253	1/1	0.94	0.09	58,58,58,58	0
57	MG	2A	3039	1/1	0.94	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	2A	3040	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3041	1/1	0.94	0.16	56,56,56,56	0
57	MG	1A	3508	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3698	1/1	0.94	0.08	51,51,51,51	0
57	MG	2a	1746	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3803	1/1	0.94	0.06	39,39,39,39	0
57	MG	2A	3259	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3260	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3100	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3979	1/1	0.94	0.15	39,39,39,39	0
57	MG	2A	3810	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3841	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3842	1/1	0.94	0.10	40,40,40,40	0
57	MG	2a	1758	1/1	0.94	0.09	62,62,62,62	0
57	MG	2a	1759	1/1	0.94	0.09	69,69,69,69	0
57	MG	1A	3843	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3586	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3506	1/1	0.94	0.07	30,30,30,30	0
57	MG	1D	312	1/1	0.94	0.16	30,30,30,30	0
57	MG	1A	3587	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3590	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3369	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3254	1/1	0.94	0.17	52,52,52,52	0
57	MG	2A	3517	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3518	1/1	0.94	0.08	35,35,35,35	0
57	MG	2a	1776	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3991	1/1	0.94	0.10	20,20,20,20	0
57	MG	2A	3837	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3593	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3512	1/1	0.94	0.09	40,40,40,40	0
57	MG	2a	1783	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3717	1/1	0.94	0.13	27,27,27,27	0
57	MG	1a	1698	1/1	0.94	0.20	49,49,49,49	0
57	MG	1A	3718	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3067	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3323	1/1	0.94	0.12	36,36,36,36	0
57	MG	1a	1701	1/1	0.94	0.23	47,47,47,47	0
57	MG	1A	3600	1/1	0.94	0.34	52,52,52,52	0
57	MG	1a	1704	1/1	0.94	0.37	58,58,58,58	0
57	MG	1G	202	1/1	0.94	0.17	55,55,55,55	0
57	MG	1G	203	1/1	0.94	0.22	58,58,58,58	0
57	MG	1I	201	1/1	0.94	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3345	1/1	0.94	0.09	56,56,56,56	0
57	MG	2a	1798	1/1	0.94	0.16	70,70,70,70	0
57	MG	2A	3550	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	4002	1/1	0.94	0.07	15,15,15,15	0
57	MG	2a	1801	1/1	0.94	0.13	61,61,61,61	0
57	MG	2A	3085	1/1	0.94	0.08	58,58,58,58	0
57	MG	1N	206	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3557	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3297	1/1	0.94	0.06	45,45,45,45	0
57	MG	2A	3088	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3564	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3602	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3376	1/1	0.94	0.18	40,40,40,40	0
57	MG	2A	3091	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3569	1/1	0.94	0.16	51,51,51,51	0
57	MG	2B	212	1/1	0.94	0.09	73,73,73,73	0
57	MG	1A	3520	1/1	0.94	0.29	31,31,31,31	0
57	MG	1A	3377	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	4011	1/1	0.94	0.07	19,19,19,19	0
57	MG	2A	3305	1/1	0.94	0.20	58,58,58,58	0
57	MG	2A	3095	1/1	0.94	0.13	55,55,55,55	0
57	MG	1R	202	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3731	1/1	0.94	0.08	59,59,59,59	0
57	MG	1a	1720	1/1	0.94	0.18	65,65,65,65	0
57	MG	1A	3346	1/1	0.94	0.30	44,44,44,44	0
57	MG	2A	3100	1/1	0.94	0.07	33,33,33,33	0
57	MG	2E	302	1/1	0.94	0.14	65,65,65,65	0
57	MG	1S	202	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3255	1/1	0.94	0.18	49,49,49,49	0
57	MG	1A	3876	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3587	1/1	0.94	0.20	65,65,65,65	0
57	MG	2A	3107	1/1	0.94	0.17	61,61,61,61	0
57	MG	2A	3594	1/1	0.94	0.17	55,55,55,55	0
57	MG	2A	3595	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3108	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3878	1/1	0.94	0.09	42,42,42,42	0
57	MG	1a	1730	1/1	0.94	0.19	52,52,52,52	0
57	MG	1a	1731	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3609	1/1	0.94	0.30	62,62,62,62	0
57	MG	2O	201	1/1	0.94	0.18	54,54,54,54	0
57	MG	1a	1733	1/1	0.94	0.28	61,61,61,61	0
57	MG	1A	3528	1/1	0.94	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1U	206	1/1	0.94	0.17	27,27,27,27	0
57	MG	1A	3741	1/1	0.94	0.14	64,64,64,64	0
57	MG	2A	3119	1/1	0.94	0.30	65,65,65,65	0
57	MG	2A	3326	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3120	1/1	0.94	0.13	57,57,57,57	0
57	MG	1V	202	1/1	0.94	0.37	35,35,35,35	0
57	MG	1A	3349	1/1	0.94	0.09	55,55,55,55	0
57	MG	2V	202	1/1	0.94	0.23	45,45,45,45	0
57	MG	2A	3123	1/1	0.94	0.32	59,59,59,59	0
57	MG	1V	206	1/1	0.94	0.10	54,54,54,54	0
57	MG	1V	207	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3466	1/1	0.94	0.19	65,65,65,65	0
57	MG	2A	3656	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3334	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3241	1/1	0.95	0.05	32,32,32,32	0
57	MG	1A	3514	1/1	0.95	0.16	28,28,28,28	0
57	MG	1A	3723	1/1	0.95	0.09	28,28,28,28	0
57	MG	2A	3399	1/1	0.95	0.28	47,47,47,47	0
57	MG	1a	1675	1/1	0.95	0.10	65,65,65,65	0
57	MG	2A	3401	1/1	0.95	0.18	47,47,47,47	0
57	MG	1A	3515	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3002	1/1	0.95	0.27	58,58,58,58	0
57	MG	1A	3186	1/1	0.95	0.11	45,45,45,45	0
57	MG	1F	311	1/1	0.95	0.05	40,40,40,40	0
57	MG	2A	3406	1/1	0.95	0.31	50,50,50,50	0
57	MG	1F	313	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3337	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	3729	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3410	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3220	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3011	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3871	1/1	0.95	0.08	19,19,19,19	0
57	MG	2A	3017	1/1	0.95	0.19	51,51,51,51	0
57	MG	1A	3442	1/1	0.95	0.23	35,35,35,35	0
57	MG	2A	3019	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3418	1/1	0.95	0.23	59,59,59,59	0
57	MG	1A	3134	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3689	1/1	0.95	0.06	62,62,62,62	0
57	MG	1A	3135	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3025	1/1	0.95	0.15	61,61,61,61	0
57	MG	2A	3028	1/1	0.95	0.12	51,51,51,51	0
57	MG	1a	1688	1/1	0.95	0.12	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	1N	205	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3877	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3387	1/1	0.95	0.09	54,54,54,54	0
57	MG	2A	3237	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3698	1/1	0.95	0.07	24,24,24,24	0
57	MG	1O	203	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3340	1/1	0.95	0.32	57,57,57,57	0
57	MG	1A	4020	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3703	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3199	1/1	0.95	0.21	40,40,40,40	0
57	MG	1A	3016	1/1	0.95	0.18	58,58,58,58	0
57	MG	1A	3531	1/1	0.95	0.13	73,73,73,73	0
57	MG	1A	4026	1/1	0.95	0.05	45,45,45,45	0
57	MG	1A	3449	1/1	0.95	0.16	41,41,41,41	0
57	MG	2A	3046	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3744	1/1	0.95	0.05	50,50,50,50	0
57	MG	1A	4030	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3442	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3203	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3019	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3455	1/1	0.95	0.20	30,30,30,30	0
57	MG	1a	1708	1/1	0.95	0.25	70,70,70,70	0
57	MG	1A	3624	1/1	0.95	0.09	24,24,24,24	0
57	MG	1U	205	1/1	0.95	0.24	35,35,35,35	0
57	MG	1A	4038	1/1	0.95	0.06	38,38,38,38	0
57	MG	1U	207	1/1	0.95	0.30	35,35,35,35	0
57	MG	2A	3458	1/1	0.95	0.18	46,46,46,46	0
57	MG	2A	3460	1/1	0.95	0.12	67,67,67,67	0
57	MG	1A	4041	1/1	0.95	0.10	68,68,68,68	0
57	MG	1A	3536	1/1	0.95	0.08	30,30,30,30	0
57	MG	2A	3061	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3456	1/1	0.95	0.14	31,31,31,31	0
57	MG	2a	1659	1/1	0.95	0.08	71,71,71,71	0
57	MG	1A	3756	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3468	1/1	0.95	0.33	52,52,52,52	0
57	MG	2A	3469	1/1	0.95	0.20	57,57,57,57	0
57	MG	2a	1665	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3065	1/1	0.95	0.20	45,45,45,45	0
57	MG	2A	3735	1/1	0.95	0.07	59,59,59,59	0
57	MG	1A	3894	1/1	0.95	0.11	31,31,31,31	0
57	MG	1A	3252	1/1	0.95	0.05	59,59,59,59	0
57	MG	1W	203	1/1	0.95	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	2A	3475	1/1	0.95	0.31	61,61,61,61	0
57	MG	2A	3741	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3034	1/1	0.95	0.30	34,34,34,34	0
57	MG	2A	3477	1/1	0.95	0.10	41,41,41,41	0
57	MG	1a	1722	1/1	0.95	0.15	48,48,48,48	0
57	MG	1a	1723	1/1	0.95	0.33	61,61,61,61	0
57	MG	2A	3480	1/1	0.95	0.20	60,60,60,60	0
57	MG	2A	3076	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3271	1/1	0.95	0.08	58,58,58,58	0
57	MG	1X	103	1/1	0.95	0.14	46,46,46,46	0
57	MG	2a	1685	1/1	0.95	0.29	64,64,64,64	0
57	MG	2A	3274	1/1	0.95	0.23	47,47,47,47	0
57	MG	1a	1725	1/1	0.95	0.09	49,49,49,49	0
57	MG	2A	3276	1/1	0.95	0.13	49,49,49,49	0
57	MG	1A	3634	1/1	0.95	0.05	32,32,32,32	0
57	MG	2a	1690	1/1	0.95	0.12	52,52,52,52	0
57	MG	1A	3347	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3900	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3492	1/1	0.95	0.30	56,56,56,56	0
57	MG	1A	3637	1/1	0.95	0.08	31,31,31,31	0
57	MG	10	101	1/1	0.95	0.08	38,38,38,38	0
57	MG	10	105	1/1	0.95	0.22	62,62,62,62	0
57	MG	2A	3498	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3903	1/1	0.95	0.09	37,37,37,37	0
57	MG	10	107	1/1	0.95	0.16	56,56,56,56	0
57	MG	1A	3906	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3461	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3908	1/1	0.95	0.09	22,22,22,22	0
57	MG	1A	3035	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3775	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3290	1/1	0.95	0.10	56,56,56,56	0
57	MG	12	101	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3292	1/1	0.95	0.10	57,57,57,57	0
57	MG	13	103	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3102	1/1	0.95	0.10	31,31,31,31	0
57	MG	1a	1746	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3465	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3647	1/1	0.95	0.05	25,25,25,25	0
57	MG	15	105	1/1	0.95	0.13	31,31,31,31	0
57	MG	2a	1718	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3406	1/1	0.95	0.27	34,34,34,34	0
57	MG	2A	3790	1/1	0.95	0.09	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	3104	1/1	0.95	0.23	52,52,52,52	0
57	MG	2A	3105	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3212	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3796	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3797	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	3408	1/1	0.95	0.22	45,45,45,45	0
57	MG	2a	1727	1/1	0.95	0.28	69,69,69,69	0
57	MG	2a	1728	1/1	0.95	0.21	61,61,61,61	0
57	MG	17	103	1/1	0.95	0.14	29,29,29,29	0
57	MG	17	104	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3801	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	4068	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3158	1/1	0.95	0.07	42,42,42,42	0
57	MG	1a	1765	1/1	0.95	0.08	63,63,63,63	0
57	MG	2A	3538	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3410	1/1	0.95	0.14	48,48,48,48	0
57	MG	1a	1768	1/1	0.95	0.05	64,64,64,64	0
57	MG	2a	1738	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3260	1/1	0.95	0.06	34,34,34,34	0
57	MG	2A	3542	1/1	0.95	0.06	53,53,53,53	0
57	MG	2A	3543	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3544	1/1	0.95	0.14	51,51,51,51	0
57	MG	1a	1773	1/1	0.95	0.19	70,70,70,70	0
57	MG	1A	3108	1/1	0.95	0.18	37,37,37,37	0
57	MG	1a	1777	1/1	0.95	0.18	66,66,66,66	0
57	MG	1A	3921	1/1	0.95	0.16	53,53,53,53	0
57	MG	2A	3553	1/1	0.95	0.08	34,34,34,34	0
57	MG	1a	1602	1/1	0.95	0.14	69,69,69,69	0
57	MG	1A	3054	1/1	0.95	0.09	40,40,40,40	0
57	MG	1a	1604	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3558	1/1	0.95	0.10	51,51,51,51	0
57	MG	2a	1753	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3125	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3126	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3359	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3219	1/1	0.95	0.06	44,44,44,44	0
57	MG	1a	1785	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3843	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	4083	1/1	0.95	0.19	40,40,40,40	0
57	MG	2A	3846	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3663	1/1	0.95	0.05	26,26,26,26	0
57	MG	2a	1766	1/1	0.95	0.05	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1767	1/1	0.95	0.09	72,72,72,72	0
57	MG	2A	3570	1/1	0.95	0.05	40,40,40,40	0
57	MG	2A	3849	1/1	0.95	0.13	56,56,56,56	0
57	MG	1a	1611	1/1	0.95	0.05	21,21,21,21	0
57	MG	1A	3793	1/1	0.95	0.06	62,62,62,62	0
57	MG	2A	3138	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3856	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3665	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3221	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3859	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3481	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3672	1/1	0.95	0.09	31,31,31,31	0
57	MG	1A	3807	1/1	0.95	0.07	16,16,16,16	0
57	MG	1a	1797	1/1	0.95	0.12	56,56,56,56	0
57	MG	1a	1798	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3936	1/1	0.95	0.05	64,64,64,64	0
57	MG	1a	1800	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3149	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3339	1/1	0.95	0.28	59,59,59,59	0
57	MG	1A	3269	1/1	0.95	0.12	60,60,60,60	0
57	MG	2A	3592	1/1	0.95	0.12	64,64,64,64	0
57	MG	2A	3593	1/1	0.95	0.16	55,55,55,55	0
57	MG	1A	3004	1/1	0.95	0.05	20,20,20,20	0
57	MG	1A	3676	1/1	0.95	0.12	35,35,35,35	0
57	MG	1a	1807	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3487	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3224	1/1	0.95	0.25	34,34,34,34	0
57	MG	1A	3322	1/1	0.95	0.16	54,54,54,54	0
57	MG	1A	3574	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3956	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3042	1/1	0.95	0.15	29,29,29,29	0
57	MG	1A	3126	1/1	0.95	0.27	38,38,38,38	0
57	MG	1a	1815	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3685	1/1	0.95	0.05	27,27,27,27	0
57	MG	2a	1808	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3327	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3689	1/1	0.95	0.06	42,42,42,42	0
57	MG	1B	216	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3612	1/1	0.95	0.09	33,33,33,33	0
57	MG	1B	217	1/1	0.95	0.13	46,46,46,46	0
57	MG	1B	218	1/1	0.95	0.06	51,51,51,51	0
57	MG	1A	3690	1/1	0.95	0.05	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	3692	1/1	0.95	0.04	18,18,18,18	0
57	MG	2F	301	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3695	1/1	0.95	0.05	18,18,18,18	0
57	MG	1A	3180	1/1	0.95	0.10	28,28,28,28	0
57	MG	1A	3969	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3495	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3835	1/1	0.95	0.26	26,26,26,26	0
57	MG	2A	3625	1/1	0.95	0.07	31,31,31,31	0
57	MG	1l	201	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3628	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3837	1/1	0.95	0.08	39,39,39,39	0
57	MG	2A	3630	1/1	0.95	0.17	46,46,46,46	0
57	MG	2A	3631	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3633	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3281	1/1	0.95	0.35	42,42,42,42	0
57	MG	2T	3501	1/1	0.95	0.35	66,66,66,66	0
57	MG	1A	3372	1/1	0.95	0.10	59,59,59,59	0
57	MG	2l	201	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3374	1/1	0.95	0.26	45,45,45,45	0
57	MG	1A	3430	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3708	1/1	0.95	0.09	19,19,19,19	0
57	MG	1A	3506	1/1	0.95	0.13	39,39,39,39	0
57	MG	1a	1654	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3230	1/1	0.95	0.15	27,27,27,27	0
57	MG	1B	236	1/1	0.95	0.07	31,31,31,31	0
57	MG	1w	104	1/1	0.95	0.07	67,67,67,67	0
57	MG	1D	302	1/1	0.95	0.18	43,43,43,43	0
57	MG	1A	3713	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3850	1/1	0.95	0.14	36,36,36,36	0
57	MG	1A	3128	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	3009	1/1	0.95	0.06	24,24,24,24	0
57	MG	1A	3716	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3378	1/1	0.95	0.13	40,40,40,40	0
57	MG	1E	308	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3653	1/1	0.95	0.10	65,65,65,65	0
58	K	1A	3570	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3131	1/1	0.95	0.09	40,40,40,40	0
59	ZN	14	102	1/1	0.95	0.13	114,114,114,114	0
57	MG	1A	3856	1/1	0.95	0.08	33,33,33,33	0
57	MG	1a	1662	1/1	0.96	0.07	56,56,56,56	0
57	MG	2A	3129	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3353	1/1	0.96	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3403	1/1	0.96	0.22	55,55,55,55	0
57	MG	2A	3132	1/1	0.96	0.26	48,48,48,48	0
57	MG	1A	3160	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	3215	1/1	0.96	0.19	50,50,50,50	0
57	MG	2A	3490	1/1	0.96	0.25	47,47,47,47	0
57	MG	1A	3124	1/1	0.96	0.17	33,33,33,33	0
57	MG	1b	301	1/1	0.96	0.05	78,78,78,78	0
57	MG	1A	3594	1/1	0.96	0.07	31,31,31,31	0
57	MG	2A	3494	1/1	0.96	0.06	72,72,72,72	0
57	MG	1a	1669	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3318	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3006	1/1	0.96	0.19	65,65,65,65	0
57	MG	1P	203	1/1	0.96	0.22	28,28,28,28	0
57	MG	1A	3166	1/1	0.96	0.17	34,34,34,34	0
57	MG	1A	3799	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3686	1/1	0.96	0.05	17,17,17,17	0
57	MG	1A	3523	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3028	1/1	0.96	0.24	29,29,29,29	0
57	MG	1R	206	1/1	0.96	0.10	41,41,41,41	0
57	MG	1S	201	1/1	0.96	0.31	41,41,41,41	0
57	MG	1A	3462	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3363	1/1	0.96	0.14	39,39,39,39	0
57	MG	2A	3511	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3693	1/1	0.96	0.10	19,19,19,19	0
57	MG	1A	3811	1/1	0.96	0.06	46,46,46,46	0
57	MG	2A	3160	1/1	0.96	0.08	35,35,35,35	0
57	MG	2A	3516	1/1	0.96	0.08	44,44,44,44	0
57	MG	1U	202	1/1	0.96	0.24	40,40,40,40	0
57	MG	1A	4055	1/1	0.96	0.04	29,29,29,29	0
57	MG	2A	3519	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3812	1/1	0.96	0.05	16,16,16,16	0
57	MG	2A	3522	1/1	0.96	0.08	37,37,37,37	0
57	MG	1w	107	1/1	0.96	0.09	64,64,64,64	0
57	MG	1A	3170	1/1	0.96	0.05	30,30,30,30	0
57	MG	1a	1690	1/1	0.96	0.16	62,62,62,62	0
57	MG	1A	3018	1/1	0.96	0.09	26,26,26,26	0
57	MG	2A	3528	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3324	1/1	0.96	0.15	25,25,25,25	0
57	MG	1A	3105	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3174	1/1	0.96	0.25	31,31,31,31	0
57	MG	1A	3930	1/1	0.96	0.03	28,28,28,28	0
57	MG	1A	3178	1/1	0.96	0.12	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	3821	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	4067	1/1	0.96	0.04	15,15,15,15	0
57	MG	1A	3132	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3177	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3282	1/1	0.96	0.15	31,31,31,31	0
57	MG	2A	3768	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3179	1/1	0.96	0.09	52,52,52,52	0
57	MG	1X	101	1/1	0.96	0.25	32,32,32,32	0
57	MG	2A	3771	1/1	0.96	0.05	51,51,51,51	0
57	MG	2A	3773	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	4070	1/1	0.96	0.05	34,34,34,34	0
57	MG	2a	1676	1/1	0.96	0.09	71,71,71,71	0
57	MG	1A	3107	1/1	0.96	0.18	36,36,36,36	0
57	MG	2A	3346	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3616	1/1	0.96	0.23	41,41,41,41	0
57	MG	1A	3830	1/1	0.96	0.06	57,57,57,57	0
57	MG	1Z	301	1/1	0.96	0.14	59,59,59,59	0
57	MG	2A	3007	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	4078	1/1	0.96	0.15	52,52,52,52	0
57	MG	1A	3475	1/1	0.96	0.10	47,47,47,47	0
57	MG	2A	3787	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3559	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3083	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3014	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3015	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3540	1/1	0.96	0.20	42,42,42,42	0
57	MG	1A	3541	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3794	1/1	0.96	0.07	61,61,61,61	0
57	MG	2A	3795	1/1	0.96	0.11	66,66,66,66	0
57	MG	2A	3567	1/1	0.96	0.12	67,67,67,67	0
57	MG	1a	1714	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3290	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3020	1/1	0.96	0.04	55,55,55,55	0
57	MG	2A	3571	1/1	0.96	0.12	31,31,31,31	0
57	MG	2A	3021	1/1	0.96	0.07	24,24,24,24	0
57	MG	2A	3802	1/1	0.96	0.11	52,52,52,52	0
57	MG	2A	3022	1/1	0.96	0.19	45,45,45,45	0
57	MG	1A	3836	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3953	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3202	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3808	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3235	1/1	0.96	0.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3368	1/1	0.96	0.05	56,56,56,56	0
57	MG	2A	3026	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3205	1/1	0.96	0.17	67,67,67,67	0
57	MG	2A	3813	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	4088	1/1	0.96	0.17	51,51,51,51	0
57	MG	2A	3815	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3838	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3817	1/1	0.96	0.06	57,57,57,57	0
57	MG	2A	3821	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3426	1/1	0.96	0.27	56,56,56,56	0
57	MG	1A	3625	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3237	1/1	0.96	0.21	30,30,30,30	0
57	MG	2A	3376	1/1	0.96	0.18	61,61,61,61	0
57	MG	15	104	1/1	0.96	0.15	33,33,33,33	0
57	MG	1A	3183	1/1	0.96	0.05	52,52,52,52	0
57	MG	1A	3629	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3846	1/1	0.96	0.18	41,41,41,41	0
57	MG	16	102	1/1	0.96	0.09	59,59,59,59	0
57	MG	1a	1729	1/1	0.96	0.18	51,51,51,51	0
57	MG	2A	3383	1/1	0.96	0.08	57,57,57,57	0
57	MG	1A	3547	1/1	0.96	0.25	49,49,49,49	0
57	MG	1B	201	1/1	0.96	0.10	53,53,53,53	0
57	MG	2A	3841	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3631	1/1	0.96	0.07	38,38,38,38	0
57	MG	2A	3603	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3728	1/1	0.96	0.09	55,55,55,55	0
57	MG	1B	205	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3222	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	1737	1/1	0.96	0.17	61,61,61,61	0
57	MG	1B	206	1/1	0.96	0.12	44,44,44,44	0
57	MG	2A	3850	1/1	0.96	0.05	57,57,57,57	0
57	MG	2A	3225	1/1	0.96	0.15	42,42,42,42	0
57	MG	2A	3610	1/1	0.96	0.11	41,41,41,41	0
57	MG	2A	3853	1/1	0.96	0.12	63,63,63,63	0
57	MG	1A	3138	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3394	1/1	0.96	0.17	64,64,64,64	0
57	MG	2A	3395	1/1	0.96	0.22	70,70,70,70	0
57	MG	1A	3633	1/1	0.96	0.06	19,19,19,19	0
57	MG	19	101	1/1	0.96	0.19	49,49,49,49	0
57	MG	1A	3486	1/1	0.96	0.13	52,52,52,52	0
57	MG	2A	3617	1/1	0.96	0.08	37,37,37,37	0
57	MG	2a	1755	1/1	0.96	0.09	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	2A	3618	1/1	0.96	0.07	32,32,32,32	0
57	MG	1a	1743	1/1	0.96	0.23	56,56,56,56	0
57	MG	1A	3139	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3142	1/1	0.96	0.10	51,51,51,51	0
57	MG	2a	1760	1/1	0.96	0.12	48,48,48,48	0
57	MG	1A	3735	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3195	1/1	0.96	0.20	26,26,26,26	0
57	MG	1A	3977	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3978	1/1	0.96	0.07	25,25,25,25	0
57	MG	2A	3064	1/1	0.96	0.18	60,60,60,60	0
57	MG	1a	1608	1/1	0.96	0.16	52,52,52,52	0
57	MG	1A	3857	1/1	0.96	0.21	52,52,52,52	0
57	MG	1A	3110	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3069	1/1	0.96	0.14	57,57,57,57	0
57	MG	2a	1770	1/1	0.96	0.06	74,74,74,74	0
57	MG	2A	3412	1/1	0.96	0.30	49,49,49,49	0
57	MG	1A	3491	1/1	0.96	0.10	36,36,36,36	0
57	MG	2a	1773	1/1	0.96	0.09	61,61,61,61	0
57	MG	2a	1774	1/1	0.96	0.13	59,59,59,59	0
57	MG	1A	3862	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3111	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3436	1/1	0.96	0.16	46,46,46,46	0
57	MG	1A	3112	1/1	0.96	0.12	27,27,27,27	0
57	MG	2A	3077	1/1	0.96	0.10	25,25,25,25	0
57	MG	2D	305	1/1	0.96	0.33	44,44,44,44	0
57	MG	2a	1782	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3419	1/1	0.96	0.26	57,57,57,57	0
57	MG	2a	1784	1/1	0.96	0.07	68,68,68,68	0
57	MG	1a	1766	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3149	1/1	0.96	0.28	29,29,29,29	0
57	MG	2A	3422	1/1	0.96	0.18	51,51,51,51	0
57	MG	2A	3080	1/1	0.96	0.09	52,52,52,52	0
57	MG	1a	1618	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3082	1/1	0.96	0.16	45,45,45,45	0
57	MG	1a	1771	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3650	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3150	1/1	0.96	0.27	40,40,40,40	0
57	MG	1A	3752	1/1	0.96	0.06	45,45,45,45	0
57	MG	2a	1795	1/1	0.96	0.14	62,62,62,62	0
57	MG	1A	3873	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3498	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3995	1/1	0.96	0.08	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	3653	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3253	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3658	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3056	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3208	1/1	0.96	0.12	32,32,32,32	0
57	MG	2A	3437	1/1	0.96	0.34	60,60,60,60	0
57	MG	1a	1784	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3664	1/1	0.96	0.08	60,60,60,60	0
57	MG	1A	3502	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3760	1/1	0.96	0.10	27,27,27,27	0
57	MG	2T	3500	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3503	1/1	0.96	0.14	34,34,34,34	0
57	MG	2A	3668	1/1	0.96	0.22	41,41,41,41	0
57	MG	1A	3575	1/1	0.96	0.27	31,31,31,31	0
57	MG	2A	3443	1/1	0.96	0.07	53,53,53,53	0
57	MG	2V	201	1/1	0.96	0.08	66,66,66,66	0
57	MG	2A	3444	1/1	0.96	0.19	44,44,44,44	0
57	MG	1A	3763	1/1	0.96	0.14	54,54,54,54	0
57	MG	1A	3661	1/1	0.96	0.13	22,22,22,22	0
57	MG	2A	3447	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3273	1/1	0.96	0.14	56,56,56,56	0
57	MG	2Y	201	1/1	0.96	0.19	61,61,61,61	0
57	MG	1E	302	1/1	0.96	0.21	45,45,45,45	0
57	MG	2A	3103	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3662	1/1	0.96	0.07	31,31,31,31	0
57	MG	2a	1824	1/1	0.96	0.17	61,61,61,61	0
57	MG	1A	4016	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3766	1/1	0.96	0.05	36,36,36,36	0
57	MG	23	101	1/1	0.96	0.14	64,64,64,64	0
57	MG	1A	3155	1/1	0.96	0.10	31,31,31,31	0
57	MG	23	103	1/1	0.96	0.06	57,57,57,57	0
57	MG	2f	201	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3459	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3280	1/1	0.96	0.08	65,65,65,65	0
57	MG	1A	3397	1/1	0.96	0.25	31,31,31,31	0
57	MG	2A	3687	1/1	0.96	0.08	34,34,34,34	0
57	MG	2k	201	1/1	0.96	0.10	67,67,67,67	0
57	MG	1E	312	1/1	0.96	0.09	25,25,25,25	0
57	MG	2l	202	1/1	0.96	0.07	74,74,74,74	0
57	MG	2A	3463	1/1	0.96	0.19	62,62,62,62	0
57	MG	27	101	1/1	0.96	0.27	61,61,61,61	0
57	MG	1A	3398	1/1	0.96	0.20	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2r	101	1/1	0.96	0.12	69,69,69,69	0
57	MG	1A	3015	1/1	0.96	0.19	36,36,36,36	0
57	MG	1a	1804	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	4023	1/1	0.96	0.06	61,61,61,61	0
57	MG	1F	301	1/1	0.96	0.19	38,38,38,38	0
57	MG	2A	3470	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3669	1/1	0.96	0.06	36,36,36,36	0
57	MG	1F	306	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	4025	1/1	0.96	0.07	75,75,75,75	0
57	MG	1A	3670	1/1	0.96	0.13	36,36,36,36	0
57	MG	2A	3701	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3036	1/1	0.96	0.08	33,33,33,33	0
57	MG	1a	1656	1/1	0.96	0.27	66,66,66,66	0
57	MG	1A	3781	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3352	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	4031	1/1	0.96	0.08	67,67,67,67	0
57	MG	1G	204	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3481	1/1	0.96	0.09	50,50,50,50	0
59	ZN	2Y	202	1/1	0.96	0.06	94,94,94,94	0
57	MG	1A	3674	1/1	0.96	0.06	38,38,38,38	0
59	ZN	2n	501	1/1	0.96	0.06	91,91,91,91	0
57	MG	1A	3137	1/1	0.97	0.21	32,32,32,32	0
57	MG	1A	3202	1/1	0.97	0.05	38,38,38,38	0
57	MG	2A	3074	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3059	1/1	0.97	0.31	57,57,57,57	0
57	MG	1A	3733	1/1	0.97	0.04	12,12,12,12	0
57	MG	1A	4037	1/1	0.97	0.11	56,56,56,56	0
57	MG	1W	201	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3273	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3014	1/1	0.97	0.05	28,28,28,28	0
57	MG	1a	1735	1/1	0.97	0.34	47,47,47,47	0
57	MG	1A	4042	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3276	1/1	0.97	0.22	38,38,38,38	0
57	MG	1A	3205	1/1	0.97	0.10	21,21,21,21	0
57	MG	1X	104	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3738	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3278	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3280	1/1	0.97	0.18	30,30,30,30	0
57	MG	2A	3496	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3516	1/1	0.97	0.20	52,52,52,52	0
57	MG	1A	3141	1/1	0.97	0.07	15,15,15,15	0
57	MG	1A	3432	1/1	0.97	0.18	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	3736	1/1	0.97	0.15	40,40,40,40	0
57	MG	10	103	1/1	0.97	0.11	37,37,37,37	0
57	MG	10	104	1/1	0.97	0.26	32,32,32,32	0
57	MG	1A	3747	1/1	0.97	0.05	47,47,47,47	0
57	MG	1a	1749	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3519	1/1	0.97	0.18	29,29,29,29	0
57	MG	1a	1752	1/1	0.97	0.05	34,34,34,34	0
57	MG	1a	1754	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3890	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3508	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3626	1/1	0.97	0.08	20,20,20,20	0
57	MG	1A	3355	1/1	0.97	0.17	27,27,27,27	0
57	MG	1A	3041	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3522	1/1	0.97	0.17	37,37,37,37	0
57	MG	2A	3514	1/1	0.97	0.07	40,40,40,40	0
57	MG	1a	1761	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3285	1/1	0.97	0.07	49,49,49,49	0
57	MG	13	102	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3525	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3287	1/1	0.97	0.10	36,36,36,36	0
57	MG	1A	3008	1/1	0.97	0.12	25,25,25,25	0
57	MG	2A	3521	1/1	0.97	0.06	40,40,40,40	0
57	MG	2a	1661	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3063	1/1	0.97	0.23	46,46,46,46	0
57	MG	2a	1663	1/1	0.97	0.06	56,56,56,56	0
57	MG	1a	1770	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3761	1/1	0.97	0.08	36,36,36,36	0
57	MG	2A	3762	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3115	1/1	0.97	0.12	34,34,34,34	0
57	MG	2a	1668	1/1	0.97	0.13	44,44,44,44	0
57	MG	15	101	1/1	0.97	0.23	33,33,33,33	0
57	MG	1A	3145	1/1	0.97	0.20	28,28,28,28	0
57	MG	1A	3905	1/1	0.97	0.04	35,35,35,35	0
57	MG	15	106	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3636	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3147	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3064	1/1	0.97	0.15	31,31,31,31	0
57	MG	1A	3043	1/1	0.97	0.29	30,30,30,30	0
57	MG	2a	1678	1/1	0.97	0.09	67,67,67,67	0
57	MG	17	101	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3294	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	4072	1/1	0.97	0.06	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3103	1/1	0.97	0.16	27,27,27,27	0
57	MG	2A	3778	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3151	1/1	0.97	0.16	36,36,36,36	0
57	MG	1A	4077	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3769	1/1	0.97	0.05	46,46,46,46	0
57	MG	2A	3545	1/1	0.97	0.10	31,31,31,31	0
57	MG	2A	3547	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3772	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3220	1/1	0.97	0.08	38,38,38,38	0
57	MG	2a	1692	1/1	0.97	0.30	61,61,61,61	0
57	MG	1A	3044	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3135	1/1	0.97	0.17	41,41,41,41	0
57	MG	2A	3552	1/1	0.97	0.08	50,50,50,50	0
57	MG	1a	1792	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3775	1/1	0.97	0.08	51,51,51,51	0
57	MG	2A	3555	1/1	0.97	0.12	58,58,58,58	0
57	MG	2a	1699	1/1	0.97	0.10	57,57,57,57	0
57	MG	1A	3001	1/1	0.97	0.10	36,36,36,36	0
57	MG	1A	3300	1/1	0.97	0.06	32,32,32,32	0
57	MG	1A	3373	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3223	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3560	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3782	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3562	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3925	1/1	0.97	0.08	39,39,39,39	0
57	MG	1a	1609	1/1	0.97	0.28	53,53,53,53	0
57	MG	1A	3452	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3655	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3075	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3109	1/1	0.97	0.21	31,31,31,31	0
57	MG	1A	3077	1/1	0.97	0.11	32,32,32,32	0
57	MG	1A	4095	1/1	0.97	0.14	47,47,47,47	0
57	MG	2A	3152	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3227	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3162	1/1	0.97	0.33	29,29,29,29	0
57	MG	2A	3157	1/1	0.97	0.18	42,42,42,42	0
57	MG	1A	3046	1/1	0.97	0.07	34,34,34,34	0
57	MG	1a	1619	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3232	1/1	0.97	0.09	43,43,43,43	0
57	MG	1a	1621	1/1	0.97	0.04	41,41,41,41	0
57	MG	2A	3819	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3794	1/1	0.97	0.05	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	1B	204	1/1	0.97	0.17	63,63,63,63	0
57	MG	1A	3937	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3938	1/1	0.97	0.12	42,42,42,42	0
57	MG	2A	3826	1/1	0.97	0.05	57,57,57,57	0
57	MG	1a	1626	1/1	0.97	0.14	53,53,53,53	0
57	MG	2A	3829	1/1	0.97	0.04	68,68,68,68	0
57	MG	1A	3939	1/1	0.97	0.10	56,56,56,56	0
57	MG	2A	3365	1/1	0.97	0.12	39,39,39,39	0
57	MG	2A	3589	1/1	0.97	0.04	44,44,44,44	0
57	MG	1A	3940	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3941	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3795	1/1	0.97	0.04	22,22,22,22	0
57	MG	1a	1824	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3310	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3944	1/1	0.97	0.09	39,39,39,39	0
57	MG	2A	3597	1/1	0.97	0.05	55,55,55,55	0
57	MG	1A	3664	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3383	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3800	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3845	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3948	1/1	0.97	0.04	12,12,12,12	0
57	MG	1A	3311	1/1	0.97	0.04	26,26,26,26	0
57	MG	2A	3180	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3802	1/1	0.97	0.07	43,43,43,43	0
57	MG	1B	220	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3030	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3955	1/1	0.97	0.07	43,43,43,43	0
57	MG	2a	1754	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3668	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3048	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3168	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3671	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3236	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3116	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3119	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3032	1/1	0.97	0.14	24,24,24,24	0
57	MG	1A	3564	1/1	0.97	0.19	33,33,33,33	0
57	MG	1A	3677	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3474	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3122	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3395	1/1	0.97	0.13	40,40,40,40	0
57	MG	2A	3621	1/1	0.97	0.05	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	1x	102	1/1	0.97	0.09	52,52,52,52	0
57	MG	1D	301	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3397	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3825	1/1	0.97	0.23	22,22,22,22	0
57	MG	1A	3033	1/1	0.97	0.29	25,25,25,25	0
57	MG	2A	3627	1/1	0.97	0.15	53,53,53,53	0
57	MG	1D	308	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3085	1/1	0.97	0.18	23,23,23,23	0
57	MG	1A	3572	1/1	0.97	0.19	32,32,32,32	0
57	MG	1A	3179	1/1	0.97	0.09	34,34,34,34	0
57	MG	2A	3632	1/1	0.97	0.09	41,41,41,41	0
57	MG	2a	1780	1/1	0.97	0.11	61,61,61,61	0
57	MG	1A	3051	1/1	0.97	0.13	31,31,31,31	0
57	MG	2B	218	1/1	0.97	0.23	76,76,76,76	0
57	MG	1A	3687	1/1	0.97	0.10	28,28,28,28	0
57	MG	1E	303	1/1	0.97	0.13	27,27,27,27	0
57	MG	2D	304	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3576	1/1	0.97	0.20	38,38,38,38	0
57	MG	1A	3127	1/1	0.97	0.21	32,32,32,32	0
57	MG	1A	3022	1/1	0.97	0.04	39,39,39,39	0
57	MG	2A	3004	1/1	0.97	0.32	55,55,55,55	0
57	MG	1A	3484	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3485	1/1	0.97	0.15	43,43,43,43	0
57	MG	2E	304	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3251	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3696	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3839	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3988	1/1	0.97	0.05	63,63,63,63	0
57	MG	2A	3013	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3129	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3990	1/1	0.97	0.11	42,42,42,42	0
57	MG	1F	305	1/1	0.97	0.18	30,30,30,30	0
57	MG	1A	3053	1/1	0.97	0.06	48,48,48,48	0
57	MG	2F	305	1/1	0.97	0.17	40,40,40,40	0
57	MG	1F	307	1/1	0.97	0.04	36,36,36,36	0
57	MG	1F	308	1/1	0.97	0.13	21,21,21,21	0
57	MG	1A	3699	1/1	0.97	0.05	26,26,26,26	0
57	MG	2A	3227	1/1	0.97	0.24	42,42,42,42	0
57	MG	1A	3588	1/1	0.97	0.05	37,37,37,37	0
57	MG	2P	202	1/1	0.97	0.06	50,50,50,50	0
57	MG	1a	1685	1/1	0.97	0.15	53,53,53,53	0
57	MG	1F	312	1/1	0.97	0.11	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	3701	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3589	1/1	0.97	0.06	44,44,44,44	0
57	MG	1G	201	1/1	0.97	0.11	35,35,35,35	0
57	MG	2A	3027	1/1	0.97	0.04	42,42,42,42	0
57	MG	1A	3703	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3185	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3017	1/1	0.97	0.10	57,57,57,57	0
57	MG	1A	3999	1/1	0.97	0.04	44,44,44,44	0
57	MG	1A	4000	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3035	1/1	0.97	0.11	37,37,37,37	0
57	MG	2A	3670	1/1	0.97	0.05	54,54,54,54	0
57	MG	2A	3241	1/1	0.97	0.12	71,71,71,71	0
57	MG	1A	3025	1/1	0.97	0.08	32,32,32,32	0
57	MG	1N	203	1/1	0.97	0.06	40,40,40,40	0
57	MG	1a	1697	1/1	0.97	0.13	43,43,43,43	0
57	MG	2A	3675	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3189	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3711	1/1	0.97	0.06	63,63,63,63	0
57	MG	1O	201	1/1	0.97	0.22	50,50,50,50	0
57	MG	1A	4004	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3190	1/1	0.97	0.15	29,29,29,29	0
57	MG	2A	3448	1/1	0.97	0.29	49,49,49,49	0
57	MG	1a	1703	1/1	0.97	0.17	48,48,48,48	0
57	MG	2A	3451	1/1	0.97	0.17	50,50,50,50	0
57	MG	1A	3259	1/1	0.97	0.06	34,34,34,34	0
57	MG	2A	3048	1/1	0.97	0.10	42,42,42,42	0
57	MG	2A	3049	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3597	1/1	0.97	0.17	29,29,29,29	0
57	MG	2A	3688	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3598	1/1	0.97	0.20	39,39,39,39	0
57	MG	1P	205	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	4012	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3192	1/1	0.97	0.06	41,41,41,41	0
57	MG	1Q	207	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3262	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3193	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3194	1/1	0.97	0.25	29,29,29,29	0
57	MG	1A	3133	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3466	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3092	1/1	0.97	0.06	21,21,21,21	0
57	MG	1A	3419	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3268	1/1	0.97	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3867	1/1	0.97	0.06	15,15,15,15	0
57	MG	1A	3868	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3504	1/1	0.97	0.15	25,25,25,25	0
57	MG	1A	3608	1/1	0.97	0.10	35,35,35,35	0
57	MG	1A	4028	1/1	0.97	0.11	57,57,57,57	0
57	MG	2A	3068	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3505	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3872	1/1	0.97	0.12	20,20,20,20	0
57	MG	1A	3039	1/1	0.97	0.27	31,31,31,31	0
57	MG	1A	3286	1/1	0.98	0.17	47,47,47,47	0
57	MG	1A	3573	1/1	0.98	0.04	15,15,15,15	0
57	MG	1a	1802	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3390	1/1	0.98	0.07	22,22,22,22	0
57	MG	1A	3191	1/1	0.98	0.23	38,38,38,38	0
57	MG	2a	1670	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3037	1/1	0.98	0.12	21,21,21,21	0
57	MG	2A	3820	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3577	1/1	0.98	0.20	42,42,42,42	0
57	MG	2A	3112	1/1	0.98	0.24	49,49,49,49	0
57	MG	2A	3452	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3578	1/1	0.98	0.19	31,31,31,31	0
57	MG	2A	3825	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3393	1/1	0.98	0.08	45,45,45,45	0
57	MG	1N	204	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3096	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3739	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	3740	1/1	0.98	0.06	20,20,20,20	0
57	MG	2A	3832	1/1	0.98	0.05	57,57,57,57	0
57	MG	2A	3639	1/1	0.98	0.10	35,35,35,35	0
57	MG	2A	3834	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	4057	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	4058	1/1	0.98	0.05	18,18,18,18	0
57	MG	1a	1655	1/1	0.98	0.03	40,40,40,40	0
57	MG	1A	3153	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	3582	1/1	0.98	0.23	36,36,36,36	0
57	MG	2a	1691	1/1	0.98	0.17	42,42,42,42	0
57	MG	1P	201	1/1	0.98	0.24	26,26,26,26	0
57	MG	1P	202	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3396	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3844	1/1	0.98	0.09	51,51,51,51	0
57	MG	1A	3584	1/1	0.98	0.15	35,35,35,35	0
57	MG	1Q	201	1/1	0.98	0.25	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	1Q	202	1/1	0.98	0.05	30,30,30,30	0
57	MG	1Q	203	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3154	1/1	0.98	0.05	34,34,34,34	0
57	MG	2A	3133	1/1	0.98	0.08	41,41,41,41	0
57	MG	1Q	205	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3746	1/1	0.98	0.04	46,46,46,46	0
57	MG	1R	201	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3453	1/1	0.98	0.21	41,41,41,41	0
57	MG	2a	1706	1/1	0.98	0.04	69,69,69,69	0
57	MG	2A	3854	1/1	0.98	0.05	43,43,43,43	0
57	MG	1R	203	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	3454	1/1	0.98	0.18	28,28,28,28	0
57	MG	1A	3954	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3196	1/1	0.98	0.22	29,29,29,29	0
57	MG	2A	3663	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3038	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3957	1/1	0.98	0.03	38,38,38,38	0
57	MG	1A	3198	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3125	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3459	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3029	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3962	1/1	0.98	0.04	47,47,47,47	0
57	MG	1A	3963	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3080	1/1	0.98	0.08	33,33,33,33	0
57	MG	1a	1684	1/1	0.98	0.12	48,48,48,48	0
57	MG	2A	3153	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3002	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3858	1/1	0.98	0.04	33,33,33,33	0
57	MG	2A	3156	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	3596	1/1	0.98	0.09	24,24,24,24	0
57	MG	1U	209	1/1	0.98	0.21	29,29,29,29	0
57	MG	1V	201	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3524	1/1	0.98	0.09	26,26,26,26	0
57	MG	1V	204	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3405	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3249	1/1	0.98	0.24	33,33,33,33	0
57	MG	1A	3163	1/1	0.98	0.21	46,46,46,46	0
57	MG	1A	3031	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3206	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3005	1/1	0.98	0.04	32,32,32,32	0
57	MG	1W	204	1/1	0.98	0.19	30,30,30,30	0
57	MG	1W	205	1/1	0.98	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1W	206	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3356	1/1	0.98	0.14	36,36,36,36	0
57	MG	1A	3104	1/1	0.98	0.11	46,46,46,46	0
57	MG	1X	102	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3770	1/1	0.98	0.04	39,39,39,39	0
57	MG	2a	1745	1/1	0.98	0.08	64,64,64,64	0
57	MG	1A	3167	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3683	1/1	0.98	0.08	37,37,37,37	0
57	MG	1X	106	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3009	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3084	1/1	0.98	0.11	25,25,25,25	0
57	MG	1A	3473	1/1	0.98	0.15	30,30,30,30	0
57	MG	2A	3012	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3211	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3704	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3010	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3476	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3780	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3213	1/1	0.98	0.13	27,27,27,27	0
57	MG	1A	3987	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3086	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3691	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3614	1/1	0.98	0.15	50,50,50,50	0
57	MG	2A	3532	1/1	0.98	0.08	46,46,46,46	0
57	MG	2A	3533	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3716	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3261	1/1	0.98	0.09	49,49,49,49	0
57	MG	2A	3535	1/1	0.98	0.06	50,50,50,50	0
57	MG	2A	3719	1/1	0.98	0.10	36,36,36,36	0
57	MG	1A	3066	1/1	0.98	0.11	31,31,31,31	0
57	MG	2A	3537	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3136	1/1	0.98	0.10	26,26,26,26	0
57	MG	1A	3217	1/1	0.98	0.14	38,38,38,38	0
57	MG	13	101	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3003	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3790	1/1	0.98	0.05	15,15,15,15	0
57	MG	1A	3317	1/1	0.98	0.18	49,49,49,49	0
57	MG	2X	102	1/1	0.98	0.08	47,47,47,47	0
57	MG	2A	3030	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3792	1/1	0.98	0.09	40,40,40,40	0
57	MG	2A	3546	1/1	0.98	0.09	29,29,29,29	0
57	MG	1A	3891	1/1	0.98	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3621	1/1	0.98	0.07	21,21,21,21	0
57	MG	2A	3034	1/1	0.98	0.06	49,49,49,49	0
57	MG	15	102	1/1	0.98	0.15	32,32,32,32	0
57	MG	15	103	1/1	0.98	0.25	22,22,22,22	0
57	MG	2A	3037	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3038	1/1	0.98	0.09	26,26,26,26	0
57	MG	1A	3176	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3267	1/1	0.98	0.23	35,35,35,35	0
57	MG	1a	1734	1/1	0.98	0.26	47,47,47,47	0
57	MG	1A	3796	1/1	0.98	0.04	22,22,22,22	0
57	MG	1A	3069	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	4005	1/1	0.98	0.04	33,33,33,33	0
57	MG	1B	227	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3897	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3071	1/1	0.98	0.12	22,22,22,22	0
57	MG	17	102	1/1	0.98	0.17	26,26,26,26	0
57	MG	1A	4008	1/1	0.98	0.04	65,65,65,65	0
57	MG	1A	3113	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	4010	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3114	1/1	0.98	0.04	29,29,29,29	0
57	MG	18	102	1/1	0.98	0.12	36,36,36,36	0
57	MG	2A	3753	1/1	0.98	0.11	51,51,51,51	0
57	MG	18	103	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3072	1/1	0.98	0.05	11,11,11,11	0
57	MG	1A	3710	1/1	0.98	0.04	27,27,27,27	0
57	MG	1a	1750	1/1	0.98	0.10	47,47,47,47	0
57	MG	1A	4014	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	4015	1/1	0.98	0.04	32,32,32,32	0
57	MG	1a	1753	1/1	0.98	0.10	30,30,30,30	0
57	MG	1A	3904	1/1	0.98	0.06	48,48,48,48	0
57	MG	1D	303	1/1	0.98	0.07	31,31,31,31	0
57	MG	1D	304	1/1	0.98	0.06	17,17,17,17	0
57	MG	1A	3803	1/1	0.98	0.04	33,33,33,33	0
57	MG	2A	3580	1/1	0.98	0.08	54,54,54,54	0
57	MG	1D	306	1/1	0.98	0.12	30,30,30,30	0
57	MG	2A	3582	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	4018	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3804	1/1	0.98	0.04	45,45,45,45	0
57	MG	1D	310	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3007	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3772	1/1	0.98	0.05	64,64,64,64	0
57	MG	1A	3274	1/1	0.98	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3117	1/1	0.98	0.14	25,25,25,25	0
57	MG	1A	3146	1/1	0.98	0.14	29,29,29,29	0
57	MG	2A	3591	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3118	1/1	0.98	0.07	35,35,35,35	0
57	MG	1a	1769	1/1	0.98	0.12	34,34,34,34	0
57	MG	2A	3780	1/1	0.98	0.04	37,37,37,37	0
57	MG	2A	3781	1/1	0.98	0.04	51,51,51,51	0
57	MG	2A	3075	1/1	0.98	0.12	40,40,40,40	0
57	MG	1E	304	1/1	0.98	0.13	27,27,27,27	0
57	MG	1E	305	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3229	1/1	0.98	0.08	27,27,27,27	0
57	MG	1E	307	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3562	1/1	0.98	0.05	48,48,48,48	0
57	MG	1a	1776	1/1	0.98	0.04	43,43,43,43	0
57	MG	1A	3279	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	3565	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3021	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3721	1/1	0.98	0.06	14,14,14,14	0
57	MG	2A	3086	1/1	0.98	0.07	47,47,47,47	0
57	MG	1A	3231	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3819	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3640	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3076	1/1	0.98	0.17	42,42,42,42	0
57	MG	1F	302	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	4035	1/1	0.98	0.04	44,44,44,44	0
57	MG	1F	304	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3822	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3824	1/1	0.98	0.04	31,31,31,31	0
57	MG	1a	1790	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3725	1/1	0.98	0.05	38,38,38,38	0
57	MG	2A	3805	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	4040	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3643	1/1	0.98	0.09	54,54,54,54	0
57	MG	1A	3284	1/1	0.98	0.29	31,31,31,31	0
57	MG	1A	3929	1/1	0.98	0.04	22,22,22,22	0
59	ZN	1n	103	1/1	0.98	0.04	66,66,66,66	0
57	MG	1A	3646	1/1	0.98	0.05	47,47,47,47	0
57	MG	1F	314	1/1	0.98	0.05	42,42,42,42	0
59	ZN	25	106	1/1	0.98	0.07	60,60,60,60	0
59	ZN	26	102	1/1	0.98	0.05	64,64,64,64	0
59	ZN	29	501	1/1	0.98	0.04	71,71,71,71	0
57	MG	1A	3121	1/1	0.98	0.37	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	SF4	1d	501	8/8	0.98	0.06	60,70,77,81	0
60	SF4	2d	303	8/8	0.98	0.06	69,79,88,91	0
57	MG	1A	3748	1/1	0.99	0.05	18,18,18,18	0
57	MG	1F	309	1/1	0.99	0.11	23,23,23,23	0
57	MG	1A	3749	1/1	0.99	0.04	21,21,21,21	0
57	MG	2Q	201	1/1	0.99	0.04	50,50,50,50	0
57	MG	1A	3306	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3919	1/1	0.99	0.04	34,34,34,34	0
57	MG	1A	3560	1/1	0.99	0.24	34,34,34,34	0
57	MG	1A	3561	1/1	0.99	0.08	23,23,23,23	0
57	MG	1A	3283	1/1	0.99	0.17	29,29,29,29	0
57	MG	1A	3923	1/1	0.99	0.07	36,36,36,36	0
57	MG	1A	3563	1/1	0.99	0.09	28,28,28,28	0
57	MG	1A	3055	1/1	0.99	0.08	30,30,30,30	0
57	MG	1a	1801	1/1	0.99	0.03	44,44,44,44	0
57	MG	1A	3240	1/1	0.99	0.13	35,35,35,35	0
57	MG	1A	3201	1/1	0.99	0.14	22,22,22,22	0
57	MG	1A	4073	1/1	0.99	0.06	23,23,23,23	0
57	MG	2A	3144	1/1	0.99	0.06	26,26,26,26	0
57	MG	1A	3758	1/1	0.99	0.06	41,41,41,41	0
57	MG	1A	3242	1/1	0.99	0.22	30,30,30,30	0
57	MG	1A	4076	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3106	1/1	0.99	0.03	23,23,23,23	0
57	MG	2A	3774	1/1	0.99	0.04	47,47,47,47	0
57	MG	1A	3140	1/1	0.99	0.10	26,26,26,26	0
57	MG	1A	3023	1/1	0.99	0.07	13,13,13,13	0
57	MG	1A	3097	1/1	0.99	0.09	15,15,15,15	0
57	MG	1A	3187	1/1	0.99	0.03	36,36,36,36	0
57	MG	10	102	1/1	0.99	0.15	41,41,41,41	0
57	MG	1A	3694	1/1	0.99	0.02	20,20,20,20	0
57	MG	1A	3805	1/1	0.99	0.05	38,38,38,38	0
57	MG	1A	4084	1/1	0.99	0.03	41,41,41,41	0
57	MG	1A	3070	1/1	0.99	0.05	14,14,14,14	0
57	MG	2A	3711	1/1	0.99	0.04	45,45,45,45	0
57	MG	1A	3156	1/1	0.99	0.14	20,20,20,20	0
57	MG	1P	204	1/1	0.99	0.11	29,29,29,29	0
57	MG	1D	307	1/1	0.99	0.15	30,30,30,30	0
57	MG	1A	3057	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3173	1/1	0.99	0.06	33,33,33,33	0
57	MG	1A	3496	1/1	0.99	0.10	34,34,34,34	0
57	MG	1a	1634	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3771	1/1	0.99	0.06	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	1760	1/1	0.99	0.09	44,44,44,44	0
57	MG	1A	4039	1/1	0.99	0.02	18,18,18,18	0
57	MG	1a	1762	1/1	0.99	0.07	38,38,38,38	0
57	MG	2A	3510	1/1	0.99	0.07	39,39,39,39	0
57	MG	1A	3011	1/1	0.99	0.12	39,39,39,39	0
57	MG	1Q	206	1/1	0.99	0.20	39,39,39,39	0
57	MG	1A	3813	1/1	0.99	0.07	15,15,15,15	0
57	MG	1A	3175	1/1	0.99	0.12	25,25,25,25	0
57	MG	2A	3173	1/1	0.99	0.14	37,37,37,37	0
57	MG	1A	3159	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3901	1/1	0.99	0.07	30,30,30,30	0
57	MG	2A	3588	1/1	0.99	0.06	27,27,27,27	0
57	MG	1A	3177	1/1	0.99	0.07	23,23,23,23	0
57	MG	2D	301	1/1	0.99	0.07	42,42,42,42	0
57	MG	1A	3641	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3950	1/1	0.99	0.06	54,54,54,54	0
57	MG	1A	3951	1/1	0.99	0.06	24,24,24,24	0
57	MG	1A	3860	1/1	0.99	0.03	52,52,52,52	0
57	MG	1A	3705	1/1	0.99	0.07	28,28,28,28	0
57	MG	1a	1775	1/1	0.99	0.06	62,62,62,62	0
57	MG	2A	3525	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3778	1/1	0.99	0.09	42,42,42,42	0
57	MG	1A	3706	1/1	0.99	0.03	22,22,22,22	0
57	MG	1U	201	1/1	0.99	0.14	30,30,30,30	0
57	MG	1A	3012	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3326	1/1	0.99	0.06	30,30,30,30	0
57	MG	2A	3818	1/1	0.99	0.03	54,54,54,54	0
59	ZN	1Y	203	1/1	0.99	0.03	57,57,57,57	0
57	MG	1E	316	1/1	0.99	0.08	41,41,41,41	0
59	ZN	15	108	1/1	0.99	0.04	41,41,41,41	0
59	ZN	16	104	1/1	0.99	0.05	48,48,48,48	0
57	MG	1A	3823	1/1	0.99	0.03	42,42,42,42	0
57	MG	1A	3074	1/1	0.99	0.08	26,26,26,26	0
57	MG	1A	3645	1/1	0.99	0.05	15,15,15,15	0
57	MG	1B	213	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3013	1/1	0.99	0.09	24,24,24,24	0
57	MG	1A	3067	1/1	0.99	0.07	28,28,28,28	0
57	MG	1A	3238	1/1	0.99	0.07	30,30,30,30	0
57	MG	1V	203	1/1	0.99	0.14	32,32,32,32	0
57	MG	2A	3828	1/1	0.99	0.04	29,29,29,29	0
59	ZN	19	102	1/1	1.00	0.04	40,40,40,40	0
57	MG	1A	3161	1/1	1.00	0.10	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.